LAMMPS Users Manual

16 Feb 2016 version

http://lammps.sandia.gov - Sandia National Laboratories

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LAMMPS Documentation

16 Feb 2016 version

Version info:

The LAMMPS "version" is the date when it was released, such as 1 May 2010. LAMMPS is updated continuously. Whenever we fix a bug or add a feature, we release it immediately, and post a notice on this page of the WWW site. Each dated copy of LAMMPS contains all the features and bug-fixes up to and including that version date. The version date is printed to the screen and logfile every time you run LAMMPS. It is also in the file src/version.h and in the LAMMPS directory name created when you unpack a tarball, and at the top of the first page of the manual (this page).

- If you browse the HTML doc pages on the LAMMPS WWW site, they always describe the most current version of LAMMPS.
- If you browse the HTML doc pages included in your tarball, they describe the version you have.
- The PDF file on the WWW site or in the tarball is updated about once per month. This is because it is large, and we don't want it to be part of every patch.
- There is also a Developer.pdf file in the doc directory, which describes the internal structure and algorithms of LAMMPS.

LAMMPS stands for Large-scale Atomic/Molecular Massively Parallel Simulator.

LAMMPS is a classical molecular dynamics simulation code designed to run efficiently on parallel computers. It was developed at Sandia National Laboratories, a US Department of Energy facility, with funding from the DOE. It is an open-source code, distributed freely under the terms of the GNU Public License (GPL).

The primary developers of LAMMPS are Steve Plimpton, Aidan Thompson, and Paul Crozier who can be contacted at sjplimp,athomps,pscrozi at sandia.gov. The LAMMPS WWW Site at http://lammps.sandia.gov has more information about the code and its uses.

The LAMMPS documentation is organized into the following sections. If you find errors or omissions in this manual or have suggestions for useful information to add, please send an email to the developers so we can improve the LAMMPS documentation.

Once you are familiar with LAMMPS, you may want to bookmark this page at Section_commands.html#comm since it gives quick access to documentation for all LAMMPS commands.

PDF file of the entire manual, generated by htmldoc

1. Introduction

This section provides an overview of what LAMMPS can and can't do, describes what it means for LAMMPS to be an open-source code, and acknowledges the funding and people who have contributed to LAMMPS over the years.

1.1 What is LAMMPS

LAMMPS is a classical molecular dynamics code that models an ensemble of particles in a liquid, solid, or gaseous state. It can model atomic, polymeric, biological, metallic, granular, and coarse-grained systems using a variety of force fields and boundary conditions.

For examples of LAMMPS simulations, see the Publications page of the LAMMPS WWW Site.

LAMMPS runs efficiently on single-processor desktop or laptop machines, but is designed for parallel computers. It will run on any parallel machine that compiles C++ and supports the MPI message-passing library. This includes distributed- or shared-memory parallel machines and Beowulf-style clusters.

LAMMPS can model systems with only a few particles up to millions or billions. See Section_perf for information on LAMMPS performance and scalability, or the Benchmarks section of the LAMMPS WWW Site.

LAMMPS is a freely-available open-source code, distributed under the terms of the GNU Public License, which means you can use or modify the code however you wish. See this section for a brief discussion of the open-source philosophy.

LAMMPS is designed to be easy to modify or extend with new capabilities, such as new force fields, atom types, boundary conditions, or diagnostics. See Section_modify for more details.

The current version of LAMMPS is written in C++. Earlier versions were written in F77 and F90. See Section_history for more information on different versions. All versions can be downloaded from the LAMMPS WWW Site.

LAMMPS was originally developed under a US Department of Energy CRADA (Cooperative Research and Development Agreement) between two DOE labs and 3 companies. It is distributed by Sandia National Labs. See this section for more information on LAMMPS funding and individuals who have contributed to LAMMPS.

In the most general sense, LAMMPS integrates Newton's equations of motion for collections of atoms, molecules, or macroscopic particles that interact via short- or long-range forces with a variety of initial and/or boundary conditions. For computational efficiency LAMMPS uses neighbor lists to keep track of nearby particles. The lists are optimized for systems with particles that are repulsive at short distances, so that the local density of particles never becomes too large. On parallel machines, LAMMPS uses spatial-decomposition techniques to partition the simulation domain into small 3d sub-domains, one of which is assigned to each processor. Processors

communicate and store "ghost" atom information for atoms that border their sub-domain. LAMMPS is most efficient (in a parallel sense) for systems whose particles fill a 3d rectangular box with roughly uniform density. Papers with technical details of the algorithms used in LAMMPS are listed in this section.

1.2 LAMMPS features

This section highlights LAMMPS features, with pointers to specific commands which give more details. If LAMMPS doesn't have your favorite interatomic potential, boundary condition, or atom type, see Section_modify, which describes how you can add it to LAMMPS.

General features

- runs on a single processor or in parallel
- distributed-memory message-passing parallelism (MPI)
- spatial-decomposition of simulation domain for parallelism
- open-source distribution
- highly portable C++
- optional libraries used: MPI and single-processor FFT
- GPU (CUDA and OpenCL), Intel(R) Xeon Phi(TM) coprocessors, and OpenMP support for many code features
- easy to extend with new features and functionality
- runs from an input script
- syntax for defining and using variables and formulas
- syntax for looping over runs and breaking out of loops
- run one or multiple simulations simultaneously (in parallel) from one script
- build as library, invoke LAMMPS thru library interface or provided Python wrapper
- couple with other codes: LAMMPS calls other code, other code calls LAMMPS, umbrella code calls both

Particle and model types

(atom style command)

- atoms
- coarse-grained particles (e.g. bead-spring polymers)
- united-atom polymers or organic molecules
- all-atom polymers, organic molecules, proteins, DNA
- metals
- granular materials
- coarse-grained mesoscale models
- finite-size spherical and ellipsoidal particles
- finite-size line segment (2d) and triangle (3d) particles
- point dipole particles
- rigid collections of particles
- hybrid combinations of these

Force fields

(pair style, bond style, angle style, dihedral style, improper style, kspace style commands)

- pairwise potentials: Lennard-Jones, Buckingham, Morse, Born-Mayer-Huggins, Yukawa, soft, class 2 (COMPASS), hydrogen bond, tabulated
- charged pairwise potentials: Coulombic, point-dipole

- manybody potentials: EAM, Finnis/Sinclair EAM, modified EAM (MEAM), embedded ion method (EIM), EDIP, ADP, Stillinger-Weber, Tersoff, REBO, AIREBO, ReaxFF, COMB, SNAP, Streitz-Mintmire, 3-body polymorphic
- long-range interactions for charge, point-dipoles, and LJ dispersion: Ewald, Wolf, PPPM (similar to particle-mesh Ewald)
- polarization models: QEq, core/shell model, Drude dipole model
- charge equilibration (QEq via dynamic, point, shielded, Slater methods)
- coarse-grained potentials: DPD, GayBerne, REsquared, colloidal, DLVO
- mesoscopic potentials: granular, Peridynamics, SPH
- electron force field (eFF, AWPMD)
- bond potentials: harmonic, FENE, Morse, nonlinear, class 2, quartic (breakable)
- angle potentials: harmonic, CHARMM, cosine, cosine/squared, cosine/periodic, class 2 (COMPASS)
- dihedral potentials: harmonic, CHARMM, multi-harmonic, helix, class 2 (COMPASS), OPLS
- improper potentials: harmonic, cvff, umbrella, class 2 (COMPASS)
- polymer potentials: all-atom, united-atom, bead-spring, breakable
- water potentials: TIP3P, TIP4P, SPC
- implicit solvent potentials: hydrodynamic lubrication, Debye
- force-field compatibility with common CHARMM, AMBER, DREIDING, OPLS, GROMACS, COMPASS options
- access to KIM archive of potentials via pair kim
- hybrid potentials: multiple pair, bond, angle, dihedral, improper potentials can be used in one simulation
- overlaid potentials: superposition of multiple pair potentials

Atom creation

(read_data, lattice, create_atoms, delete_atoms, displace_atoms, replicate commands)

- read in atom coords from files
- create atoms on one or more lattices (e.g. grain boundaries)
- delete geometric or logical groups of atoms (e.g. voids)
- replicate existing atoms multiple times
- displace atoms

Ensembles, constraints, and boundary conditions

(fix command)

- 2d or 3d systems
- orthogonal or non-orthogonal (triclinic symmetry) simulation domains
- constant NVE, NVT, NPT, NPH, Parinello/Rahman integrators
- thermostatting options for groups and geometric regions of atoms
- pressure control via Nose/Hoover or Berendsen barostatting in 1 to 3 dimensions
- simulation box deformation (tensile and shear)
- harmonic (umbrella) constraint forces
- rigid body constraints
- SHAKE bond and angle constraints
- Monte Carlo bond breaking, formation, swapping
- atom/molecule insertion and deletion
- walls of various kinds
- non-equilibrium molecular dynamics (NEMD)
- variety of additional boundary conditions and constraints

Integrators

(run, run_style, minimize commands)

- velocity-Verlet integrator
- Brownian dynamics
- rigid body integration
- energy minimization via conjugate gradient or steepest descent relaxation
- rRESPA hierarchical timestepping
- rerun command for post-processing of dump files

Diagnostics

- see the various flavors of the fix and compute commands

Output

(dump, restart commands)

- log file of thermodynamic info
- text dump files of atom coords, velocities, other per-atom quantities
- binary restart files
- parallel I/O of dump and restart files
- per-atom quantities (energy, stress, centro-symmetry parameter, CNA, etc)
- user-defined system-wide (log file) or per-atom (dump file) calculations
- spatial and time averaging of per-atom quantities
- time averaging of system-wide quantities
- atom snapshots in native, XYZ, XTC, DCD, CFG formats

Multi-replica models

nudged elastic band parallel replica dynamics temperature accelerated dynamics parallel tempering

Pre- and post-processing

- Various pre- and post-processing serial tools are packaged with LAMMPS; see these doc pages.
- Our group has also written and released a separate toolkit called Pizza.py which provides tools for doing setup, analysis, plotting, and visualization for LAMMPS simulations. Pizza.py is written in Python and is available for download from the Pizza.py WWW site.

Specialized features

These are LAMMPS capabilities which you may not think of as typical molecular dynamics options:

- static and dynamic load-balancing
- generalized aspherical particles
- stochastic rotation dynamics (SRD)
- real-time visualization and interactive MD
- calculate virtual diffraction patterns
- atom-to-continuum coupling with finite elements
- coupled rigid body integration via the POEMS library
- QM/MM coupling
- path-integral molecular dynamics (PIMD) and this as well

- Monte Carlo via GCMC and tfMC and atom swapping
- Direct Simulation Monte Carlo for low-density fluids
- Peridynamics mesoscale modeling
- Lattice Boltzmann fluid
- targeted and steered molecular dynamics
- two-temperature electron model

1.3 LAMMPS non-features

LAMMPS is designed to efficiently compute Newton's equations of motion for a system of interacting particles. Many of the tools needed to pre- and post-process the data for such simulations are not included in the LAMMPS kernel for several reasons:

- the desire to keep LAMMPS simple
- they are not parallel operations
- other codes already do them
- limited development resources

Specifically, LAMMPS itself does not:

- run thru a GUI
- build molecular systems
- assign force-field coefficients automagically
- perform sophisticated analyses of your MD simulation
- visualize your MD simulation
- plot your output data

A few tools for pre- and post-processing tasks are provided as part of the LAMMPS package; they are described in this section. However, many people use other codes or write their own tools for these tasks.

As noted above, our group has also written and released a separate toolkit called Pizza.py which addresses some of the listed bullets. It provides tools for doing setup, analysis, plotting, and visualization for LAMMPS simulations. Pizza.py is written in Python and is available for download from the Pizza.py WWW site.

LAMMPS requires as input a list of initial atom coordinates and types, molecular topology information, and force-field coefficients assigned to all atoms and bonds. LAMMPS will not build molecular systems and assign force-field parameters for you.

For atomic systems LAMMPS provides a create_atoms command which places atoms on solid-state lattices (fcc, bcc, user-defined, etc). Assigning small numbers of force field coefficients can be done via the pair coeff, bond coeff, angle coeff, etc commands. For molecular systems or more complicated simulation geometries, users typically use another code as a builder and convert its output to LAMMPS input format, or write their own code to generate atom coordinate and molecular topology for LAMMPS to read in.

For complicated molecular systems (e.g. a protein), a multitude of topology information and hundreds of force-field coefficients must typically be specified. We suggest you use a program like CHARMM or AMBER or other molecular builders to setup such problems and dump its information to a file. You can then reformat the file as LAMMPS input. Some of the tools in this section can assist in this process.

Similarly, LAMMPS creates output files in a simple format. Most users post-process these files with their own analysis tools or re-format them for input into other programs, including visualization packages. If you are

convinced you need to compute something on-the-fly as LAMMPS runs, see Section_modify for a discussion of how you can use the dump and compute and fix commands to print out data of your choosing. Keep in mind that complicated computations can slow down the molecular dynamics timestepping, particularly if the computations are not parallel, so it is often better to leave such analysis to post-processing codes.

A very simple (yet fast) visualizer is provided with the LAMMPS package - see the xmovie tool in this section. It creates xyz projection views of atomic coordinates and animates them. We find it very useful for debugging purposes. For high-quality visualization we recommend the following packages:

- VMD
- AtomEye
- PyMol
- Raster3d
- RasMol

Other features that LAMMPS does not yet (and may never) support are discussed in Section_history.

Finally, these are freely-available molecular dynamics codes, most of them parallel, which may be well-suited to the problems you want to model. They can also be used in conjunction with LAMMPS to perform complementary modeling tasks.

- CHARMM
- AMBER
- NAMD
- NWCHEM
- DL_POLY
- Tinker

CHARMM, AMBER, NAMD, NWCHEM, and Tinker are designed primarily for modeling biological molecules. CHARMM and AMBER use atom-decomposition (replicated-data) strategies for parallelism; NAMD and NWCHEM use spatial-decomposition approaches, similar to LAMMPS. Tinker is a serial code. DL_POLY includes potentials for a variety of biological and non-biological materials; both a replicated-data and spatial-decomposition version exist.

1.4 Open source distribution

LAMMPS comes with no warranty of any kind. As each source file states in its header, it is a copyrighted code that is distributed free-of- charge, under the terms of the GNU Public License (GPL). This is often referred to as open-source distribution - see www.gnu.org or www.opensource.org for more details. The legal text of the GPL is in the LICENSE file that is included in the LAMMPS distribution.

Here is a summary of what the GPL means for LAMMPS users:

(1) Anyone is free to use, modify, or extend LAMMPS in any way they choose, including for commercial purposes.

(2) If you distribute a modified version of LAMMPS, it must remain open-source, meaning you distribute it under the terms of the GPL. You should clearly annotate such a code as a derivative version of LAMMPS.

(3) If you release any code that includes LAMMPS source code, then it must also be open-sourced, meaning you distribute it under the terms of the GPL.

(4) If you give LAMMPS files to someone else, the GPL LICENSE file and source file headers (including the copyright and GPL notices) should remain part of the code.

In the spirit of an open-source code, these are various ways you can contribute to making LAMMPS better. You can send email to the developers on any of these items.

- Point prospective users to the LAMMPS WWW Site. Mention it in talks or link to it from your WWW site.
- If you find an error or omission in this manual or on the LAMMPS WWW Site, or have a suggestion for something to clarify or include, send an email to the developers.
- If you find a bug, Section_errors 2 describes how to report it.
- If you publish a paper using LAMMPS results, send the citation (and any cool pictures or movies if you like) to add to the Publications, Pictures, and Movies pages of the LAMMPS WWW Site, with links and attributions back to you.
- Create a new Makefile.machine that can be added to the src/MAKE directory.
- The tools sub-directory of the LAMMPS distribution has various stand-alone codes for pre- and post-processing of LAMMPS data. More details are given in Section_tools. If you write a new tool that users will find useful, it can be added to the LAMMPS distribution.
- LAMMPS is designed to be easy to extend with new code for features like potentials, boundary conditions, diagnostic computations, etc. This section gives details. If you add a feature of general interest, it can be added to the LAMMPS distribution.
- The Benchmark page of the LAMMPS WWW Site lists LAMMPS performance on various platforms. The files needed to run the benchmarks are part of the LAMMPS distribution. If your machine is sufficiently different from those listed, your timing data can be added to the page.
- You can send feedback for the User Comments page of the LAMMPS WWW Site. It might be added to the page. No promises.
- Cash. Small denominations, unmarked bills preferred. Paper sack OK. Leave on desk. VISA also accepted. Chocolate chip cookies encouraged.

1.5 Acknowledgments and citations

LAMMPS development has been funded by the US Department of Energy (DOE), through its CRADA, LDRD, ASCI, and Genomes-to-Life programs and its OASCR and OBER offices.

Specifically, work on the latest version was funded in part by the US Department of Energy's Genomics:GTL program (www.doegenomestolife.org) under the project, "Carbon Sequestration in Synechococcus Sp.: From Molecular Machines to Hierarchical Modeling".

The following paper describe the basic parallel algorithms used in LAMMPS. If you use LAMMPS results in your published work, please cite this paper and include a pointer to the LAMMPS WWW Site (http://lammps.sandia.gov):

S. J. Plimpton, **Fast Parallel Algorithms for Short-Range Molecular Dynamics**, J Comp Phys, 117, 1-19 (1995).

Other papers describing specific algorithms used in LAMMPS are listed under the Citing LAMMPS link of the LAMMPS WWW page.

The Publications link on the LAMMPS WWW page lists papers that have cited LAMMPS. If your paper is not listed there for some reason, feel free to send us the info. If the simulations in your paper produced cool pictures or animations, we'll be pleased to add them to the Pictures or Movies pages of the LAMMPS WWW site.

The core group of LAMMPS developers is at Sandia National Labs:

- Steve Plimpton, sjplimp at sandia.gov
- Aidan Thompson, athomps at sandia.gov
- Paul Crozier, pscrozi at sandia.gov

The following folks are responsible for significant contributions to the code, or other aspects of the LAMMPS development effort. Many of the packages they have written are somewhat unique to LAMMPS and the code would not be as general-purpose as it is without their expertise and efforts.

- Axel Kohlmeyer (Temple U), akohlmey at gmail.com, SVN and Git repositories, indefatigable mail list responder, USER-CG-CMM and USER-OMP packages
- Roy Pollock (LLNL), Ewald and PPPM solvers
- Mike Brown (ORNL), brownw at ornl.gov, GPU package
- Greg Wagner (Sandia), gjwagne at sandia.gov, MEAM package for MEAM potential
- Mike Parks (Sandia), mlparks at sandia.gov, PERI package for Peridynamics
- Rudra Mukherjee (JPL), Rudranarayan.M.Mukherjee at jpl.nasa.gov, POEMS package for articulated rigid body motion
- Reese Jones (Sandia) and collaborators, rjones at sandia.gov, USER-ATC package for atom/continuum coupling
- Ilya Valuev (JIHT), valuev at physik.hu-berlin.de, USER-AWPMD package for wave-packet MD
- Christian Trott (U Tech Ilmenau), christian.trott at tu-ilmenau.de, USER-CUDA package
- Andres Jaramillo-Botero (Caltech), ajaramil at wag.caltech.edu, USER-EFF package for electron force field
- Christoph Kloss (JKU), Christoph.Kloss at jku.at, USER-LIGGGHTS package for granular models and granular/fluid coupling
- Metin Aktulga (LBL), hmaktulga at lbl.gov, USER-REAXC package for C version of ReaxFF
- Georg Gunzenmuller (EMI), georg.ganzenmueller at emi.fhg.de, USER-SPH package

As discussed in Section_history, LAMMPS originated as a cooperative project between DOE labs and industrial partners. Folks involved in the design and testing of the original version of LAMMPS were the following:

- John Carpenter (Mayo Clinic, formerly at Cray Research)
- Terry Stouch (Lexicon Pharmaceuticals, formerly at Bristol Myers Squibb)
- Steve Lustig (Dupont)
- Jim Belak (LLNL)

2. Getting Started

This section describes how to build and run LAMMPS, for both new and experienced users.

2.1 What's in the LAMMPS distribution

When you download a LAMMPS tarball you will need to unzip and untar the downloaded file with the following commands, after placing the tarball in an appropriate directory.

```
gunzip lammps*.tar.gz
tar xvf lammps*.tar
```

This will create a LAMMPS directory containing two files and several sub-directories:

README	text file
LICENSE	the GNU General Public License (GPL)
bench	benchmark problems
doc	documentation
examples	simple test problems
potentials	embedded atom method (EAM) potential files
src	source files
tools	pre- and post-processing tools

Note that the download page also has links to download Windows exectubles and installers, as well as pre-built executables for a few specific Linux distributions. It also has instructions for how to download/install LAMMPS for Macs (via Homebrew), and to download and update LAMMPS from SVN and Git repositories, which gives you the same files that are in the download tarball.

The Windows and Linux executables for serial or parallel only include certain packages and bug-fixes/upgrades listed on this page up to a certain date, as stated on the download page. If you want an executable with non-included packages or that is more current, then you'll need to build LAMMPS yourself, as discussed in the next section.

Skip to the Running LAMMPS sections for info on how to launch a LAMMPS Windows executable on a Windows box.

2.2 Making LAMMPS

This section has the following sub-sections:

Read this first:

If you want to avoid building LAMMPS yourself, read the preceeding section about options available for downloading and installing executables. Details are discussed on the download page.

Building LAMMPS can be simple or not-so-simple. If all you need are the default packages installed in LAMMPS, and MPI is already installed on your machine, or you just want to run LAMMPS in serial, then you can typically use the Makefile.mpi or Makefile.serial files in src/MAKE by typing one of these lines (from the src dir):

```
make mpi
make serial
```

Note that on a facility supercomputer, there are often "modules" loaded in your environment that provide the compilers and MPI you should use. In this case, the "mpicxx" compile/link command in Makefile.mpi should just work by accessing those modules.

It may be the case that one of the other Makefile.machine files in the src/MAKE sub-directories is a better match to your system (type "make" to see a list), you can use it as-is by typing (for example):

```
make stampede
```

If any of these builds (with an existing Makefile.machine) works on your system, then you're done!

If you want to do one of the following:

- use optional LAMMPS features that require additional libraries
- use optional packages that require additional libraries
- use optional accelerator packages that require special compiler/linker settings
- run on a specialized platform that has its own compilers, settings, or other libs to use

then building LAMMPS is more complicated. You may need to find where auxiliary libraries exist on your machine or install them if they don't. You may need to build additional libraries that are part of the LAMMPS package, before building LAMMPS. You may need to edit a Makefile.machine file to make it compatible with your system.

Note that there is a Make.py tool in the src directory that automates several of these steps, but you still have to know what you are doing. Section 2.4 below describes the tool. It is a convenient way to work with installing/un-installing various packages, the Makefile.machine changes required by some packages, and the auxiliary libraries some of them use.

Please read the following sections carefully. If you are not comfortable with makefiles, or building codes on a Unix platform, or running an MPI job on your machine, please find a local expert to help you. Many compilation, linking, and run problems that users have are often not really LAMMPS issues - they are peculiar to the user's system, compilers, libraries, etc. Such questions are better answered by a local expert.

If you have a build problem that you are convinced is a LAMMPS issue (e.g. the compiler complains about a line of LAMMPS source code), then please post the issue to the LAMMPS mail list.

If you succeed in building LAMMPS on a new kind of machine, for which there isn't a similar machine Makefile included in the src/MAKE/MACHINES directory, then send it to the developers and we can include it in the LAMMPS distribution.

Steps to build a LAMMPS executable:

Step 0

The src directory contains the C++ source and header files for LAMMPS. It also contains a top-level Makefile and a MAKE sub-directory with low-level Makefile.* files for many systems and machines. See the src/MAKE/README file for a quick overview of what files are available and what sub-directories they are in.

The src/MAKE dir has a few files that should work as-is on many platforms. The src/MAKE/OPTIONS dir has more that invoke additional compiler, MPI, and other setting options commonly used by LAMMPS, to illustrate their syntax. The src/MAKE/MACHINES dir has many more that have been tweaked or optimized for specific machines. These files are all good starting points if you find you need to change them for your machine. Put any file you edit into the src/MAKE/MINE directory and it will be never be touched by any LAMMPS updates.

>From within the src directory, type "make" or "gmake". You should see a list of available choices from src/MAKE and all of its sub-directories. If one of those has the options you want or is the machine you want, you can type a command like:

```
make mpi
or
make serial_icc
or
gmake mac
```

Note that the corresponding Makefile.machine can exist in src/MAKE or any of its sub-directories. If a file with the same name appears in multiple places (not a good idea), the order they are used is as follows: src/MAKE/MINE, src/MAKE, src/MAKE/OPTIONS, src/MAKE/MACHINES. This gives preference to a file you have created/edited and put in src/MAKE/MINE.

Note that on a multi-processor or multi-core platform you can launch a parallel make, by using the "-j" switch with the make command, which will build LAMMPS more quickly.

If you get no errors and an executable like lmp_mpi or lmp_g++_serial or lmp_mac is produced, then you're done; it's your lucky day.

Note that by default only a few of LAMMPS optional packages are installed. To build LAMMPS with optional packages, see this section below.

Step 1

If Step 0 did not work, you will need to create a low-level Makefile for your machine, like Makefile.foo. You should make a copy of an existing Makefile.* in src/MAKE or one of its sub-directories as a starting point. The only portions of the file you need to edit are the first line, the "compiler/linker settings" section, and the "LAMMPS-specific settings" section. When it works, put the edited file in src/MAKE/MINE and it will not be altered by any future LAMMPS updates.

Step 2

Change the first line of Makefile.foo to list the word "foo" after the "#", and whatever other options it will set. This is the line you will see if you just type "make".

Step 3

The "compiler/linker settings" section lists compiler and linker settings for your C++ compiler, including optimization flags. You can use g++, the open-source GNU compiler, which is available on all Unix systems. You can also use mpicxx which will typically be available if MPI is installed on your system, though you should check which actual compiler it wraps. Vendor compilers often produce faster code. On boxes with Intel CPUs, we suggest using the Intel icc compiler, which can be downloaded from Intel's compiler site.

If building a C++ code on your machine requires additional libraries, then you should list them as part of the LIB variable. You should not need to do this if you use mpicxx.

The DEPFLAGS setting is what triggers the C++ compiler to create a dependency list for a source file. This speeds re-compilation when source (*.cpp) or header (*.h) files are edited. Some compilers do not support dependency file creation, or may use a different switch than -D. GNU g++ and Intel icc works with -D. If your compiler can't create dependency files, then you'll need to create a Makefile.foo patterned after Makefile.storm, which uses different rules that do not involve dependency files. Note that when you build LAMMPS for the first time on a new platform, a long list of *.d files will be printed out rapidly. This is not an error; it is the Makefile doing its normal creation of dependencies.

Step 4

The "system-specific settings" section has several parts. Note that if you change any -D setting in this section, you should do a full re-compile, after typing "make clean" (which will describe different clean options).

The LMP_INC variable is used to include options that turn on ifdefs within the LAMMPS code. The options that are currently recogized are:

- -DLAMMPS_GZIP
- -DLAMMPS_JPEG
- -DLAMMPS_PNG
- -DLAMMPS_FFMPEG
- -DLAMMPS_MEMALIGN
- -DLAMMPS_XDR
- -DLAMMPS_SMALLBIG
- -DLAMMPS_BIGBIG
- -DLAMMPS_SMALLSMALL
- -DLAMMPS_LONGLONG_TO_LONG
- -DPACK_ARRAY
- -DPACK_POINTER
- -DPACK_MEMCPY

The read_data and dump commands will read/write gzipped files if you compile with -DLAMMPS_GZIP. It requires that your machine supports the "popen()" function in the standard runtime library and that a gzip executable can be found by LAMMPS during a run.

NOTE: on some clusters with high-speed networks, using the fork() library calls (required by popen()) can interfere with the fast communication library and lead to simulations using compressed output or input to hang or crash. For selected operations, compressed file I/O is also available using a compression library instead, which are provided in the COMPRESS package. From more details about compiling LAMMPS with packages, please see below.

If you use -DLAMMPS_JPEG, the dump image command will be able to write out JPEG image files. For JPEG files, you must also link LAMMPS with a JPEG library, as described below. If you use -DLAMMPS_PNG, the dump image command will be able to write out PNG image files. For PNG files, you must also link LAMMPS with a PNG library, as described below. If neither of those two defines are used, LAMMPS will only be able to write out uncompressed PPM image files.

If you use -DLAMMPS_FFMPEG, the dump movie command will be available to support on-the-fly generation of rendered movies the need to store intermediate image files. It requires that your machines supports the "popen" function in the standard runtime library and that an FFmpeg executable can be found by LAMMPS during the run.

NOTE: Similar to the note above, this option can conflict with high-speed networks, because it uses popen().

Using -DLAMMPS_MEMALIGN= enables the use of the posix_memalign() call instead of malloc() when large chunks or memory are allocated by LAMMPS. This can help to make more efficient use of vector instructions of modern CPUS, since dynamically allocated memory has to be aligned on larger than default byte boundaries (e.g. 16 bytes instead of 8 bytes on x86 type platforms) for optimal performance.

If you use -DLAMMPS_XDR, the build will include XDR compatibility files for doing particle dumps in XTC format. This is only necessary if your platform does have its own XDR files available. See the Restrictions section of the dump command for details.

Use at most one of the -DLAMMPS_SMALLBIG, -DLAMMPS_BIGBIG, -DLAMMPS_SMALLSMALL settings. The default is -DLAMMPS_SMALLBIG. These settings refer to use of 4-byte (small) vs 8-byte (big) integers within LAMMPS, as specified in src/lmptype.h. The only reason to use the BIGBIG setting is to enable simulation of huge molecular systems (which store bond topology info) with more than 2 billion atoms, or to track the image flags of moving atoms that wrap around a periodic box more than 512 times. Normally, the only reason to use SMALLSMALL is if your machine does not support 64-bit integers, though you can use SMALLSMALL setting if you are running in serial or on a desktop machine or small cluster where you will never run large systems or for long time (more than 2 billion atoms, more than 2 billion timesteps). See the Additional build tips section below for more details on these settings.

Note that two packages, USER-ATC and USER-CUDA are not currently compatible with -DLAMMPS_BIGBIG. Also the GPU package requires the lib/gpu library to be compiled with the same setting, or the link will fail.

The -DLAMMPS_LONGLONG_TO_LONG setting may be needed if your system or MPI version does not recognize "long long" data types. In this case a "long" data type is likely already 64-bits, in which case this setting will convert to that data type.

Using one of the -DPACK_ARRAY, -DPACK_POINTER, and -DPACK_MEMCPY options can make for faster parallel FFTs (in the PPPM solver) on some platforms. The -DPACK_ARRAY setting is the default. See the kspace_style command for info about PPPM. See Step 6 below for info about building LAMMPS with an FFT library.

Step 5

The 3 MPI variables are used to specify an MPI library to build LAMMPS with. Note that you do not need to set these if you use the MPI compiler mpicxx for your CC and LINK setting in the section above. The MPI wrapper knows where to find the needed files.

If you want LAMMPS to run in parallel, you must have an MPI library installed on your platform. If MPI is installed on your system in the usual place (under /usr/local), you also may not need to specify these 3 variables, assuming /usr/local is in your path. On some large parallel machines which use "modules" for their compile/link environements, you may simply need to include the correct module in your build environment, before building LAMMPS. Or the parallel machine may have a vendor-provided MPI which the compiler has no trouble finding.

Failing this, these 3 variables can be used to specify where the mpi.h file (MPI_INC) and the MPI library file (MPI_PATH) are found and the name of the library file (MPI_LIB).

If you are installing MPI yourself, we recommend Argonne's MPICH2 or OpenMPI. MPICH can be downloaded from the Argonne MPI site. OpenMPI can be downloaded from the OpenMPI site. Other MPI packages should also work. If you are running on a big parallel platform, your system people or the vendor should have already installed a version of MPI, which is likely to be faster than a self-installed MPICH or OpenMPI, so find out how to build and link with it. If you use MPICH or OpenMPI, you will have to configure and build it for your platform. The MPI configure script should have compiler options to enable you to use the same compiler you are using for the LAMMPS build, which can avoid problems that can arise when linking LAMMPS to the MPI library.

If you just want to run LAMMPS on a single processor, you can use the dummy MPI library provided in src/STUBS, since you don't need a true MPI library installed on your system. See src/MAKE/Makefile.serial for how to specify the 3 MPI variables in this case. You will also need to build the STUBS library for your platform before making LAMMPS itself. Note that if you are building with src/MAKE/Makefile.serial, e.g. by typing "make serial", then the STUBS library is built for you.

To build the STUBS library from the src directory, type "make mpi-stubs", or from the src/STUBS dir, type "make". This should create a libmpi_stubs.a file suitable for linking to LAMMPS. If the build fails, you will need to edit the STUBS/Makefile for your platform.

The file STUBS/mpi.c provides a CPU timer function called MPI_Wtime() that calls gettimeofday() . If your system doesn't support gettimeofday() , you'll need to insert code to call another timer. Note that the ANSI-standard function clock() rolls over after an hour or so, and is therefore insufficient for timing long LAMMPS simulations.

Step 6

The 3 FFT variables allow you to specify an FFT library which LAMMPS uses (for performing 1d FFTs) when running the particle-particle particle-mesh (PPPM) option for long-range Coulombics via the kspace_style command.

LAMMPS supports various open-source or vendor-supplied FFT libraries for this purpose. If you leave these 3 variables blank, LAMMPS will use the open-source KISS FFT library, which is included in the LAMMPS distribution. This library is portable to all platforms and for typical LAMMPS simulations is almost as fast as FFTW or vendor optimized libraries. If you are not including the KSPACE package in your build, you can also leave the 3 variables blank.

Otherwise, select which kinds of FFTs to use as part of the FFT_INC setting by a switch of the form

-DFFT_XXX. Recommended values for XXX are: MKL, SCSL, FFTW2, and FFTW3. Legacy options are: INTEL, SGI, ACML, and T3E. For backward compatability, using -DFFT_FFTW will use the FFTW2 library. Using -DFFT_NONE will use the KISS library described above.

You may also need to set the FFT_INC, FFT_PATH, and FFT_LIB variables, so the compiler and linker can find the needed FFT header and library files. Note that on some large parallel machines which use "modules" for their compile/link environements, you may simply need to include the correct module in your build environment. Or the parallel machine may have a vendor-provided FFT library which the compiler has no trouble finding.

FFTW is a fast, portable library that should also work on any platform. You can download it from www.fftw.org. Both the legacy version 2.1.X and the newer 3.X versions are supported as -DFFT_FFTW2 or -DFFT_FFTW3. Building FFTW for your box should be as simple as ./configure; make. Note that on some platforms FFTW2 has been pre-installed, and uses renamed files indicating the precision it was compiled with, e.g. sfftw.h, or dfftw.h instead of fftw.h. In this case, you can specify an additional define variable for FFT_INC called -DFFTW_SIZE, which will select the correct include file. In this case, for FFT_LIB you must also manually specify the correct library, namely -lsfftw or -ldfftw.

The FFT_INC variable also allows for a -DFFT_SINGLE setting that will use single-precision FFTs with PPPM, which can speed-up long-range calulations, particularly in parallel or on GPUs. Fourier transform and related PPPM operations are somewhat insensitive to floating point truncation errors and thus do not always need to be performed in double precision. Using the -DFFT_SINGLE setting trades off a little accuracy for reduced memory use and parallel communication costs for transposing 3d FFT data. Note that single precision FFTs have only been tested with the FFTW3, FFTW2, MKL, and KISS FFT options.

Step 7

The 3 JPG variables allow you to specify a JPEG and/or PNG library which LAMMPS uses when writing out JPEG or PNG files via the dump image command. These can be left blank if you do not use the -DLAMMPS_JPEG or -DLAMMPS_PNG switches discussed above in Step 4, since in that case JPEG/PNG output will be disabled.

A standard JPEG library usually goes by the name libjpeg.a or libjpeg.so and has an associated header file jpeglib.h. Whichever JPEG library you have on your platform, you'll need to set the appropriate JPG_INC, JPG_PATH, and JPG_LIB variables, so that the compiler and linker can find it.

A standard PNG library usually goes by the name libpng.a or libpng.so and has an associated header file png.h. Whichever PNG library you have on your platform, you'll need to set the appropriate JPG_INC, JPG_PATH, and JPG_LIB variables, so that the compiler and linker can find it.

As before, if these header and library files are in the usual place on your machine, you may not need to set these variables.

Step 8

Note that by default only a few of LAMMPS optional packages are installed. To build LAMMPS with optional packages, see this section below, before proceeding to Step 9.

Step 9

That's it. Once you have a correct Makefile.foo, and you have pre-built any other needed libraries (e.g. MPI, FFT, etc) all you need to do from the src directory is type something like this:

```
make foo
```

```
or
gmake foo
```

You should get the executable lmp_foo when the build is complete.

Errors that can occur when making LAMMPS:

NOTE: If an error occurs when building LAMMPS, the compiler or linker will state very explicitly what the problem is. The error message should give you a hint as to which of the steps above has failed, and what you need to do in order to fix it. Building a code with a Makefile is a very logical process. The compiler and linker need to find the appropriate files and those files need to be compatible with LAMMPS source files. When a make fails, there is usually a very simple reason, which you or a local expert will need to fix.

Here are two non-obvious errors that can occur:

(1) If the make command breaks immediately with errors that indicate it can't find files with a "*" in their names, this can be because your machine's native make doesn't support wildcard expansion in a makefile. Try gmake instead of make. If that doesn't work, try using a -f switch with your make command to use a pre-generated Makefile.list which explicitly lists all the needed files, e.g.

```
make makelist
make -f Makefile.list linux
gmake -f Makefile.list mac
```

The first "make" command will create a current Makefile.list with all the file names in your src dir. The 2nd "make" command (make or gmake) will use it to build LAMMPS. Note that you should include/exclude any desired optional packages before using the "make makelist" command.

(2) If you get an error that says something like 'identifier "atoll" is undefined', then your machine does not support "long long" integers. Try using the -DLAMMPS_LONGLONG_TO_LONG setting described above in Step 4.

Additional build tips:

(1) Building LAMMPS for multiple platforms.

You can make LAMMPS for multiple platforms from the same src directory. Each target creates its own object sub-directory called Obj_target where it stores the system-specific *.o files.

(2) Cleaning up.

Typing "make clean-all" or "make clean-machine" will delete *.o object files created when LAMMPS is built, for either all builds or for a particular machine.

(3) Changing the LAMMPS size limits via -DLAMMPS_SMALLBIG or -DLAMMPS_BIGBIG or -DLAMMPS_SMALLSMALL

As explained above, any of these 3 settings can be specified on the LMP_INC line in your low-level src/MAKE/Makefile.foo.

The default is -DLAMMPS_SMALLBIG which allows for systems with up to 2^63 atoms and 2^63 timesteps (about 9e18). The atom limit is for atomic systems which do not store bond topology info and thus do not require atom IDs. If you use atom IDs for atomic systems (which is the default) or if you use a molecular model, which stores bond topology info and thus requires atom IDs, the limit is 2^31 atoms (about 2 billion). This is because the

IDs are stored in 32-bit integers.

Likewise, with this setting, the 3 image flags for each atom (see the dump doc page for a discussion) are stored in a 32-bit integer, which means the atoms can only wrap around a periodic box (in each dimension) at most 512 times. If atoms move through the periodic box more than this many times, the image flags will "roll over", e.g. from 511 to -512, which can cause diagnostics like the mean-squared displacement, as calculated by the compute msd command, to be faulty.

To allow for larger atomic systems with atom IDs or larger molecular systems or larger image flags, compile with -DLAMMPS_BIGBIG. This stores atom IDs and image flags in 64-bit integers. This enables atomic or molecular systems with atom IDS of up to 2^63 atoms (about 9e18). And image flags will not "roll over" until they reach 2^20 = 1048576.

If your system does not support 8-byte integers, you will need to compile with the -DLAMMPS_SMALLSMALL setting. This will restrict the total number of atoms (for atomic or molecular systems) and timesteps to 2^31 (about 2 billion). Image flags will roll over at 2^9 = 512.

Note that in src/lmptype.h there are definitions of all these data types as well as the MPI data types associated with them. The MPI types need to be consistent with the associated C data types, or else LAMMPS will generate a run-time error. As far as we know, the settings defined in src/lmptype.h are portable and work on every current system.

In all cases, the size of problem that can be run on a per-processor basis is limited by 4-byte integer storage to 2^31 atoms per processor (about 2 billion). This should not normally be a limitation since such a problem would have a huge per-processor memory footprint due to neighbor lists and would run very slowly in terms of CPU secs/timestep.

Building for a Mac:

OS X is BSD Unix, so it should just work. See the src/MAKE/MACHINES/Makefile.mac and Makefile.mac_mpi files.

Building for Windows:

The LAMMPS download page has an option to download both a serial and parallel pre-built Windows executable. See the Running LAMMPS section for instructions on running these executables on a Windows box.

The pre-built executables hosted on the LAMMPS download page are built with a subset of the available packages; see the download page for the list. These are single executable files. No examples or documentation in included. You will need to download the full source code package to obtain those.

As an alternative, you can download "daily builds" (and some older versions) of the installer packages from rpm.lammps.org/windows.html. These executables are built with most optional packages and the download includes documentation, some tools and most examples.

If you want a Windows version with specific packages included and excluded, you can build it yourself.

One way to do this is install and use cygwin to build LAMMPS with a standard unix style make program, just as you would on a Linux box; see src/MAKE/MACHINES/Makefile.cygwin.

2.3 Making LAMMPS with optional packages

This section has the following sub-sections:

- Package basics
- Including/excluding packages
- Packages that require extra libraries
- Packages that require Makefile.machine settings

Note that the following Section 2.4 describes the Make.py tool which can be used to install/un-install packages and build the auxiliary libraries which some of them use. It can also auto-edit a Makefile.machine to add settings needed by some packages.

Package basics:

The source code for LAMMPS is structured as a set of core files which are always included, plus optional packages. Packages are groups of files that enable a specific set of features. For example, force fields for molecular systems or granular systems are in packages.

You can see the list of all packages by typing "make package" from within the src directory of the LAMMPS distribution. This also lists various make commands that can be used to manipulate packages.

If you use a command in a LAMMPS input script that is specific to a particular package, you must have built LAMMPS with that package, else you will get an error that the style is invalid or the command is unknown. Every command's doc page specfies if it is part of a package. You can also type

```
lmp_machine -h
```

to run your executable with the optional -h command-line switch for "help", which will simply list the styles and commands known to your executable, and immediately exit.

There are two kinds of packages in LAMMPS, standard and user packages. More information about the contents of standard and user packages is given in Section_packages of the manual. The difference between standard and user packages is as follows:

Standard packages, such as molecule or kspace, are supported by the LAMMPS developers and are written in a syntax and style consistent with the rest of LAMMPS. This means we will answer questions about them, debug and fix them if necessary, and keep them compatible with future changes to LAMMPS.

User packages, such as user-atc or user-omp, have been contributed by users, and always begin with the user prefix. If they are a single command (single file), they are typically in the user-misc package. Otherwise, they are a a set of files grouped together which add a specific functionality to the code.

User packages don't necessarily meet the requirements of the standard packages. If you have problems using a feature provided in a user package, you may need to contact the contributor directly to get help. Information on how to submit additions you make to LAMMPS as single files or either a standard or user-contributed package are given in this section of the documentation.

Some packages (both standard and user) require additional auxiliary libraries when building LAMMPS. See more details below.

Including/excluding packages:

To use (or not use) a package you must include it (or exclude it) before building LAMMPS. From the src directory, this is typically as simple as:

```
make yes-colloid
make g++
```

or

```
make no-manybody
make g++
```

NOTE: You should NOT include/exclude packages and build LAMMPS in a single make command using multiple targets, e.g. make yes-colloid g++. This is because the make procedure creates a list of source files that will be out-of-date for the build if the package configuration changes within the same command.

Some packages have individual files that depend on other packages being included. LAMMPS checks for this and does the right thing. I.e. individual files are only included if their dependencies are already included. Likewise, if a package is excluded, other files dependent on that package are also excluded.

If you will never run simulations that use the features in a particular packages, there is no reason to include it in your build. For some packages, this will keep you from having to build auxiliary libraries (see below), and will also produce a smaller executable which may run a bit faster.

When you download a LAMMPS tarball, these packages are pre-installed in the src directory: KSPACE, MANYBODY,MOLECULE. When you download LAMMPS source files from the SVN or Git repositories, no packages are pre-installed.

Packages are included or excluded by typing "make yes-name" or "make no-name", where "name" is the name of the package in lower-case, e.g. name = kspace for the KSPACE package or name = user-atc for the USER-ATC package. You can also type "make yes-standard", "make no-standard", "make yes-std", "make no-std", "make yes-user", "make no-user", "make yes-all" or "make no-all" to include/exclude various sets of packages. Type "make package" to see the all of the package-related make options.

NOTE: Inclusion/exclusion of a package works by simply moving files back and forth between the main src directory and sub-directories with the package name (e.g. src/KSPACE, src/USER-ATC), so that the files are seen or not seen when LAMMPS is built. After you have included or excluded a package, you must re-build LAMMPS.

Additional package-related make options exist to help manage LAMMPS files that exist in both the src directory and in package sub-directories. You do not normally need to use these commands unless you are editing LAMMPS files or have downloaded a patch from the LAMMPS WWW site.

Typing "make package-update" or "make pu" will overwrite src files with files from the package sub-directories if the package has been included. It should be used after a patch is installed, since patches only update the files in the package sub-directory, but not the src files. Typing "make package-overwrite" will overwrite files in the package sub-directories with src files.

Typing "make package-status" or "make ps" will show which packages are currently included. Of those that are included, it will list files that are different in the src directory and package sub-directory. Typing "make package-diff" lists all differences between these files. Again, type "make package" to see all of the package-related make options.

Packages that require extra libraries:

A few of the standard and user packages require additional auxiliary libraries. Many of them are provided with LAMMPS, in which case they must be compiled first, before LAMMPS is built, if you wish to include that package. If you get a LAMMPS build error about a missing library, this is likely the reason. See the Section_packages doc page for a list of packages that have these kinds of auxiliary libraries.

The lib directory in the distribution has sub-directories with package names that correspond to the needed auxiliary libs, e.g. lib/gpu. Each sub-directory has a README file that gives more details. Code for most of the auxiliary libraries is included in that directory. Examples are the USER-ATC and MEAM packages.

A few of the lib sub-directories do not include code, but do include instructions (and sometimes scripts) that automate the process of downloading the auxiliary library and installing it so LAMMPS can link to it. Examples are the KIM, VORONOI, USER-MOLFILE, and USER-SMD packages.

The lib/python directory (for the PYTHON package) contains only a choice of Makefile.lammps.* files. This is because no auxiliary code or libraries are needed, only the Python library and other system libs that should already available on your system. However, the Makefile.lammps file is needed to tell LAMMPS which libs to use and where to find them.

For libraries with provided code, the sub-directory README file (e.g. lib/atc/README) has instructions on how to build that library. Typically this is done by typing something like:

```
make -f Makefile.g++
```

If one of the provided Makefiles is not appropriate for your system you will need to edit or add one. Note that all the Makefiles have a setting for EXTRAMAKE at the top that specifies a Makefile.lammps.* file.

If the library build is successful, it will produce 2 files in the lib directory:

```
libpackage.a
Makefile.lammps
```

The Makefile.lammps file will be a copy of the EXTRAMAKE file setting specified in the library Makefile.* you used.

Note that you must insure that the settings in Makefile.lammps are appropriate for your system. If they are not, the LAMMPS build will fail.

As explained in the lib/package/README files, the settings in Makefile.lammps are used to specify additional system libraries and their locations so that LAMMPS can build with the auxiliary library. For example, if the MEAM package is used, the auxiliary library consists of F90 code, built with a Fortran complier. To link that library with LAMMPS (a C++ code) via whatever C++ compiler LAMMPS is built with, typically requires additional Fortran-to-C libraries be included in the link. Another example are the BLAS and LAPACK libraries needed to use the USER-ATC or USER-AWPMD packages.

For libraries without provided code, the sub-directory README file has information on where to download the library and how to build it, e.g. lib/voronoi/README and lib/smd/README. The README files also describe how you must either (a) create soft links, via the "ln" command, in those directories to point to where you built or installed the packages, or (b) check or edit the Makefile.lammps file in the same directory to provide that information.

Some of the sub-directories, e.g. lib/voronoi, also have an install.py script which can be used to automate the process of downloading/building/installing the auxiliary library, and setting the needed soft links. Type "python install.py" for further instructions.

As with the sub-directories containing library code, if the soft links or settings in the lib/package/Makefile.lammps files are not correct, the LAMMPS build will typically fail.

Packages that require Makefile.machine settings

A few packages require specific settings in Makefile.machine, to either build or use the package effectively. These are the USER-INTEL, KOKKOS, USER-OMP, and OPT packages. The details of what flags to add or what variables to define are given on the doc pages that describe each of these accelerator packages in detail:

- USER-INTEL package
- KOKKOS package
- USER-OMP package
- OPT package

Here is a brief summary of what Makefile.machine changes are needed. Note that the Make.py tool, described in the next Section 2.4 can automatically add the needed info to an existing machine Makefile, using simple command-line arguments.

In src/MAKE/OPTIONS see the following Makefiles for examples of the changes described below:

- Makefile.intel_cpu
- Makefile.intel_phi
- Makefile.kokkos_omp
- Makefile.kokkos_cuda
- Makefile.kokkos_phi
- Makefile.omp

For the USER-INTEL package, you have 2 choices when building. You can build with CPU or Phi support. The latter uses Xeon Phi chips in "offload" mode. Each of these modes requires additional settings in your Makefile.machine for CCFLAGS and LINKFLAGS.

For CPU mode (if using an Intel compiler):

- CCFLAGS: add -fopenmp, -DLAMMPS_MEMALIGN=64, -restrict, -xHost, -fno-alias, -ansi-alias, -override-limits
- LINKFLAGS: add -fopenmp

For Phi mode add the following in addition to the CPU mode flags:

- CCFLAGS: add -DLMP_INTEL_OFFLOAD and
- LINKFLAGS: add -offload

And also add this to CCFLAGS:

```
-offload-option,mic,compiler,"-fp-model fast=2 -mGLOB_default_function_attrs=\"gather_scatter_loop_u
```

For the KOKKOS package, you have 3 choices when building. You can build with OMP or Cuda or Phi support. Phi support uses Xeon Phi chips in "native" mode. This can be done by setting the following variables in your Makefile.machine:

- for OMP support, set OMP = yes
- for Cuda support, set OMP = yes and CUDA = yes

- for Phi support, set OMP = yes and MIC = yes

These can also be set as additional arguments to the make command, e.g.

```
make g++ OMP=yes MIC=yes
```

Building the KOKKOS package with CUDA support requires a Makefile machine that uses the NVIDIA "nvcc" compiler, as well as an appropriate "arch" setting appropriate to the GPU hardware and NVIDIA software you have on your machine. See src/MAKE/OPTIONS/Makefile.kokkos_cuda for an example of such a machine Makefile.

For the USER-OMP package, your Makefile.machine needs additional settings for CCFLAGS and LINKFLAGS.

- CCFLAGS: add -fopenmp and -restrict
- LINKFLAGS: add -fopenmp

For the OPT package, your Makefile.machine needs an additional settings for CCFLAGS.

- CCFLAGS: add -restrict

2.4 Building LAMMPS via the Make.py tool

The src directory includes a Make.py script, written in Python, which can be used to automate various steps of the build process. It is particularly useful for working with the accelerator packages, as well as other packages which require auxiliary libraries to be built.

The goal of the Make.py tool is to allow any complex multi-step LAMMPS build to be performed as a single Make.py command. And you can archive the commands, so they can be re-invoked later via the -r (redo) switch. If you find some LAMMPS build procedure that can't be done in a single Make.py command, let the developers know, and we'll see if we can augment the tool.

You can run Make.py from the src directory by typing either:

```
Make.py -h
python Make.py -h
```

which will give you help info about the tool. For the former to work, you may need to edit the first line of Make.py to point to your local Python. And you may need to insure the script is executable:

```
chmod +x Make.py
```

Here are examples of build tasks you can perform with Make.py:

Install/uninstall packages	Make.py -p no-lib kokkos omp intel
Build specific auxiliary libs	Make.py -a lib-atc lib-meam
Build libs for all installed packages	Make.py -p cuda gpu -gpu mode=double arch=31 -a lib-all
Create a Makefile from scratch with compiler and MPI settings	Make.py -m none -cc g++ -mpi mpich -a file
Augment Makefile.serial with settings for installed packages	Make.py -p intel -intel cpu -m serial -a file
Add JPG and FFTW support to Makefile.mpi	Make.py -m mpi -jpg -fft fftw -a file
Build LAMMPS with a parallel make using Makefile.mpi	Make.py -j 16 -m mpi -a exe

Build LAMMPS and libs it needs using Makefile.serial with accelerator settings	Make.py -p gpu intel -intel cpu -a lib-all file serial

The bench and examples directories give Make.py commands that can be used to build LAMMPS with the various packages and options needed to run all the benchmark and example input scripts. See these files for more details:

- bench/README
- bench/FERMI/README
- bench/KEPLER/README
- bench/PHI/README
- examples/README
- examples/accelerate/README
- examples/accelerate/make.list

All of the Make.py options and syntax help can be accessed by using the "-h" switch.

E.g. typing "Make.py -h" gives

```
Syntax: Make.py switch args ...
  switches can be listed in any order
  help switch:
    -h prints help and syntax for all other specified switches
  switch for actions:
    -a lib-all, lib-dir, clean, file, exe or machine
    list one or more actions, in any order
    machine is a Makefile.machine suffix, must be last if used
  one-letter switches:
    -d (dir), -j (jmake), -m (makefile), -o (output),
    -p (packages), -r (redo), -s (settings), -v (verbose)
  switches for libs:
    -atc, -awpmd, -colvars, -cuda
    -gpu, -meam, -poems, -qmmm, -reax
  switches for build and makefile options:
    -intel, -kokkos, -cc, -mpi, -fft, -jpg, -png
```

Using the "-h" switch with other switches and actions gives additional info on all the other specified switches or actions. The "-h" can be anywhere in the command-line and the other switches do not need their arguments. E.g. type "Make.py -h -d -atc -intel" will print:

```
-d dir
  dir = LAMMPS home dir
  if -d not specified, working dir must be lammps/src

-atc make=suffix lammps=suffix2
  all args are optional and can be in any order
  make = use Makefile.suffix (def = g++)
  lammps = use Makefile.lammps.suffix2 (def = EXTRAMAKE in makefile)

-intel mode
  mode = cpu or phi (def = cpu)
    build Intel package for CPU or Xeon Phi
```

Note that Make.py never overwrites an existing Makefile.machine. Instead, it creates src/MAKE/MINE/Makefile.auto, which you can save or rename if desired. Likewise it creates an executable named src/lmp_auto, which you can rename using the -o switch if desired.

The most recently executed Make.py commmand is saved in src/Make.py.last. You can use the "-r" switch (for redo) to re-invoke the last command, or you can save a sequence of one or more Make.py commands to a file and invoke the file of commands using "-r". You can also label the commands in the file and invoke one or more of them by name.

A typical use of Make.py is to start with a valid Makefile.machine for your system, that works for a vanilla LAMMPS build, i.e. when optional packages are not installed. You can then use Make.py to add various settings (FFT, JPG, PNG) to the Makefile.machine as well as change its compiler and MPI options. You can also add additional packages to the build, as well as build the needed supporting libraries.

You can also use Make.py to create a new Makefile.machine from scratch, using the "-m none" switch, if you also specify what compiler and MPI options to use, via the "-cc" and "-mpi" switches.

2.5 Building LAMMPS as a library

LAMMPS can be built as either a static or shared library, which can then be called from another application or a scripting language. See this section for more info on coupling LAMMPS to other codes. See this section for more info on wrapping and running LAMMPS from Python.

Static library:

To build LAMMPS as a static library (*.a file on Linux), type

```
make foo mode=lib
```

where foo is the machine name. This kind of library is typically used to statically link a driver application to LAMMPS, so that you can insure all dependencies are satisfied at compile time. This will use the ARCHIVE and ARFLAGS settings in src/MAKE/Makefile.foo. The build will create the file liblammps_foo.a which another application can link to. It will also create a soft link liblammps.a, which will point to the most recently built static library.

Shared library:

To build LAMMPS as a shared library (*.so file on Linux), which can be dynamically loaded, e.g. from Python, type

```
make foo mode=shlib
```

where foo is the machine name. This kind of library is required when wrapping LAMMPS with Python; see Section_python for details. This will use the SHFLAGS and SHLIBFLAGS settings in src/MAKE/Makefile.foo and perform the build in the directory Obj_shared_foo. This is so that each file can be compiled with the -fPIC flag which is required for inclusion in a shared library. The build will create the file liblammps_foo.so which another application can link to dyamically. It will also create a soft link liblammps.so, which will point to the most recently built shared library. This is the file the Python wrapper loads by default.

Note that for a shared library to be usable by a calling program, all the auxiliary libraries it depends on must also exist as shared libraries. This will be the case for libraries included with LAMMPS, such as the dummy MPI library in src/STUBS or any package libraries in lib/packages, since they are always built as shared libraries using the -fPIC switch. However, if a library like MPI or FFTW does not exist as a shared library, the shared library build will generate an error. This means you will need to install a shared library version of the auxiliary library. The build instructions for the library should tell you how to do this.

Here is an example of such errors when the system FFTW or provided lib/colvars library have not been built as shared libraries:

```
/usr/bin/ld: /usr/local/lib/libfftw3.a(mapflags.o): relocation
R_X86_64_32 against `.rodata' can not be used when making a shared
object; recompile with -fPIC
/usr/local/lib/libfftw3.a: could not read symbols: Bad value

/usr/bin/ld: ../../lib/colvars/libcolvars.a(colvarmodule.o):
relocation R_X86_64_32 against `__pthread_key_create' can not be used
when making a shared object; recompile with -fPIC
../../lib/colvars/libcolvars.a: error adding symbols: Bad value
```

As an example, here is how to build and install the MPICH library, a popular open-source version of MPI, distributed by Argonne National Labs, as a shared library in the default /usr/local/lib location:

```
./configure --enable-shared
make
make install
```

You may need to use "sudo make install" in place of the last line if you do not have write privileges for /usr/local/lib. The end result should be the file /usr/local/lib/libmpich.so.

Additional requirement for using a shared library:

The operating system finds shared libraries to load at run-time using the environment variable LD_LIBRARY_PATH. So you may wish to copy the file src/liblammps.so or src/liblammps_g++.so (for example) to a place the system can find it by default, such as /usr/local/lib, or you may wish to add the LAMMPS src directory to LD_LIBRARY_PATH, so that the current version of the shared library is always available to programs that use it.

For the csh or tcsh shells, you would add something like this to your ~/.cshrc file:

```
setenv LD_LIBRARY_PATH ${LD_LIBRARY_PATH}:/home/sjplimp/lammps/src
```

Calling the LAMMPS library:

Either flavor of library (static or shared) allows one or more LAMMPS objects to be instantiated from the calling program.

When used from a C++ program, all of LAMMPS is wrapped in a LAMMPS_NS namespace; you can safely use any of its classes and methods from within the calling code, as needed.

When used from a C or Fortran program or a scripting language like Python, the library has a simple function-style interface, provided in src/library.cpp and src/library.h.

See the sample codes in examples/COUPLE/simple for examples of C++ and C and Fortran codes that invoke LAMMPS thru its library interface. There are other examples as well in the COUPLE directory which are discussed in Section_howto 10 of the manual. See Section_python of the manual for a description of the Python wrapper provided with LAMMPS that operates through the LAMMPS library interface.

The files src/library.cpp and library.h define the C-style API for using LAMMPS as a library. See Section_howto 19 of the manual for a description of the interface and how to extend it for your needs.

2.6 Running LAMMPS

By default, LAMMPS runs by reading commands from standard input. Thus if you run the LAMMPS executable by itself, e.g.

```
lmp_linux
```

it will simply wait, expecting commands from the keyboard. Typically you should put commands in an input script and use I/O redirection, e.g.

```
lmp_linux <in.file
```

For parallel environments this should also work. If it does not, use the '-in' command-line switch, e.g.

```
lmp_linux -in in.file
```

This section describes how input scripts are structured and what commands they contain.

You can test LAMMPS on any of the sample inputs provided in the examples or bench directory. Input scripts are named in.* and sample outputs are named log.*.name.P where name is a machine and P is the number of processors it was run on.

Here is how you might run a standard Lennard-Jones benchmark on a Linux box, using mpirun to launch a parallel job:

```
cd src
make linux
cp lmp_linux ../bench
cd ../bench
mpirun -np 4 lmp_linux -in in.lj
```

See this page for timings for this and the other benchmarks on various platforms. Note that some of the example scripts require LAMMPS to be built with one or more of its optional packages.

On a Windows box, you can skip making LAMMPS and simply download an executable, as described above, though the pre-packaged executables include only certain packages.

To run a LAMMPS executable on a Windows machine, first decide whether you want to download the non-MPI (serial) or the MPI (parallel) version of the executable. Download and save the version you have chosen.

For the non-MPI version, follow these steps:

- Get a command prompt by going to Start->Run... , then typing "cmd".
- Move to the directory where you have saved lmp_win_no-mpi.exe (e.g. by typing: cd "Documents").
- At the command prompt, type "lmp_win_no-mpi -in in.lj", replacing in.lj with the name of your LAMMPS input script.

For the MPI version, which allows you to run LAMMPS under Windows on multiple processors, follow these steps:

- Download and install MPICH2 for Windows.
- You'll need to use the mpiexec.exe and smpd.exe files from the MPICH2 package. Put them in same directory (or path) as the LAMMPS Windows executable.
- Get a command prompt by going to Start->Run... , then typing "cmd".

- Move to the directory where you have saved lmp_win_mpi.exe (e.g. by typing: cd "Documents").
- Then type something like this: "mpiexec -localonly 4 lmp_win_mpi -in in.lj", replacing in.lj with the name of your LAMMPS input script.
- Note that you may need to provide smpd with a passphrase (it doesn't matter what you type).
- In this mode, output may not immediately show up on the screen, so if your input script takes a long time to execute, you may need to be patient before the output shows up. :l Alternatively, you can still use this executable to run on a single processor by typing something like: "lmp_win_mpi -in in.lj".

The screen output from LAMMPS is described in a section below. As it runs, LAMMPS also writes a log.lammps file with the same information.

Note that this sequence of commands copies the LAMMPS executable (lmp_linux) to the directory with the input files. This may not be necessary, but some versions of MPI reset the working directory to where the executable is, rather than leave it as the directory where you launch mpirun from (if you launch lmp_linux on its own and not under mpirun). If that happens, LAMMPS will look for additional input files and write its output files to the executable directory, rather than your working directory, which is probably not what you want.

If LAMMPS encounters errors in the input script or while running a simulation it will print an ERROR message and stop or a WARNING message and continue. See Section_errors for a discussion of the various kinds of errors LAMMPS can or can't detect, a list of all ERROR and WARNING messages, and what to do about them.

LAMMPS can run a problem on any number of processors, including a single processor. In theory you should get identical answers on any number of processors and on any machine. In practice, numerical round-off can cause slight differences and eventual divergence of molecular dynamics phase space trajectories.

LAMMPS can run as large a problem as will fit in the physical memory of one or more processors. If you run out of memory, you must run on more processors or setup a smaller problem.

2.7 Command-line options

At run time, LAMMPS recognizes several optional command-line switches which may be used in any order. Either the full word or a one-or-two letter abbreviation can be used:

- -c or -cuda
- -e or -echo
- -h or -help
- -i or -in
- -k or -kokkos
- -l or -log
- -nc or -nocite
- -pk or -package
- -p or -partition
- -pl or -plog
- -ps or -pscreen
- -r or -restart
- -ro or -reorder
- -sc or -screen
- -sf or -suffix
- -v or -var

For example, lmp_ibm might be launched as follows:

```
mpirun -np 16 lmp_ibm -v f tmp.out -l my.log -sc none -in in.alloy
mpirun -np 16 lmp_ibm -var f tmp.out -log my.log -screen none -in in.alloy
```

Here are the details on the options:

```
-cuda on/off
```

Explicitly enable or disable CUDA support, as provided by the USER-CUDA package. Even if LAMMPS is built with this package, as described above in Section 2.3, this switch must be set to enable running with the CUDA-enabled styles the package provides. If the switch is not set (the default), LAMMPS will operate as if the USER-CUDA package were not installed; i.e. you can run standard LAMMPS or with the GPU package, for testing or benchmarking purposes.

```
-echo style
```

Set the style of command echoing. The style can be *none* or *screen* or *log* or *both*. Depending on the style, each command read from the input script will be echoed to the screen and/or logfile. This can be useful to figure out which line of your script is causing an input error. The default value is *log*. The echo style can also be set by using the echo command in the input script itself.

```
-help
```

Print a brief help summary and a list of options compiled into this executable for each LAMMPS style (atom_style, fix, compute, pair_style, bond_style, etc). This can tell you if the command you want to use was included via the appropriate package at compile time. LAMMPS will print the info and immediately exit if this switch is used.

```
-in file
```

Specify a file to use as an input script. This is an optional switch when running LAMMPS in one-partition mode. If it is not specified, LAMMPS reads its script from standard input, typically from a script via I/O redirection; e.g. lmp_linux < in.run. I/O redirection should also work in parallel, but if it does not (in the unlikely case that an MPI implementation does not support it), then use the -in flag. Note that this is a required switch when running LAMMPS in multi-partition mode, since multiple processors cannot all read from stdin.

```
-kokkos on/off keyword/value ...
```

Explicitly enable or disable KOKKOS support, as provided by the KOKKOS package. Even if LAMMPS is built with this package, as described above in Section 2.3, this switch must be set to enable running with the KOKKOS-enabled styles the package provides. If the switch is not set (the default), LAMMPS will operate as if the KOKKOS package were not installed; i.e. you can run standard LAMMPS or with the GPU or USER-CUDA or USER-OMP packages, for testing or benchmarking purposes.

Additional optional keyword/value pairs can be specified which determine how Kokkos will use the underlying hardware on your platform. These settings apply to each MPI task you launch via the "mpirun" or "mpiexec" command. You may choose to run one or more MPI tasks per physical node. Note that if you are running on a desktop machine, you typically have one physical node. On a cluster or supercomputer there may be dozens or 1000s of physical nodes.

Either the full word or an abbreviation can be used for the keywords. Note that the keywords do not use a leading minus sign. I.e. the keyword is "t", not "-t". Also note that each of the keywords has a default setting. Example of when to use these options and what settings to use on different platforms is given in Section 5.8.

- d or device

- g or gpus
- t or threads
- n or numa

```
device Nd
```

This option is only relevant if you built LAMMPS with CUDA=yes, you have more than one GPU per node, and if you are running with only one MPI task per node. The Nd setting is the ID of the GPU on the node to run on. By default Nd = 0. If you have multiple GPUs per node, they have consecutive IDs numbered as 0,1,2,etc. This setting allows you to launch multiple independent jobs on the node, each with a single MPI task per node, and assign each job to run on a different GPU.

```
gpus Ng Ns
```

This option is only relevant if you built LAMMPS with CUDA=yes, you have more than one GPU per node, and you are running with multiple MPI tasks per node (up to one per GPU). The Ng setting is how many GPUs you will use. The Ns setting is optional. If set, it is the ID of a GPU to skip when assigning MPI tasks to GPUs. This may be useful if your desktop system reserves one GPU to drive the screen and the rest are intended for computational work like running LAMMPS. By default Ng = 1 and Ns is not set.

Depending on which flavor of MPI you are running, LAMMPS will look for one of these 3 environment variables

```
SLURM_LOCALID (various MPI variants compiled with SLURM support)
MV2_COMM_WORLD_LOCAL_RANK (Mvapich)
OMPI_COMM_WORLD_LOCAL_RANK (OpenMPI)
```

which are initialized by the "srun", "mpirun" or "mpiexec" commands. The environment variable setting for each MPI rank is used to assign a unique GPU ID to the MPI task.

```
threads Nt
```

This option assigns Nt number of threads to each MPI task for performing work when Kokkos is executing in OpenMP or pthreads mode. The default is Nt = 1, which essentially runs in MPI-only mode. If there are Np MPI tasks per physical node, you generally want Np*Nt = the number of physical cores per node, to use your available hardware optimally. This also sets the number of threads used by the host when LAMMPS is compiled with CUDA=yes.

```
numa Nm
```

This option is only relevant when using pthreads with hwloc support. In this case Nm defines the number of NUMA regions (typicaly sockets) on a node which will be utilizied by a single MPI rank. By default Nm = 1. If this option is used the total number of worker-threads per MPI rank is threads*numa. Currently it is always almost better to assign at least one MPI rank per NUMA region, and leave numa set to its default value of 1. This is because letting a single process span multiple NUMA regions induces a significant amount of cross NUMA data traffic which is slow.

```
-log file
```

Specify a log file for LAMMPS to write status information to. In one-partition mode, if the switch is not used, LAMMPS writes to the file log.lammps. If this switch is used, LAMMPS writes to the specified file. In multi-partition mode, if the switch is not used, a log.lammps file is created with hi-level status information. Each partition also writes to a log.lammps.N file where N is the partition ID. If the switch is specified in multi-partition mode, the hi-level logfile is named "file" and each partition also logs information to a file.N. For both one-partition and multi-partition mode, if the specified file is "none", then no log files are created. Using a log

command in the input script will override this setting. Option -plog will override the name of the partition log files file.N.

```
-nocite
```

Disable writing the log.cite file which is normally written to list references for specific cite-able features used during a LAMMPS run. See the citation page for more details.

```
-package style args ....
```

Invoke the package command with style and args. The syntax is the same as if the command appeared at the top of the input script. For example "-package gpu 2" or "-pk gpu 2" is the same as package gpu 2 in the input script. The possible styles and args are documented on the package doc page. This switch can be used multiple times, e.g. to set options for the USER-INTEL and USER-OMP packages which can be used together.

Along with the "-suffix" command-line switch, this is a convenient mechanism for invoking accelerator packages and their options without having to edit an input script.

```
-partition 8x2 4 5 ...
```

Invoke LAMMPS in multi-partition mode. When LAMMPS is run on P processors and this switch is not used, LAMMPS runs in one partition, i.e. all P processors run a single simulation. If this switch is used, the P processors are split into separate partitions and each partition runs its own simulation. The arguments to the switch specify the number of processors in each partition. Arguments of the form MxN mean M partitions, each with N processors. Arguments of the form N mean a single partition with N processors. The sum of processors in all partitions must equal P. Thus the command "-partition 8x2 4 5" has 10 partitions and runs on a total of 25 processors.

Running with multiple partitions can e useful for running multi-replica simulations, where each replica runs on on one or a few processors. Note that with MPI installed on a machine (e.g. your desktop), you can run on more (virtual) processors than you have physical processors.

To run multiple independent simulatoins from one input script, using multiple partitions, see Section_howto 4 of the manual. World- and universe-style variables are useful in this context.

```
-plog file
```

Specify the base name for the partition log files, so partition N writes log information to file.N. If file is none, then no partition log files are created. This overrides the filename specified in the -log command-line option. This option is useful when working with large numbers of partitions, allowing the partition log files to be suppressed (-plog none) or placed in a sub-directory (-plog replica_files/log.lammps) If this option is not used the log file for partition N is log.lammps.N or whatever is specified by the -log command-line option.

```
-pscreen file
```

Specify the base name for the partition screen file, so partition N writes screen information to file.N. If file is none, then no partition screen files are created. This overrides the filename specified in the -screen command-line option. This option is useful when working with large numbers of partitions, allowing the partition screen files to be suppressed (-pscreen none) or placed in a sub-directory (-pscreen replica_files/screen). If this option is not used the screen file for partition N is screen.N or whatever is specified by the -screen command-line option.

```
-restart restartfile remap datafile keyword value ...
```

Convert the restart file into a data file and immediately exit. This is the same operation as if the following 2-line input script were run:

```
read_restart restartfile remap
write_data datafile keyword value ...
```

Note that the specified restartfile and datafile can have wild-card characters ("*",%") as described by the read_restart and write_data commands. But a filename such as file.* will need to be enclosed in quotes to avoid shell expansion of the "*" character.

Note that following restartfile, the optional flag *remap* can be used. This has the same effect as adding it to the read_restart command, as explained on its doc page. This is only useful if the reading of the restart file triggers an error that atoms have been lost. In that case, use of the remap flag should allow the data file to still be produced.

Also note that following datafile, the same optional keyword/value pairs can be listed as used by the write_data command.

```
-reorder nth N
-reorder custom filename
```

Reorder the processors in the MPI communicator used to instantiate LAMMPS, in one of several ways. The original MPI communicator ranks all P processors from 0 to P-1. The mapping of these ranks to physical processors is done by MPI before LAMMPS begins. It may be useful in some cases to alter the rank order. E.g. to insure that cores within each node are ranked in a desired order. Or when using the run_style verlet/split command with 2 partitions to insure that a specific Kspace processor (in the 2nd partition) is matched up with a specific set of processors in the 1st partition. See the Section_accelerate doc pages for more details.

If the keyword *nth* is used with a setting *N*, then it means every Nth processor will be moved to the end of the ranking. This is useful when using the run_style verlet/split command with 2 partitions via the -partition command-line switch. The first set of processors will be in the first partition, the 2nd set in the 2nd partition. The -reorder command-line switch can alter this so that the 1st N procs in the 1st partition and one proc in the 2nd partition will be ordered consecutively, e.g. as the cores on one physical node. This can boost performance. For example, if you use "-reorder nth 4" and "-partition 9 3" and you are running on 12 processors, the processors will be reordered from

```
0 1 2 3 4 5 6 7 8 9 10 11
```

to

```
0 1 2 4 5 6 8 9 10 3 7 11
```

so that the processors in each partition will be

```
0 1 2 4 5 6 8 9 10
3 7 11
```

See the "processors" command for how to insure processors from each partition could then be grouped optimally for quad-core nodes.

If the keyword is *custom*, then a file that specifies a permutation of the processor ranks is also specified. The format of the reorder file is as follows. Any number of initial blank or comment lines (starting with a "#" character) can be present. These should be followed by P lines of the form:

```
I J
```

where P is the number of processors LAMMPS was launched with. Note that if running in multi-partition mode (see the -partition switch above) P is the total number of processors in all partitions. The I and J values describe a permutation of the P processors. Every I and J should be values from 0 to P-1 inclusive. In the set of P I values, every proc ID should appear exactly once. Ditto for the set of P J values. A single I,J pairing means that the physical processor with rank I in the original MPI communicator will have rank J in the reordered communicator.

Note that rank ordering can also be specified by many MPI implementations, either by environment variables that specify how to order physical processors, or by config files that specify what physical processors to assign to each MPI rank. The -reorder switch simply gives you a portable way to do this without relying on MPI itself. See the processors out command for how to output info on the final assignment of physical processors to the LAMMPS simulation domain.

```
-screen file
```

Specify a file for LAMMPS to write its screen information to. In one-partition mode, if the switch is not used, LAMMPS writes to the screen. If this switch is used, LAMMPS writes to the specified file instead and you will see no screen output. In multi-partition mode, if the switch is not used, hi-level status information is written to the screen. Each partition also writes to a screen.N file where N is the partition ID. If the switch is specified in multi-partition mode, the hi-level screen dump is named "file" and each partition also writes screen information to a file.N. For both one-partition and multi-partition mode, if the specified file is "none", then no screen output is performed. Option -pscreen will override the name of the partition screen files file.N.

```
-suffix style args
```

Use variants of various styles if they exist. The specified style can be *cuda*, *gpu*, *intel*, *kk*, *omp*, *opt*, or *hybrid*. These refer to optional packages that LAMMPS can be built with, as described above in Section 2.3. The "cuda" style corresponds to the USER-CUDA package, the "gpu" style to the GPU package, the "intel" style to the USER-INTEL package, the "kk" style to the KOKKOS package, the "opt" style to the OPT package, and the "omp" style to the USER-OMP package. The hybrid style is the only style that accepts arguments. It allows for two packages to be specified. The first package specified is the default and will be used if it is available. If no style is available for the first package, the style for the second package will be used if available. For example, "-suffix hybrid intel omp" will use styles from the USER-INTEL package if they are installed and available, but styles for the USER-OMP package otherwise.

Along with the "-package" command-line switch, this is a convenient mechanism for invoking accelerator packages and their options without having to edit an input script.

As an example, all of the packages provide a pair_style lj/cut variant, with style names lj/cut/cuda, lj/cut/gpu, lj/cut/intel, lj/cut/kk, lj/cut/omp, and lj/cut/opt. A variant style can be specified explicitly in your input script, e.g. pair_style lj/cut/gpu. If the -suffix switch is used the specified suffix (cuda,gpu,intel,kk,omp,opt) is automatically appended whenever your input script command creates a new atom, pair, fix, compute, or run style. If the variant version does not exist, the standard version is created.

For the GPU package, using this command-line switch also invokes the default GPU settings, as if the command "package gpu 1" were used at the top of your input script. These settings can be changed by using the "-package gpu" command-line switch or the package gpu command in your script.

For the USER-INTEL package, using this command-line switch also invokes the default USER-INTEL settings, as if the command "package intel 1" were used at the top of your input script. These settings can be changed by using the "-package intel" command-line switch or the package intel command in your script. If the USER-OMP package is also installed, the hybrid style with "intel omp" arguments can be used to make the omp suffix a second choice, if a requested style is not available in the USER-INTEL package. It will also invoke the default USER-OMP settings, as if the command "package omp 0" were used at the top of your input script. These settings

can be changed by using the "-package omp" command-line switch or the package omp command in your script.

For the KOKKOS package, using this command-line switch also invokes the default KOKKOS settings, as if the command "package kokkos" were used at the top of your input script. These settings can be changed by using the "-package kokkos" command-line switch or the package kokkos command in your script.

For the OMP package, using this command-line switch also invokes the default OMP settings, as if the command "package omp 0" were used at the top of your input script. These settings can be changed by using the "-package omp" command-line switch or the package omp command in your script.

The suffix command can also be used within an input script to set a suffix, or to turn off or back on any suffix setting made via the command line.

```
-var name value1 value2 ...
```

Specify a variable that will be defined for substitution purposes when the input script is read. This switch can be used multiple times to define multiple variables. "Name" is the variable name which can be a single character (referenced as $x in the input script) or a full string (referenced as ${abc}). An index-style variable will be created and populated with the subsequent values, e.g. a set of filenames. Using this command-line option is equivalent to putting the line "variable name index value1 value2 ..." at the beginning of the input script. Defining an index variable as a command-line argument overrides any setting for the same index variable in the input script, since index variables cannot be re-defined. See the variable command for more info on defining index and other kinds of variables and this section for more info on using variables in input scripts.

NOTE: Currently, the command-line parser looks for arguments that start with "-" to indicate new switches. Thus you cannot specify multiple variable values if any of they start with a "-", e.g. a negative numeric value. It is OK if the first value1 starts with a "-", since it is automatically skipped.

2.8 LAMMPS screen output

As LAMMPS reads an input script, it prints information to both the screen and a log file about significant actions it takes to setup a simulation. When the simulation is ready to begin, LAMMPS performs various initializations and prints the amount of memory (in MBytes per processor) that the simulation requires. It also prints details of the initial thermodynamic state of the system. During the run itself, thermodynamic information is printed periodically, every few timesteps. When the run concludes, LAMMPS prints the final thermodynamic state and a total run time for the simulation. It then appends statistics about the CPU time and storage requirements for the simulation. An example set of statistics is shown here:

Loop time of 2.81192 on 4 procs for 300 steps with 2004 atoms

```
Performance: 18.436 ns/day  1.302 hours/ns  106.689 timesteps/s
97.0% CPU use with 4 MPI tasks x no OpenMP threads

MPI task timings breakdown:
Section |  min time  |  avg time  |  max time  |%varavg| %total
---------------------------------------------------------------
Pair    | 1.9808     | 2.0134     | 2.0318     |   1.4 | 71.60
Bond    | 0.0021894  | 0.0060319  | 0.010058   |   4.7 |  0.21
Kspace  | 0.3207     | 0.3366     | 0.36616    |   3.1 | 11.97
Neigh   | 0.28411    | 0.28464    | 0.28516    |   0.1 | 10.12
Comm    | 0.075732   | 0.077018   | 0.07883    |   0.4 |  2.74
Output  | 0.00030518 | 0.00042665 | 0.00078821 |   1.0 |  0.02
Modify  | 0.086606   | 0.086631   | 0.086668   |   0.0 |  3.08
Other   |            | 0.007178   |            |       |  0.26
```

```
Nlocal:    501 ave 508 max 490 min
Histogram: 1 0 0 0 0 0 1 1 0 1
Nghost:    6586.25 ave 6628 max 6548 min
Histogram: 1 0 1 0 0 0 1 0 0 1
Neighs:    177007 ave 180562 max 170212 min
Histogram: 1 0 0 0 0 0 0 1 1 1

Total # of neighbors = 708028
Ave neighs/atom = 353.307
Ave special neighs/atom = 2.34032
Neighbor list builds = 26
Dangerous builds = 0
```

The first section provides a global loop timing summary. The loop time is the total wall time for the section. The *Performance* line is provided for convenience to help predicting the number of loop continuations required and for comparing performance with other similar MD codes. The CPU use line provides the CPU utilzation per MPI task; it should be close to 100% times the number of OpenMP threads (or 1). Lower numbers correspond to delays due to file I/O or insufficient thread utilization.

The MPI task section gives the breakdown of the CPU run time (in seconds) into major categories:

- *Pair* stands for all non-bonded force computation
- *Bond* stands for bonded interactions: bonds, angles, dihedrals, impropers
- *Kspace* stands for reciprocal space interactions: Ewald, PPPM, MSM
- *Neigh* stands for neighbor list construction
- *Comm* stands for communicating atoms and their properties
- *Output* stands for writing dumps and thermo output
- *Modify* stands for fixes and computes called by them
- *Other* is the remaining time

For each category, there is a breakdown of the least, average and most amount of wall time a processor spent on this section. Also you have the variation from the average time. Together these numbers allow to gauge the amount of load imbalance in this segment of the calculation. Ideally the difference between minimum, maximum and average is small and thus the variation from the average close to zero. The final column shows the percentage of the total loop time is spent in this section.

When using the timer full setting, an additional column is present that also prints the CPU utilization in percent. In addition, when using *timer full* and the package omp command are active, a similar timing summary of time spent in threaded regions to monitor thread utilization and load balance is provided. A new entry is the *Reduce* section, which lists the time spend in reducing the per-thread data elements to the storage for non-threaded computation. These thread timings are taking from the first MPI rank only and and thus, as the breakdown for MPI tasks can change from MPI rank to MPI rank, this breakdown can be very different for individual ranks. Here is an example output for this section:

Thread timings breakdown (MPI rank 0): Total threaded time 0.6846 / 90.6% Section | min time | avg time | max time |%varavg| %total --- Pair | 0.5127 | 0.5147 | 0.5167 | 0.3 | 75.18 Bond | 0.0043139 | 0.0046779 | 0.0050418 | 0.5 | 0.68 Kspace | 0.070572 | 0.074541 | 0.07851 | 1.5 | 10.89 Neigh | 0.084778 | 0.086969 | 0.089161 | 0.7 | 12.70 Reduce | 0.0036485 | 0.003737 | 0.0038254 | 0.1 | 0.55

The third section lists the number of owned atoms (Nlocal), ghost atoms (Nghost), and pair-wise neighbors stored per processor. The max and min values give the spread of these values across processors with a 10-bin histogram showing the distribution. The total number of histogram counts is equal to the number of processors.

The last section gives aggregate statistics for pair-wise neighbors and special neighbors that LAMMPS keeps

track of (see the special_bonds command). The number of times neighbor lists were rebuilt during the run is given as well as the number of potentially "dangerous" rebuilds. If atom movement triggered neighbor list rebuilding (see the neigh_modify command), then dangerous reneighborings are those that were triggered on the first timestep atom movement was checked for. If this count is non-zero you may wish to reduce the delay factor to insure no force interactions are missed by atoms moving beyond the neighbor skin distance before a rebuild takes place.

If an energy minimization was performed via the minimize command, additional information is printed, e.g.

```
Minimization stats:
  Stopping criterion = linesearch alpha is zero
  Energy initial, next-to-last, final =
         -6372.3765206     -8328.46998942     -8328.46998942
  Force two-norm initial, final = 1059.36 5.36874
  Force max component initial, final = 58.6026 1.46872
  Final line search alpha, max atom move = 2.7842e-10 4.0892e-10
  Iterations, force evaluations = 701 1516
```

The first line prints the criterion that determined the minimization to be completed. The third line lists the initial and final energy, as well as the energy on the next-to-last iteration. The next 2 lines give a measure of the gradient of the energy (force on all atoms). The 2-norm is the "length" of this force vector; the inf-norm is the largest component. Then some information about the line search and statistics on how many iterations and force-evaluations the minimizer required. Multiple force evaluations are typically done at each iteration to perform a 1d line minimization in the search direction.

If a kspace_style long-range Coulombics solve was performed during the run (PPPM, Ewald), then additional information is printed, e.g.

```
FFT time (% of Kspce) = 0.200313 (8.34477)
FFT Gflps 3d 1d-only = 2.31074 9.19989
```

The first line gives the time spent doing 3d FFTs (4 per timestep) and the fraction it represents of the total KSpace time (listed above). Each 3d FFT requires computation (3 sets of 1d FFTs) and communication (transposes). The total flops performed is 5Nlog_2(N), where N is the number of points in the 3d grid. The FFTs are timed with and without the communication and a Gflop rate is computed. The 3d rate is with communication; the 1d rate is without (just the 1d FFTs). Thus you can estimate what fraction of your FFT time was spent in communication, roughly 75% in the example above.

2.9 Tips for users of previous LAMMPS versions

The current C++ began with a complete rewrite of LAMMPS 2001, which was written in F90. Features of earlier versions of LAMMPS are listed in Section_history. The F90 and F77 versions (2001 and 99) are also freely distributed as open-source codes; check the LAMMPS WWW Site for distribution information if you prefer those versions. The 99 and 2001 versions are no longer under active development; they do not have all the features of C++ LAMMPS.

If you are a previous user of LAMMPS 2001, these are the most significant changes you will notice in C++ LAMMPS:

(1) The names and arguments of many input script commands have changed. All commands are now a single word (e.g. read_data instead of read data).

(2) All the functionality of LAMMPS 2001 is included in C++ LAMMPS, but you may need to specify the relevant commands in different ways.

(3) The format of the data file can be streamlined for some problems. See the read_data command for details. The data file section "Nonbond Coeff" has been renamed to "Pair Coeff" in C++ LAMMPS.

(4) Binary restart files written by LAMMPS 2001 cannot be read by C++ LAMMPS with a read_restart command. This is because they were output by F90 which writes in a different binary format than C or C++ writes or reads. Use the *restart2data* tool provided with LAMMPS 2001 to convert the 2001 restart file to a text data file. Then edit the data file as necessary before using the C++ LAMMPS read_data command to read it in.

(5) There are numerous small numerical changes in C++ LAMMPS that mean you will not get identical answers when comparing to a 2001 run. However, your initial thermodynamic energy and MD trajectory should be close if you have setup the problem for both codes the same.

3. Commands

This section describes how a LAMMPS input script is formatted and the input script commands used to define a LAMMPS simulation.

3.1 LAMMPS input script

LAMMPS executes by reading commands from a input script (text file), one line at a time. When the input script ends, LAMMPS exits. Each command causes LAMMPS to take some action. It may set an internal variable, read in a file, or run a simulation. Most commands have default settings, which means you only need to use the command if you wish to change the default.

In many cases, the ordering of commands in an input script is not important. However the following rules apply:

(1) LAMMPS does not read your entire input script and then perform a simulation with all the settings. Rather, the input script is read one line at a time and each command takes effect when it is read. Thus this sequence of commands:

```
timestep 0.5
run      100
run      100
```

does something different than this sequence:

```
run      100
timestep 0.5
run      100
```

In the first case, the specified timestep (0.5 fmsec) is used for two simulations of 100 timesteps each. In the 2nd case, the default timestep (1.0 fmsec) is used for the 1st 100 step simulation and a 0.5 fmsec timestep is used for the 2nd one.

(2) Some commands are only valid when they follow other commands. For example you cannot set the temperature of a group of atoms until atoms have been defined and a group command is used to define which atoms belong to the group.

(3) Sometimes command B will use values that can be set by command A. This means command A must precede command B in the input script if it is to have the desired effect. For example, the read_data command initializes the system by setting up the simulation box and assigning atoms to processors. If default values are not desired, the processors and boundary commands need to be used before read_data to tell LAMMPS how to map processors to the simulation box.

Many input script errors are detected by LAMMPS and an ERROR or WARNING message is printed. This section gives more information on what errors mean. The documentation for each command lists restrictions on how the command can be used.

3.2 Parsing rules

Each non-blank line in the input script is treated as a command. LAMMPS commands are case sensitive. Command names are lower-case, as are specified command arguments. Upper case letters may be used in file names or user-chosen ID strings.

Here is how each line in the input script is parsed by LAMMPS:

(1) If the last printable character on the line is a "&" character, the command is assumed to continue on the next line. The next line is concatenated to the previous line by removing the "&" character and line break. This allows long commands to be continued across two or more lines. See the discussion of triple quotes in (6) for how to continue a command across multiple line without using "&" characters.

(2) All characters from the first "#" character onward are treated as comment and discarded. See an exception in (6). Note that a comment after a trailing "&" character will prevent the command from continuing on the next line. Also note that for multi-line commands a single leading "#" will comment out the entire command.

(3) The line is searched repeatedly for $ characters, which indicate variables that are replaced with a text string. See an exception in (6).

If the $ is followed by curly brackets, then the variable name is the text inside the curly brackets. If no curly brackets follow the $, then the variable name is the single character immediately following the $. Thus ${myTemp} and $x refer to variable names "myTemp" and "x".

How the variable is converted to a text string depends on what style of variable it is; see the variable doc page for details. It can be a variable that stores multiple text strings, and return one of them. The returned text string can be multiple "words" (space separated) which will then be interpreted as multiple arguments in the input command. The variable can also store a numeric formula which will be evaluated and its numeric result returned as a string.

As a special case, if the $ is followed by parenthesis, then the text inside the parenthesis is treated as an "immediate" variable and evaluated as an equal-style variable. This is a way to use numeric formulas in an input script without having to assign them to variable names. For example, these 3 input script lines:

```
variable X equal (xlo+xhi)/2+sqrt(v_area)
region 1 block $X 2 INF INF EDGE EDGE
variable X delete
```

can be replaced by

```
region 1 block $((xlo+xhi)/2+sqrt(v_area)) 2 INF INF EDGE EDGE
```

so that you do not have to define (or discard) a temporary variable X.

Note that neither the curly-bracket or immediate form of variables can contain nested $ characters for other variables to substitute for. Thus you cannot do this:

```
variable        a equal 2
variable        b2 equal 4
print           "B2 = ${b$a}"
```

Nor can you specify this $($x-1.0) for an immediate variable, but you could use $(v_x-1.0), since the latter is valid syntax for an equal-style variable.

See the variable command for more details of how strings are assigned to variables and evaluated, and how they can be used in input script commands.

(4) The line is broken into "words" separated by whitespace (tabs, spaces). Note that words can thus contain letters, digits, underscores, or punctuation characters.

(5) The first word is the command name. All successive words in the line are arguments.

(6) If you want text with spaces to be treated as a single argument, it can be enclosed in either single or double or triple quotes. A long single argument enclosed in single or double quotes can span multiple lines if the "&" character is used, as described above. When the lines are concatenated together (and the "&" characters and line breaks removed), the text will become a single line. If you want multiple lines of an argument to retain their line breaks, the text can be enclosed in triple quotes, in which case "&" characters are not needed. For example:

```
print "Volume = $v"
print 'Volume = $v'
if "${steps} > 1000" then quit
variable a string "red green blue &
                   purple orange cyan"
print """
System volume = $v
System temperature = $t
"""
```

In each case, the single, double, or triple quotes are removed when the single argument they enclose is stored internally.

See the dump modify format, print, if, and python commands for examples.

A "#" or "$" character that is between quotes will not be treated as a comment indicator in (2) or substituted for as a variable in (3).

NOTE: If the argument is itself a command that requires a quoted argument (e.g. using a print command as part of an if or run every command), then single, double, or triple quotes can be nested in the usual manner. See the doc pages for those commands for examples. Only one of level of nesting is allowed, but that should be sufficient for most use cases.

3.3 Input script structure

This section describes the structure of a typical LAMMPS input script. The "examples" directory in the LAMMPS distribution contains many sample input scripts; the corresponding problems are discussed in Section_example, and animated on the LAMMPS WWW Site.

A LAMMPS input script typically has 4 parts:

1. Initialization
2. Atom definition
3. Settings
4. Run a simulation

The last 2 parts can be repeated as many times as desired. I.e. run a simulation, change some settings, run some more, etc. Each of the 4 parts is now described in more detail. Remember that almost all the commands need only be used if a non-default value is desired.

(1) Initialization

Set parameters that need to be defined before atoms are created or read-in from a file.

The relevant commands are units, dimension, newton, processors, boundary, atom_style, atom_modify.

If force-field parameters appear in the files that will be read, these commands tell LAMMPS what kinds of force fields are being used: pair_style, bond_style, angle_style, dihedral_style, improper_style.

(2) Atom definition

There are 3 ways to define atoms in LAMMPS. Read them in from a data or restart file via the read_data or read_restart commands. These files can contain molecular topology information. Or create atoms on a lattice (with no molecular topology), using these commands: lattice, region, create_box, create_atoms. The entire set of atoms can be duplicated to make a larger simulation using the replicate command.

(3) Settings

Once atoms and molecular topology are defined, a variety of settings can be specified: force field coefficients, simulation parameters, output options, etc.

Force field coefficients are set by these commands (they can also be set in the read-in files): pair_coeff, bond_coeff, angle_coeff, dihedral_coeff, improper_coeff, kspace_style, dielectric, special_bonds.

Various simulation parameters are set by these commands: neighbor, neigh_modify, group, timestep, reset_timestep, run_style, min_style, min_modify.

Fixes impose a variety of boundary conditions, time integration, and diagnostic options. The fix command comes in many flavors.

Various computations can be specified for execution during a simulation using the compute, compute_modify, and variable commands.

Output options are set by the thermo, dump, and restart commands.

(4) Run a simulation

A molecular dynamics simulation is run using the run command. Energy minimization (molecular statics) is performed using the minimize command. A parallel tempering (replica-exchange) simulation can be run using the temper command.

3.4 Commands listed by category

This section lists all LAMMPS commands, grouped by category. The next section lists the same commands alphabetically. Note that some style options for some commands are part of specific LAMMPS packages, which means they cannot be used unless the package was included when LAMMPS was built. Not all packages are included in a default LAMMPS build. These dependencies are listed as Restrictions in the command's

documentation.

Initialization:

atom_modify, atom_style, boundary, dimension, newton, processors, units

Atom definition:

create_atoms, create_box, lattice, read_data, read_dump, read_restart, region, replicate

Force fields:

angle_coeff, angle_style, bond_coeff, bond_style, dielectric, dihedral_coeff, dihedral_style, improper_coeff, improper_style, kspace_modify, kspace_style, pair_coeff, pair_modify, pair_style, pair_write, special_bonds

Settings:

comm_style, group, mass, min_modify, min_style, neigh_modify, neighbor, reset_timestep, run_style, set, timestep, velocity

Fixes:

fix, fix_modify, unfix

Computes:

compute, compute_modify, uncompute

Output:

dump, dump image, dump_modify, dump movie, restart, thermo, thermo_modify, thermo_style, undump, write_data, write_dump, write_restart

Actions:

delete_atoms, delete_bonds, displace_atoms, change_box, minimize, neb prd, rerun, run, temper

Miscellaneous:

clear, echo, if, include, jump, label, log, next, print, shell, variable

---

3.5 Individual commands

This section lists all LAMMPS commands alphabetically, with a separate listing below of styles within certain commands. The previous section lists the same commands, grouped by category. Note that some style options for some commands are part of specific LAMMPS packages, which means they cannot be used unless the package was included when LAMMPS was built. Not all packages are included in a default LAMMPS build. These dependencies are listed as Restrictions in the command's documentation.

angle_coeff	angle_style	atom_modify	atom_style	balance	bond_coeff
bond_style	boundary	box	change_box	clear	comm_modify
comm_style	compute	compute_modify	create_atoms	create_bonds	create_box

delete_atoms	delete_bonds	dielectric	dihedral_coeff	dihedral_style	dimension
displace_atoms	dump	dump image	dump_modify	dump movie	echo
fix	fix_modify	group	if	info	improper_coeff
improper_style	include	jump	kspace_modify	kspace_style	label
lattice	log	mass	minimize	min_modify	min_style
molecule	neb	neigh_modify	neighbor	newton	next
package	pair_coeff	pair_modify	pair_style	pair_write	partition
prd	print	processors	python	quit	read_data
read_dump	read_restart	region	replicate	rerun	reset_timestep
restart	run	run_style	set	shell	special_bonds
suffix	tad	temper	thermo	thermo_modify	thermo_style
timer	timestep	uncompute	undump	unfix	units
variable	velocity	write_data	write_dump	write_restart	

These are additional commands in USER packages, which can be used if LAMMPS is built with the appropriate package.

group2ndx

Fix styles

See the fix command for one-line descriptions of each style or click on the style itself for a full description. Some of the styles have accelerated versions, which can be used if LAMMPS is built with the appropriate accelerated package. This is indicated by additional letters in parenthesis: c = USER-CUDA, g = GPU, i = USER-INTEL, k = KOKKOS, o = USER-OMP, t = OPT.

adapt	addforce (c)	append/atoms	atom/swap	aveforce (c)	ave/atom	ave/chunk	ave/correla
ave/histo	ave/histo/weight	ave/spatial	ave/time	balance	bond/break	bond/create	bond/swa
box/relax	deform (k)	deposit	drag	dt/reset	efield	enforce2d (c)	evaporate
external	freeze (c)	gcmc	gld	gravity (co)	heat	indent	langevin (
lineforce	momentum	move	msst	neb	nph (ko)	nphug (o)	nph/asphe (o)
nph/body	nph/sphere (o)	npt (ckio)	npt/asphere (o)	npt/body	npt/sphere (o)	nve (ckio)	nve/asphere
nve/asphere/noforce	nve/body	nve/limit	nve/line	nve/noforce	nve/sphere (o)	nve/tri	nvt (ciko
nvt/asphere (o)	nvt/body	nvt/sllod (io)	nvt/sphere (o)	oneway	orient/fcc	planeforce	poems
pour	press/berendsen	print	property/atom	qeq/comb (o)	qeq/dynamic	qeq/fire	qeq/point
qeq/shielded	qeq/slater	rattle	reax/bonds	recenter	restrain	rigid (o)	rigid/nph (
rigid/npt (o)	rigid/nve (o)	rigid/nvt (o)	rigid/small (o)	rigid/small/nph	rigid/small/npt	rigid/small/nve	rigid/small/
setforce (ck)	shake (c)	spring	spring/rg	spring/self	srd	store/force	store/stat
temp/berendsen (c)	temp/csld	temp/csvr	temp/rescale (c)	tfmc	thermal/conductivity	tmd	ttm
tune/kspace	vector	viscosity	viscous (c)	wall/colloid	wall/gran	wall/harmonic	wall/lj104
wall/lj126	wall/lj93	wall/piston	wall/reflect (k)	wall/region	wall/srd		

These are additional fix styles in USER packages, which can be used if LAMMPS is built with the appropriate package.

adapt/fep	addtorque	atc	ave/correlate/long	ave/spatial/sphere	colv
drude	drude/transform/direct	drude/transform/reverse	eos/cv	eos/table	gle
imd	ipi	langevin/drude	langevin/eff	lb/fluid	lb/mom
lb/pc	lb/rigid/pc/sphere	lb/viscous	meso	meso/stationary	nph/
npt/eff	nve/eff	nvt/eff	nvt/sllod/eff	phonon	pim
qbmsst	qeq/reax	qmmm	qtb	reax/c/bonds	reax/c/s
saed/vtk	shardlow	smd	smd/adjust/dt	smd/integrate/tlsph	smd/integr
smd/move/triangulated/surface	smd/setvel	smd/tlsph/reference/configuration	smd/wall/surface	temp/rescale/eff	ti/r
ti/spring	ttm/mod				

Compute styles

See the compute command for one-line descriptions of each style or click on the style itself for a full description. Some of the styles have accelerated versions, which can be used if LAMMPS is built with the appropriate accelerated package. This is indicated by additional letters in parenthesis: c = USER-CUDA, g = GPU, i = USER-INTEL, k = KOKKOS, o = USER-OMP, t = OPT.

angle/local	angmom/chunk	body/local	bond/local	centro/atom	chunk/atom
cluster/atom	cna/atom	com	com/chunk	contact/atom	coord/atom
damage/atom	dihedral/local	dilatation/atom	displace/atom	erotate/asphere	erotate/rigid
erotate/sphere	erotate/sphere/atom	event/displace	group/group	gyration	gyration/chunk
heat/flux	hexorder/atom	improper/local	inertia/chunk	ke	ke/atom
ke/rigid	msd	msd/chunk	msd/nongauss	omega/chunk	orientorder/atom
pair	pair/local	pe (c)	pe/atom	plasticity/atom	pressure (c)
property/atom	property/local	property/chunk	rdf	reduce	reduce/region
slice	sna/atom	snad/atom	snav/atom	stress/atom	temp (ck)
temp/asphere	temp/body	temp/chunk	temp/com	temp/deform	temp/partial (c)
temp/profile	temp/ramp	temp/region	temp/sphere	ti	torque/chunk
vacf	vcm/chunk	voronoi/atom			

These are additional compute styles in USER packages, which can be used if LAMMPS is built with the appropriate package.

ackland/atom	basal/atom	dpd	dpd/atom	fep	force/tally
heat/flux/tally	ke/eff	ke/atom/eff	meso/e/atom	meso/rho/atom	meso/t/atom
pe/tally	saed	smd/contact/radius	smd/damage	smd/hourglass/error	smd/internal/energy
smd/plastic/strain	smd/plastic/strain/rate	smd/rho	smd/tlsph/defgrad	smd/tlsph/dt	smd/tlsph/num/neighs
smd/tlsph/shape	smd/tlsph/strain	smd/tlsph/strain/rate	smd/tlsph/stress	smd/triangle/mesh/vertices	smd/ulsph/num/neighs
smd/ulsph/strain	smd/ulsph/strain/rate	smd/ulsph/stress	smd/vol	stress/tally	temp/drude
temp/eff	temp/deform/eff	temp/region/eff	temp/rotate	xrd	

Pair_style potentials

See the pair_style command for an overview of pair potentials. Click on the style itself for a full description. Many of the styles have accelerated versions, which can be used if LAMMPS is built with the appropriate accelerated package. This is indicated by additional letters in parenthesis: c = USER-CUDA, g = GPU, i = USER-INTEL, k = KOKKOS, o = USER-OMP, t = OPT.

none	hybrid	hybrid/overlay	adp (o)
airebo (o)	beck (go)	body	bop
born (go)	born/coul/long (cgo)	born/coul/long/cs	born/coul/msm (o)
born/coul/wolf (go)	brownian (o)	brownian/poly (o)	buck (cgkio)
buck/coul/cut (cgkio)	buck/coul/long (cgkio)	buck/coul/long/cs	buck/coul/msm (o)
buck/long/coul/long (o)	colloid (go)	comb (o)	comb3
coul/cut (gko)	coul/debye (gko)	coul/dsf (gko)	coul/long (gko)
coul/long/cs	coul/msm	coul/streitz	coul/wolf (ko)
dpd (o)	dpd/tstat (o)	dsmc	eam (cgkot)
eam/alloy (cgkot)	eam/fs (cgkot)	eim (o)	gauss (go)
gayberne (gio)	gran/hertz/history (o)	gran/hooke (co)	gran/hooke/history (o)
hbond/dreiding/lj (o)	hbond/dreiding/morse (o)	kim	lcbop
line/lj	lj/charmm/coul/charmm (cko)	lj/charmm/coul/charmm/implicit (cko)	lj/charmm/coul/long (cgiko)
lj/charmm/coul/msm	lj/class2 (cgko)	lj/class2/coul/cut (cko)	lj/class2/coul/long (cgko)
lj/cubic (go)	lj/cut (cgikot)	lj/cut/coul/cut (cgko)	lj/cut/coul/debye (cgko)
lj/cut/coul/dsf (gko)	lj/cut/coul/long (cgikot)	lj/cut/coul/long/cs	lj/cut/coul/msm (go)
lj/cut/dipole/cut (go)	lj/cut/dipole/long	lj/cut/tip4p/cut (o)	lj/cut/tip4p/long (ot)
lj/expand (cgko)	lj/gromacs (cgko)	lj/gromacs/coul/gromacs (cko)	lj/long/coul/long (o)
lj/long/dipole/long	lj/long/tip4p/long	lj/smooth (co)	lj/smooth/linear (o)
lj96/cut (cgo)	lubricate (o)	lubricate/poly (o)	lubricateU
lubricateU/poly	meam (o)	mie/cut (o)	morse (cgot)
nb3b/harmonic (o)	nm/cut (o)	nm/cut/coul/cut (o)	nm/cut/coul/long (o)
peri/eps	peri/lps (o)	peri/pmb (o)	peri/ves
polymorphic	reax	rebo (o)	resquared (go)
snap	soft (go)	sw (cgkio)	table (gko)
tersoff (cgkio)	tersoff/mod (ko)	tersoff/zbl (ko)	tip4p/cut (o)
tip4p/long (o)	tri/lj	vashishta (o)	yukawa (go)
yukawa/colloid (go)	zbl (go)		

These are additional pair styles in USER packages, which can be used if LAMMPS is built with the appropriate package.

awpmd/cut	buck/mdf	coul/cut/soft (o)	coul/diel (o)
coul/long/soft (o)	dpd/conservative	dpd/fdt	dpd/fdt/energy
eam/cd (o)	edip (o)	eff/cut	gauss/cut
lennard/mdf	list	lj/charmm/coul/long/soft (o)	lj/cut/coul/cut/soft (o)
lj/cut/coul/long/soft (o)	lj/cut/dipole/sf (go)	lj/cut/soft (o)	lj/cut/tip4p/long/soft (o)
lj/mdf	lj/sdk (gko)	lj/sdk/coul/long (go)	lj/sdk/coul/msm (o)
lj/sf (o)	meam/spline	meam/sw/spline	mgpt
quip	reax/c	smd/hertz	smd/tlsph
smd/triangulated/surface	smd/ulsph	smtbq	sph/heatconduction
sph/idealgas	sph/lj	sph/rhosum	sph/taitwater

sph/taitwater/morris	srp	tersoff/table (o)	thole
tip4p/long/soft (o)			

Bond_style potentials

See the bond_style command for an overview of bond potentials. Click on the style itself for a full description. Some of the styles have accelerated versions, which can be used if LAMMPS is built with the appropriate accelerated package. This is indicated by additional letters in parenthesis: c = USER-CUDA, g = GPU, i = USER-INTEL, k = KOKKOS, o = USER-OMP, t = OPT.

none	hybrid	class2 (o)	fene (ko)
fene/expand (o)	harmonic (ko)	morse (o)	nonlinear (o)
quartic (o)	table (o)		

These are additional bond styles in USER packages, which can be used if LAMMPS is built with the appropriate package.

harmonic/shift (o)	harmonic/shift/cut (o)

Angle_style potentials

See the angle_style command for an overview of angle potentials. Click on the style itself for a full description. Some of the styles have accelerated versions, which can be used if LAMMPS is built with the appropriate accelerated package. This is indicated by additional letters in parenthesis: c = USER-CUDA, g = GPU, i = USER-INTEL, k = KOKKOS, o = USER-OMP, t = OPT.

none	hybrid	charmm (ko)	class2 (o)
cosine (o)	cosine/delta (o)	cosine/periodic (o)	cosine/squared (o)
harmonic (iko)	table (o)		

These are additional angle styles in USER packages, which can be used if LAMMPS is built with the appropriate package.

cosine/shift (o)	cosine/shift/exp (o)	dipole (o)	fourier (o)
fourier/simple (o)	quartic (o)	sdk	

Dihedral_style potentials

See the dihedral_style command for an overview of dihedral potentials. Click on the style itself for a full description. Some of the styles have accelerated versions, which can be used if LAMMPS is built with the appropriate accelerated package. This is indicated by additional letters in parenthesis: c = USER-CUDA, g = GPU, i = USER-INTEL, k = KOKKOS, o = USER-OMP, t = OPT.

none	hybrid	charmm (ko)	class2 (o)
harmonic (io)	helix (o)	multi/harmonic (o)	opls (iko)

These are additional dihedral styles in USER packages, which can be used if LAMMPS is built with the appropriate package.

cosine/shift/exp (o)	fourier (o)	nharmonic (o)	quadratic (o)
table (o)			

Improper_style potentials

See the improper_style command for an overview of improper potentials. Click on the style itself for a full description. Some of the styles have accelerated versions, which can be used if LAMMPS is built with the appropriate accelerated package. This is indicated by additional letters in parenthesis: c = USER-CUDA, g = GPU, i = USER-INTEL, k = KOKKOS, o = USER-OMP, t = OPT.

none	hybrid	class2 (o)	cvff (io)
harmonic (ko)	umbrella (o)		

These are additional improper styles in USER packages, which can be used if LAMMPS is built with the appropriate package.

cossq (o)	distance	fourier (o)	ring (o)

Kspace solvers

See the kspace_style command for an overview of Kspace solvers. Click on the style itself for a full description. Some of the styles have accelerated versions, which can be used if LAMMPS is built with the appropriate accelerated package. This is indicated by additional letters in parenthesis: c = USER-CUDA, g = GPU, i = USER-INTEL, k = KOKKOS, o = USER-OMP, t = OPT.

ewald (o)	ewald/disp	msm (o)	msm/cg (o)
pppm (cgo)	pppm/cg (o)	pppm/disp	pppm/disp/tip4p
pppm/stagger	pppm/tip4p (o)		

4. Packages

This section gives a quick overview of the add-on packages that extend LAMMPS functionality.

LAMMPS includes many optional packages, which are groups of files that enable a specific set of features. For example, force fields for molecular systems or granular systems are in packages. You can see the list of all packages by typing "make package" from within the src directory of the LAMMPS distribution.

See Section_start 3 of the manual for details on how to include/exclude specific packages as part of the LAMMPS build process, and for more details about the differences between standard packages and user packages.

Unless otherwise noted below, every package is independent of all the others. I.e. any package can be included or excluded in a LAMMPS build, independent of all other packages. However, note that some packages include commands derived from commands in other packages. If the other package is not installed, the derived command from the new package will also not be installed when you include the new one. E.g. the pair lj/cut/coul/long/omp command from the USER-OMP package will not be installed as part of the USER-OMP package if the KSPACE package is not also installed, since it contains the pair lj/cut/coul/long command. If you later install the KSPACE pacakge and the USER-OMP package is already installed, both the pair lj/cut/coul/long and lj/cut/coul/long/omp commands will be installed.

The two tables below list currently available packages in LAMMPS, with a one-line descriptions of each. The sections below give a few more details, including instructions for building LAMMPS with the package, either via the make command or the Make.py tool described in Section 2.4.

4.1 Standard packages

The current list of standard packages is as follows.

Package	Description	Author(s)	Doc page	Example	Library
ASPHERE	aspherical particles	-	Section_howto 6.14	ellipse	-
BODY	body-style particles	-	body	body	-
CLASS2	class 2 force fields	-	pair_style lj/class2	-	-
COLLOID	colloidal particles	-	atom_style colloid	colloid	-
COMPRESS	I/O compression	Axel Kohlmeyer (Temple U)	dump */gz	-	-
CORESHELL	adiabatic core/shell model	Hendrik Heenen (Technical U of Munich)	Section_howto 6.25	coreshell	-
DIPOLE	point dipole particles	-	pair_style dipole/cut	dipole	-
FLD	Fast Lubrication Dynamics	Kumar & Bybee & Higdon (1)	pair_style lubricateU	-	-
GPU	GPU-enabled styles	Mike Brown (ORNL)	Section accelerate	gpu	lib/gpu
GRANULAR	granular systems	-	Section_howto 6.6	pour	-
KIM	openKIM potentials		pair_style kim	kim	KIM

		Smirichinski & Elliot & Tadmor (3)			
KOKKOS	Kokkos-enabled styles	Trott & Edwards (4)	Section_accelerate	kokkos	lib/kokkos
KSPACE	long-range Coulombic solvers	-	kspace_style	peptide	-
MANYBODY	many-body potentials	-	pair_style tersoff	shear	-
MEAM	modified EAM potential	Greg Wagner (Sandia)	pair_style meam	meam	lib/meam
MC	Monte Carlo options	-	fix gcmc	-	-
MOLECULE	molecular system force fields	-	Section_howto 6.3	peptide	-
OPT	optimized pair styles	Fischer & Richie & Natoli (2)	Section accelerate	-	-
PERI	Peridynamics models	Mike Parks (Sandia)	pair_style peri	peri	-
POEMS	coupled rigid body motion	Rudra Mukherjee (JPL)	fix poems	rigid	lib/poems
PYTHON	embed Python code in an input script	-	python	python	lib/python
REAX	ReaxFF potential	Aidan Thompson (Sandia)	pair_style reax	reax	lib/reax
REPLICA	multi-replica methods	-	Section_howto 6.5	tad	-
RIGID	rigid bodies	-	fix rigid	rigid	-
SHOCK	shock loading methods	-	fix msst	-	-
SNAP	quantum-fit potential	Aidan Thompson (Sandia)	pair snap	snap	-
SRD	stochastic rotation dynamics	-	fix srd	srd	-
VORONOI	Voronoi tesselations	Daniel Schwen (LANL)	compute voronoi/atom	-	Voro++
XTC	dumps in XTC format	-	dump	-	-

The "Authors" column lists a name(s) if a specific person is responible for creating and maintaining the package. More details on multiple authors are give below.

(1) The FLD package was created by Amit Kumar and Michael Bybee from Jonathan Higdon's group at UIUC.

(2) The OPT package was created by James Fischer (High Performance Technologies), David Richie, and Vincent Natoli (Stone Ridge Technolgy).

(3) The KIM package was created by Valeriu Smirichinski, Ryan Elliott, and Ellad Tadmor (U Minn).

(4) The KOKKOS package was created primarily by Christian Trott (Sandia). It uses the Kokkos library which was developed by Carter Edwards, Christian, and collaborators at Sandia.

The "Doc page" column links to either a portion of the Section_howto of the manual, or an input script command implemented as part of the package.

The "Example" column is a sub-directory in the examples directory of the distribution which has an input script that uses the package. E.g. "peptide" refers to the examples/peptide directory.

The "Library" column lists an external library which must be built first and which LAMMPS links to when it is built. If it is listed as lib/package, then the code for the library is under the lib directory of the LAMMPS distribution. See the lib/package/README file for info on how to build the library. If it is not listed as lib/package, then it is a third-party library not included in the LAMMPS distribution. See the src/package/README or src/package/Makefile.lammps file for info on where to download the library. Section start of the manual also gives details on how to build LAMMPS with both kinds of auxiliary libraries.

Except where explained below, all of these packages can be installed, and LAMMPS re-built, by issuing these commands from the src dir.

```
make yes-package
make machine
or
Make.py -p package -a machine
```

To un-install the package and re-build LAMMPS without it:

```
make no-package
make machine
or
Make.py -p ^package -a machine
```

"Package" is the name of the package in lower-case letters, e.g. asphere or rigid, and "machine" is the build target, e.g. mpi or serial.

Build instructions for COMPRESS package

Build instructions for GPU package

Build instructions for KIM package

Build instructions for KOKKOS package

Build instructions for KSPACE package

Build instructions for MEAM package

Build instructions for POEMS package

Build instructions for PYTHON package

Build instructions for REAX package

Build instructions for VORONOI package

Build instructions for XTC package

4.2 User packages

The current list of user-contributed packages is as follows:

Package	Description	Author(s)	Doc page	Example	Pic/movie	Lib
USER-ATC	atom-to-continuum coupling	Jones & Templeton & Zimmerman (1)	fix atc	USER/atc	atc	lib/
USER-AWPMD	wave-packet MD	Ilya Valuev (JIHT)	pair_style awpmd/cut	USER/awpmd	-	lib/aw
USER-CG-CMM	coarse-graining model	Axel Kohlmeyer (Temple U)	pair_style lj/sdk	USER/cg-cmm	cg	-
USER-COLVARS	collective variables	Fiorin & Henin & Kohlmeyer (2)	fix colvars	USER/colvars	colvars	lib/co
USER-CUDA	NVIDIA GPU styles	Christian Trott (U Tech Ilmenau)	Section accelerate	USER/cuda	-	lib/c
USER-DIFFRACTION	virutal x-ray and electron diffraction	Shawn Coleman (ARL)	compute xrd	USER/diffraction	-	-
USER-DPD	dissipative particle dynamics (DPD)	Larentzos & Mattox & Brennan (5)	src/USER-DPD/README	USER/dpd	-	-
USER-DRUDE	Drude oscillators	Dequidt & Devemy & Padua (3)	tutorial	USER/drude	-	-
USER-EFF	electron force field	Andres Jaramillo-Botero (Caltech)	pair_style eff/cut	USER/eff	eff	-
USER-FEP	free energy perturbation	Agilio Padua (U Blaise Pascal Clermont-Ferrand)	compute fep	USER/fep	-	-
USER-H5MD	dump output via HDF5	Pierre de Buyl (KU Leuven)	dump h5md	-	-	lib/h
USER-INTEL	Vectorized CPU and Intel(R) coprocessor styles	W. Michael Brown (Intel)	Section accelerate	examples/intel	-	-
USER-LB	Lattice Boltzmann fluid	Colin Denniston (U Western Ontario)	fix lb/fluid	USER/lb	-	-
USER-MGPT	fast MGPT multi-ion potentials	Tomas Oppelstrup & John Moriarty (LLNL)	pair_style mgpt	USER/mgpt	-	-
USER-MISC	single-file contributions	USER-MISC/README	USER-MISC/README	-	-	-
USER-MOLFILE	VMD molfile plug-ins	Axel Kohlmeyer (Temple U)	dump molfile	-	-	VMD-M
USER-OMP	OpenMP threaded styles	Axel Kohlmeyer (Temple U)	Section accelerate	-	-	-
USER-PHONON	phonon dynamical matrix	Ling-Ti Kong (Shanghai Jiao Tong U)	fix phonon	USER/phonon	-	-
USER-QMMM	QM/MM coupling	Axel Kohlmeyer (Temple U)	fix qmmm	USER/qmmm	-	lib/q
USER-QTB	quantum nuclear effects	Yuan Shen (Stanford)	fix qtb fix_qbmsst	qtb	-	-
USER-QUIP	QUIP/libatoms	Albert Bartok-Partay (U	pair_style quip	USER/quip	-	lib/c

	interface	Cambridge)				
USER-REAXC	C version of ReaxFF	Metin Aktulga (LBNL)	pair_style reaxc	reax	-	-
USER-SMD	smoothed Mach dynamics	Georg Ganzenmuller (EMI)	userguide.pdf	USER/smd	-	-
USER-SMTBQ	Second Moment Tight Binding - QEq potential	Salles & Maras & Politano & Tetot (4)	pair_style smtbq	USER/smtbq	-	-
USER-SPH	smoothed particle hydrodynamics	Georg Ganzenmuller (EMI)	userguide.pdf	USER/sph	sph	-
USER-TALLY	Pairwise tallied computes	Axel Kohlmeyer (Temple U)	compute /tally	USER/tally	-	-

The "Authors" column lists a name(s) if a specific person is responible for creating and maintaining the package.

(1) The ATC package was created by Reese Jones, Jeremy Templeton, and Jon Zimmerman (Sandia).

(2) The COLVARS package was created by Axel Kohlmeyer (Temple U) using the colvars module library written by Giacomo Fiorin (Temple U) and Jerome Henin (LISM, Marseille, France).

(3) The DRUDE package was created by Alain Dequidt (U Blaise Pascal Clermont-Ferrand) and co-authors Julien Devemy (CNRS) and Agilio Padua (U Blaise Pascal).

(4) The SMTBQ package was created by Nicolas Salles, Emile Maras, Olivier Politano, and Robert Tetot (LAAS-CNRS, France).

(4) The USER-DPD package was created by James Larentzos, Timothy Mattox, and John Brennan (Army Research Lab (ARL) and Engility Corp).

If the Library is not listed as lib/package, then it is a third-party library not included in the LAMMPS distribution. See the src/package/Makefile.lammps file for info on where to download the library from.

The "Doc page" column links to either a portion of the Section_howto of the manual, or an input script command implemented as part of the package, or to additional documentation provided within the package.

The "Example" column is a sub-directory in the examples directory of the distribution which has an input script that uses the package. E.g. "peptide" refers to the examples/peptide directory. USER/cuda refers to the examples/USER/cuda directory.

The "Library" column lists an external library which must be built first and which LAMMPS links to when it is built. If it is listed as lib/package, then the code for the library is under the lib directory of the LAMMPS distribution. See the lib/package/README file for info on how to build the library. If it is not listed as lib/package, then it is a third-party library not included in the LAMMPS distribution. See the src/package/Makefile.lammps file for info on where to download the library. Section start of the manual also gives details on how to build LAMMPS with both kinds of auxiliary libraries.

Except where explained below, all of these packages can be installed, and LAMMPS re-built, by issuing these commands from the src dir.

```
make yes-user-package
make machine
or
Make.py -p package -a machine
```

To un-install the package and re-build LAMMPS without it:

```
make no-user-package
make machine
or
Make.py -p ^package -a machine
```

"Package" is the name of the package (in this case without the user prefix) in lower-case letters, e.g. drude or phonon, and "machine" is the build target, e.g. mpi or serial.

USER-ATC package

This package implements a "fix atc" command which can be used in a LAMMPS input script. This fix can be employed to either do concurrent coupling of MD with FE-based physics surrogates or on-the-fly post-processing of atomic information to continuum fields.

See the doc page for the fix atc command to get started. At the bottom of the doc page are many links to additional documentation contained in the doc/USER/atc directory.

There are example scripts for using this package in examples/USER/atc.

This package uses an external library in lib/atc which must be compiled before making LAMMPS. See the lib/atc/README file and the LAMMPS manual for information on building LAMMPS with external libraries.

The primary people who created this package are Reese Jones (rjones at sandia.gov), Jeremy Templeton (jatempl at sandia.gov) and Jon Zimmerman (jzimmer at sandia.gov) at Sandia. Contact them directly if you have questions.

USER-AWPMD package

This package contains a LAMMPS implementation of the Antisymmetrized Wave Packet Molecular Dynamics (AWPMD) method.

See the doc page for the pair_style awpmd/cut command to get started.

There are example scripts for using this package in examples/USER/awpmd.

This package uses an external library in lib/awpmd which must be compiled before making LAMMPS. See the lib/awpmd/README file and the LAMMPS manual for information on building LAMMPS with external libraries.

The person who created this package is Ilya Valuev at the JIHT in Russia (valuev at physik.hu-berlin.de). Contact him directly if you have questions.

USER-CG-CMM package

This package implements 3 commands which can be used in a LAMMPS input script:

- pair_style lj/sdk
- pair_style lj/sdk/coul/long
- angle_style sdk

These styles allow coarse grained MD simulations with the parametrization of Shinoda, DeVane, Klein, Mol Sim, 33, 27 (2007) (SDK), with extensions to simulate ionic liquids, electrolytes, lipids and charged amino acids.

See the doc pages for these commands for details.

There are example scripts for using this package in examples/USER/cg-cmm.

This is the second generation implementation reducing the the clutter of the previous version. For many systems with electrostatics, it will be faster to use pair_style hybrid/overlay with lj/sdk and coul/long instead of the combined lj/sdk/coul/long style. since the number of charged atom types is usually small. For any other coulomb interactions this is now required. To exploit this property, the use of the kspace_style pppm/cg is recommended over regular pppm. For all new styles, input file backward compatibility is provided. The old implementation is still available through appending the /old suffix. These will be discontinued and removed after the new implementation has been fully validated.

The current version of this package should be considered beta quality. The CG potentials work correctly for "normal" situations, but have not been testing with all kinds of potential parameters and simulation systems.

The person who created this package is Axel Kohlmeyer at Temple U (akohlmey at gmail.com). Contact him directly if you have questions.

USER-COLVARS package

This package implements the "fix colvars" command which can be used in a LAMMPS input script.

This fix allows to use "collective variables" to implement Adaptive Biasing Force, Metadynamics, Steered MD, Umbrella Sampling and Restraints. This code consists of two parts:

- A portable collective variable module library written and maintained
- by Giacomo Fiorin (ICMS, Temple University, Philadelphia, PA, USA) and
- Jerome Henin (LISM, CNRS, Marseille, France). This code is located in
- the directory lib/colvars and needs to be compiled first. The colvars
- fix and an interface layer, exchanges information between LAMMPS and
- the collective variable module.

See the doc page of fix colvars for more details.

There are example scripts for using this package in examples/USER/colvars

This is a very new interface that does not yet support all features in the module and will see future optimizations and improvements. The colvars module library is also available in NAMD has been thoroughly used and tested there. Bugs and problems are likely due to the interface layers code. Thus the current version of this package should be considered beta quality.

The person who created this package is Axel Kohlmeyer at Temple U (akohlmey at gmail.com). Contact him directly if you have questions.

USER-CUDA package

This package provides acceleration of various LAMMPS pair styles, fix styles, compute styles, and long-range Coulombics via PPPM for NVIDIA GPUs.

See this section of the manual to get started:

Section_accelerate

There are example scripts for using this package in examples/USER/cuda.

This package uses an external library in lib/cuda which must be compiled before making LAMMPS. See the lib/cuda/README file and the LAMMPS manual for information on building LAMMPS with external libraries.

The person who created this package is Christian Trott at the University of Technology Ilmenau, Germany (christian.trott at tu-ilmenau.de). Contact him directly if you have questions.

USER-DIFFRACTION package

This package contains the commands neeed to calculate x-ray and electron diffraction intensities based on kinematic diffraction theory.

See these doc pages and their related commands to get started:

- compute xrd
- compute saed
- fix saed/vtk

The person who created this package is Shawn P. Coleman (shawn.p.coleman8.ctr at mail.mil) while at the University of Arkansas. Contact him directly if you have questions.

USER-DPD package

This package implements the dissipative particle dynamics (DPD) method under isothermal, isoenergetic, isobaric and isenthalpic conditions. The DPD equations of motion are integrated efficiently through the Shardlow splitting algorithm.

See these doc pages and their related commands to get started:

- compute dpd
- compute dpd/atom
- fix_eos/cv
- fix_eos/table
- fix_shardlow
- pair_dpd/conservative
- pair_dpd/fdt
- pair_dpd/fdt/energy

There are example scripts for using this package in examples/USER/dpd.

The people who created this package are James Larentzos (james.p.larentzos.civ at mail.mil), Timothy Mattox (Timothy.Mattox at engilitycorp.com) and John Brennan (john.k.brennan.civ at mail.mil). Contact them directly if you have questions.

USER-DRUDE package

This package implements methods for simulating polarizable systems in LAMMPS using thermalized Drude oscillators.

See these doc pages and their related commands to get started:

- Drude tutorial
- fix drude
- compute temp/drude
- fix langevin/drude
- fix drude/transform/...
- pair thole

There are auxiliary tools for using this package in tools/drude.

The person who created this package is Alain Dequidt at Universite Blaise Pascal Clermont-Ferrand (alain.dequidt at univ-bpclermont.fr) Contact him directly if you have questions. Co-authors: Julien Devemy, Agilio Padua.

USER-EFF package

This package contains a LAMMPS implementation of the electron Force Field (eFF) currently under development at Caltech, as described in A. Jaramillo-Botero, J. Su, Q. An, and W.A. Goddard III, JCC, 2010. The eFF potential was first introduced by Su and Goddard, in 2007.

eFF can be viewed as an approximation to QM wave packet dynamics and Fermionic molecular dynamics, combining the ability of electronic structure methods to describe atomic structure, bonding, and chemistry in materials, and of plasma methods to describe nonequilibrium dynamics of large systems with a large number of highly excited electrons. We classify it as a mixed QM-classical approach rather than a conventional force field method, which introduces QM-based terms (a spin-dependent repulsion term to account for the Pauli exclusion principle and the electron wavefunction kinetic energy associated with the Heisenberg principle) that reduce, along with classical electrostatic terms between nuclei and electrons, to the sum of a set of effective pairwise potentials. This makes eFF uniquely suited to simulate materials over a wide range of temperatures and pressures where electronically excited and ionized states of matter can occur and coexist.

The necessary customizations to the LAMMPS core are in place to enable the correct handling of explicit electron properties during minimization and dynamics.

See the doc page for the pair_style eff/cut command to get started.

There are example scripts for using this package in examples/USER/eff.

There are auxiliary tools for using this package in tools/eff.

The person who created this package is Andres Jaramillo-Botero at CalTech (ajaramil at wag.caltech.edu). Contact him directly if you have questions.

USER-FEP package

This package provides methods for performing free energy perturbation simulations with soft-core pair potentials in LAMMPS.

See these doc pages and their related commands to get started:

- fix adapt/fep
- compute fep
- soft pair styles

The person who created this package is Agilio Padua at Universite Blaise Pascal Clermont-Ferrand (agilio.padua at univ-bpclermont.fr) Contact him directly if you have questions.

USER-H5MD package

This package contains a dump h5md command for performing a dump of atom properties in HDF5 format. HDF5 files are binary, portable and self-describing and can be examined and used by a variety of auxiliary tools. The output HDF5 files are structured in a format called H5MD, which was designed to store molecular data, and can be used and produced by various MD and MD-related codes. The dump h5md command gives a citation to a paper describing the format.

The person who created this package and the underlying H5MD format is Pierre de Buyl at KU Leuven (see http://pdebuyl.be). Contact him directly if you have questions.

USER-INTEL package

This package provides options for performing neighbor list and non-bonded force calculations in single, mixed, or double precision and also a capability for accelerating calculations with an Intel(R) Xeon Phi(TM) coprocessor.

See this section of the manual to get started:

Section_accelerate

The person who created this package is W. Michael Brown at Intel (michael.w.brown at intel.com). Contact him directly if you have questions.

USER-LB package

This package contains a LAMMPS implementation of a background Lattice-Boltzmann fluid, which can be used to model MD particles influenced by hydrodynamic forces.

See this doc page and its related commands to get started:

fix lb/fluid

The people who created this package are Frances Mackay (fmackay at uwo.ca) and Colin (cdennist at uwo.ca) Denniston, University of Western Ontario. Contact them directly if you have questions.

USER-MGPT package

This package contains a fast implementation for LAMMPS of quantum-based MGPT multi-ion potentials. The MGPT or model GPT method derives from first-principles DFT-based generalized pseudopotential theory (GPT) through a series of systematic approximations valid for mid-period transition metals with nearly half-filled d bands. The MGPT method was originally developed by John Moriarty at Lawrence Livermore National Lab (LLNL).

In the general matrix representation of MGPT, which can also be applied to f-band actinide metals, the multi-ion potentials are evaluated on the fly during a simulation through d- or f-state matrix multiplication, and the forces that move the ions are determined analytically. The *mgpt* pair style in this package calculates forces and energies using an optimized matrix-MGPT algorithm due to Tomas Oppelstrup at LLNL.

See this doc page to get started:

pair_style mgpt

The persons who created the USER-MGPT package are Tomas Oppelstrup (oppelstrup2@llnl.gov) and John Moriarty (moriarty2@llnl.gov) Contact them directly if you have any questions.

USER-MISC package

The files in this package are a potpourri of (mostly) unrelated features contributed to LAMMPS by users. Each feature is a single pair of files (*.cpp and *.h).

More information about each feature can be found by reading its doc page in the LAMMPS doc directory. The doc page which lists all LAMMPS input script commands is as follows:

Section_commands

User-contributed features are listed at the bottom of the fix, compute, pair, etc sections.

The list of features and author of each is given in the src/USER-MISC/README file.

You should contact the author directly if you have specific questions about the feature or its coding.

USER-MOLFILE package

This package contains a dump molfile command which uses molfile plugins that are bundled with the VMD molecular visualization and analysis program, to enable LAMMPS to dump its information in formats compatible with various molecular simulation tools.

The package only provides the interface code, not the plugins. These can be obtained from a VMD installation which has to match the platform that you are using to compile LAMMPS for. By adding plugins to VMD, support for new file formats can be added to LAMMPS (or VMD or other programs that use them) without having to recompile the application itself.

See this doc page to get started:

dump molfile

The person who created this package is Axel Kohlmeyer at Temple U (akohlmey at gmail.com). Contact him directly if you have questions.

USER-OMP package

This package provides OpenMP multi-threading support and other optimizations of various LAMMPS pair styles, dihedral styles, and fix styles.

See this section of the manual to get started:

Section_accelerate

The person who created this package is Axel Kohlmeyer at Temple U (akohlmey at gmail.com). Contact him directly if you have questions.

USER-PHONON package

This package contains a fix phonon command that calculates dynamical matrices, which can then be used to compute phonon dispersion relations, directly from molecular dynamics simulations.

See this doc page to get started:

fix phonon

The person who created this package is Ling-Ti Kong (konglt at sjtu.edu.cn) at Shanghai Jiao Tong University. Contact him directly if you have questions.

USER-QMMM package

This package provides a fix qmmm command which allows LAMMPS to be used in a QM/MM simulation, currently only in combination with pw.x code from the Quantum ESPRESSO package.

The current implementation only supports an ONIOM style mechanical coupling to the Quantum ESPRESSO plane wave DFT package. Electrostatic coupling is in preparation and the interface has been written in a manner that coupling to other QM codes should be possible without changes to LAMMPS itself.

See this doc page to get started:

fix qmmm

as well as the lib/qmmm/README file.

The person who created this package is Axel Kohlmeyer at Temple U (akohlmey at gmail.com). Contact him directly if you have questions.

USER-QTB package

This package provides a self-consistent quantum treatment of the vibrational modes in a classical molecular dynamics simulation. By coupling the MD simulation to a colored thermostat, it introduces zero point energy into the system, alter the energy power spectrum and the heat capacity towards their quantum nature. This package could be of interest if one wants to model systems at temperatures lower than their classical limits or when temperatures ramp up across the classical limits in the simulation.

See these two doc pages to get started:

fix qtb provides quantum nulcear correction through a colored thermostat and can be used with other time integration schemes like fix nve or fix nph.

fix qbmsst enables quantum nuclear correction of a multi-scale shock technique simulation by coupling the quantum thermal bath with the shocked system.

The person who created this package is Yuan Shen (sy0302 at stanford.edu) at Stanford University. Contact him directly if you have questions.

USER-REAXC package

This package contains a implementation for LAMMPS of the ReaxFF force field. ReaxFF uses distance-dependent bond-order functions to represent the contributions of chemical bonding to the potential energy. It was originally developed by Adri van Duin and the Goddard group at CalTech.

The USER-REAXC version of ReaxFF (pair_style reax/c), implemented in C, should give identical or very similar results to pair_style reax, which is a ReaxFF implementation on top of a Fortran library, a version of which library was originally authored by Adri van Duin.

The reax/c version should be somewhat faster and more scalable, particularly with respect to the charge equilibration calculation. It should also be easier to build and use since there are no complicating issues with Fortran memory allocation or linking to a Fortran library.

For technical details about this implemention of ReaxFF, see this paper:

Parallel and Scalable Reactive Molecular Dynamics: Numerical Methods and Algorithmic Techniques, H. M. Aktulga, J. C. Fogarty, S. A. Pandit, A. Y. Grama, Parallel Computing, in press (2011).

See the doc page for the pair_style reax/c command for details of how to use it in LAMMPS.

The person who created this package is Hasan Metin Aktulga (hmaktulga at lbl.gov), while at Purdue University. Contact him directly, or Aidan Thompson at Sandia (athomps at sandia.gov), if you have questions.

USER-SMD package

This package implements smoothed Mach dynamics (SMD) in LAMMPS. Currently, the package has the following features:

* Does liquids via traditional Smooth Particle Hydrodynamics (SPH)

* Also solves solids mechanics problems via a state of the art stabilized meshless method with hourglass control.

* Can specify hydrostatic interactions independently from material strength models, i.e. pressure and deviatoric stresses are separated.

* Many material models available (Johnson-Cook, plasticity with hardening, Mie-Grueneisen, Polynomial EOS). Easy to add new material models.

* Rigid boundary conditions (walls) can be loaded as surface geometries from *.STL files.

See the file doc/PDF/SMD_LAMMPS_userguide.pdf to get started.

There are example scripts for using this package in examples/USER/smd.

The person who created this package is Georg Ganzenmuller at the Fraunhofer-Institute for High-Speed Dynamics, Ernst Mach Institute in Germany (georg.ganzenmueller at emi.fhg.de). Contact him directly if you have questions.

USER-SMTBQ package

This package implements the Second Moment Tight Binding - QEq (SMTB-Q) potential for the description of ionocovalent bonds in oxides.

There are example scripts for using this package in examples/USER/smtbq.

See this doc page to get started:

pair_style smtbq

The persons who created the USER-SMTBQ package are Nicolas Salles, Emile Maras, Olivier Politano, Robert Tetot, who can be contacted at these email addreses: lammps@u-bourgogne.fr, nsalles@laas.fr. Contact them directly if you have any questions.

USER-SPH package

This package implements smoothed particle hydrodynamics (SPH) in LAMMPS. Currently, the package has the following features:

* Tait, ideal gas, Lennard-Jones equation of states, full support for complete (i.e. internal-energy dependent) equations of state

* Plain or Monaghans XSPH integration of the equations of motion

* Density continuity or density summation to propagate the density field

* Commands to set internal energy and density of particles from the input script

* Output commands to access internal energy and density for dumping and thermo output

See the file doc/PDF/SPH_LAMMPS_userguide.pdf to get started.

There are example scripts for using this package in examples/USER/sph.

The person who created this package is Georg Ganzenmuller at the Fraunhofer-Institute for High-Speed Dynamics, Ernst Mach Institute in Germany (georg.ganzenmueller at emi.fhg.de). Contact him directly if you have questions.

5. Accelerating LAMMPS performance

This section describes various methods for improving LAMMPS performance for different classes of problems running on different kinds of machines.

There are two thrusts to the discussion that follows. The first is using code options that implement alternate algorithms that can speed-up a simulation. The second is to use one of the several accelerator packages provided with LAMMPS that contain code optimized for certain kinds of hardware, including multi-core CPUs, GPUs, and Intel Xeon Phi coprocessors.

The Benchmark page of the LAMMPS web site gives performance results for the various accelerator packages discussed in Section 5.2, for several of the standard LAMMPS benchmark problems, as a function of problem size and number of compute nodes, on different hardware platforms.

5.1 Measuring performance

Before trying to make your simulation run faster, you should understand how it currently performs and where the bottlenecks are.

The best way to do this is run the your system (actual number of atoms) for a modest number of timesteps (say 100 steps) on several different processor counts, including a single processor if possible. Do this for an equilibrium version of your system, so that the 100-step timings are representative of a much longer run. There is typically no need to run for 1000s of timesteps to get accurate timings; you can simply extrapolate from short runs.

For the set of runs, look at the timing data printed to the screen and log file at the end of each LAMMPS run. This section of the manual has an overview.

Running on one (or a few processors) should give a good estimate of the serial performance and what portions of the timestep are taking the most time. Running the same problem on a few different processor counts should give an estimate of parallel scalability. I.e. if the simulation runs 16x faster on 16 processors, its 100% parallel efficient; if it runs 8x faster on 16 processors, it's 50% efficient.

The most important data to look at in the timing info is the timing breakdown and relative percentages. For example, trying different options for speeding up the long-range solvers will have little impact if they only consume 10% of the run time. If the pairwise time is dominating, you may want to look at GPU or OMP versions of the pair style, as discussed below. Comparing how the percentages change as you increase the processor count gives you a sense of how different operations within the timestep are scaling. Note that if you are running with a

Kspace solver, there is additional output on the breakdown of the Kspace time. For PPPM, this includes the fraction spent on FFTs, which can be communication intensive.

Another important detail in the timing info are the histograms of atoms counts and neighbor counts. If these vary widely across processors, you have a load-imbalance issue. This often results in inaccurate relative timing data, because processors have to wait when communication occurs for other processors to catch up. Thus the reported times for "Communication" or "Other" may be higher than they really are, due to load-imbalance. If this is an issue, you can uncomment the MPI_Barrier() lines in src/timer.cpp, and recompile LAMMPS, to obtain synchronized timings.

5.2 General strategies

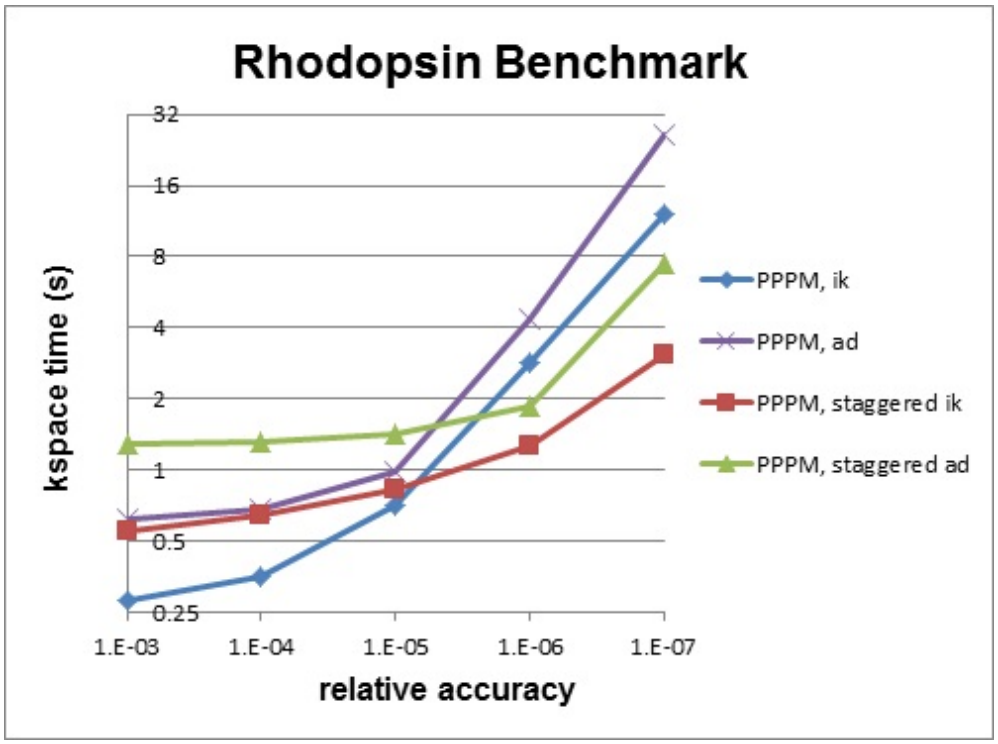
NOTE: this section 5.2 is still a work in progress

Here is a list of general ideas for improving simulation performance. Most of them are only applicable to certain models and certain bottlenecks in the current performance, so let the timing data you generate be your guide. It is hard, if not impossible, to predict how much difference these options will make, since it is a function of problem size, number of processors used, and your machine. There is no substitute for identifying performance bottlenecks, and trying out various options.

- rRESPA
- 2-FFT PPPM
- Staggered PPPM
- single vs double PPPM
- partial charge PPPM
- verlet/split run style
- processor command for proc layout and numa layout
- load-balancing: balance and fix balance

2-FFT PPPM, also called *analytic differentiation* or *ad* PPPM, uses 2 FFTs instead of the 4 FFTs used by the default *ik differentiation* PPPM. However, 2-FFT PPPM also requires a slightly larger mesh size to achieve the same accuracy as 4-FFT PPPM. For problems where the FFT cost is the performance bottleneck (typically large problems running on many processors), 2-FFT PPPM may be faster than 4-FFT PPPM.

Staggered PPPM performs calculations using two different meshes, one shifted slightly with respect to the other. This can reduce force aliasing errors and increase the accuracy of the method, but also doubles the amount of work required. For high relative accuracy, using staggered PPPM allows one to half the mesh size in each dimension as compared to regular PPPM, which can give around a 4x speedup in the kspace time. However, for low relative accuracy, using staggered PPPM gives little benefit and can be up to 2x slower in the kspace time. For example, the rhodopsin benchmark was run on a single processor, and results for kspace time vs. relative accuracy for the different methods are shown in the figure below. For this system, staggered PPPM (using ik differentiation) becomes useful when using a relative accuracy of slightly greater than 1e-5 and above.



NOTE: Using staggered PPPM may not give the same increase in accuracy of energy and pressure as it does in forces, so some caution must be used if energy and/or pressure are quantities of interest, such as when using a barostat.

5.3 Packages with optimized styles

Accelerated versions of various pair_style, fixes, computes, and other commands have been added to LAMMPS, which will typically run faster than the standard non-accelerated versions. Some require appropriate hardware to be present on your system, e.g. GPUs or Intel Xeon Phi coprocessors.

All of these commands are in packages provided with LAMMPS. An overview of packages is give in Section packages.

These are the accelerator packages currently in LAMMPS, either as standard or user packages:

USER-CUDA	for NVIDIA GPUs
GPU	for NVIDIA GPUs as well as OpenCL support
USER-INTEL	for Intel CPUs and Intel Xeon Phi
KOKKOS	for GPUs, Intel Xeon Phi, and OpenMP threading
USER-OMP	for OpenMP threading
OPT	generic CPU optimizations

Inverting this list, LAMMPS currently has acceleration support for three kinds of hardware, via the listed packages:

Many-core CPUs	USER-INTEL, KOKKOS, USER-OMP, OPT packages
NVIDIA GPUs	USER-CUDA, GPU, KOKKOS packages
Intel Phi	USER-INTEL, KOKKOS packages

Which package is fastest for your hardware may depend on the size problem you are running and what commands

(accelerated and non-accelerated) are invoked by your input script. While these doc pages include performance guidelines, there is no substitute for trying out the different packages appropriate to your hardware.

Any accelerated style has the same name as the corresponding standard style, except that a suffix is appended. Otherwise, the syntax for the command that uses the style is identical, their functionality is the same, and the numerical results it produces should also be the same, except for precision and round-off effects.

For example, all of these styles are accelerated variants of the Lennard-Jones pair_style lj/cut:

- pair_style lj/cut/cuda
- pair_style lj/cut/gpu
- pair_style lj/cut/intel
- pair_style lj/cut/kk
- pair_style lj/cut/omp
- pair_style lj/cut/opt

To see what accelerate styles are currently available, see Section_commands 5 of the manual. The doc pages for individual commands (e.g. pair lj/cut or fix nve) also list any accelerated variants available for that style.

To use an accelerator package in LAMMPS, and one or more of the styles it provides, follow these general steps. Details vary from package to package and are explained in the individual accelerator doc pages, listed above:

build the accelerator library	only for USER-CUDA and GPU packages
install the accelerator package	make yes-opt, make yes-user-intel, etc
add compile/link flags to Makefile.machine	in src/MAKE, only for USER-INTEL, KOKKOS, USER-OMP, OPT packages
re-build LAMMPS	make machine
run a LAMMPS simulation	lmp_machine < in.script mpirun -np 32 lmp_machine -in in.script
enable the accelerator package	via "-c on" and "-k on" command-line switches, only for USER-CUDA and KOKKOS packages
set any needed options for the package	via "-pk" command-line switch or package command, only if defaults need to be changed
use accelerated styles in your input script	via "-sf" command-line switch or suffix command

Note that the first 4 steps can be done as a single command, using the src/Make.py tool. This tool is discussed in Section 2.4 of the manual, and its use is illustrated in the individual accelerator sections. Typically these steps only need to be done once, to create an executable that uses one or more accelerator packages.

The last 4 steps can all be done from the command-line when LAMMPS is launched, without changing your input script, as illustrated in the individual accelerator sections. Or you can add package and suffix commands to your input script.

NOTE: With a few exceptions, you can build a single LAMMPS executable with all its accelerator packages installed. Note however that the USER-INTEL and KOKKOS packages require you to choose one of their hardware options when building for a specific platform. I.e. CPU or Phi option for the USER-INTEL package. Or the OpenMP, Cuda, or Phi option for the KOKKOS package.

These are the exceptions. You cannot build a single executable with:

- both the USER-INTEL Phi and KOKKOS Phi options
- the USER-INTEL Phi or Kokkos Phi option, and either the USER-CUDA or GPU packages

See the examples/accelerate/README and make.list files for sample Make.py commands that build LAMMPS with any or all of the accelerator packages. As an example, here is a command that builds with all the GPU related packages installed (USER-CUDA, GPU, KOKKOS with Cuda), including settings to build the needed auxiliary USER-CUDA and GPU libraries for Kepler GPUs:

```
Make.py -j 16 -p omp gpu cuda kokkos -cc nvcc wrap=mpi   -cuda mode=double arch=35 -gpu mode=double
```

The examples/accelerate directory also has input scripts that can be used with all of the accelerator packages. See its README file for details.

Likewise, the bench directory has FERMI and KEPLER and PHI sub-directories with Make.py commands and input scripts for using all the accelerator packages on various machines. See the README files in those dirs.

As mentioned above, the Benchmark page of the LAMMPS web site gives performance results for the various accelerator packages for several of the standard LAMMPS benchmark problems, as a function of problem size and number of compute nodes, on different hardware platforms.

Here is a brief summary of what the various packages provide. Details are in the individual accelerator sections.

- Styles with a "cuda" or "gpu" suffix are part of the USER-CUDA or GPU packages, and can be run on NVIDIA GPUs. The speed-up on a GPU depends on a variety of factors, discussed in the accelerator sections.
- Styles with an "intel" suffix are part of the USER-INTEL package. These styles support vectorized single and mixed precision calculations, in addition to full double precision. In extreme cases, this can provide speedups over 3.5x on CPUs. The package also supports acceleration in "offload" mode to Intel(R) Xeon Phi(TM) coprocessors. This can result in additional speedup over 2x depending on the hardware configuration.
- Styles with a "kk" suffix are part of the KOKKOS package, and can be run using OpenMP on multicore CPUs, on an NVIDIA GPU, or on an Intel Xeon Phi in "native" mode. The speed-up depends on a variety of factors, as discussed on the KOKKOS accelerator page.
- Styles with an "omp" suffix are part of the USER-OMP package and allow a pair-style to be run in multi-threaded mode using OpenMP. This can be useful on nodes with high-core counts when using less MPI processes than cores is advantageous, e.g. when running with PPPM so that FFTs are run on fewer MPI processors or when the many MPI tasks would overload the available bandwidth for communication.
- Styles with an "opt" suffix are part of the OPT package and typically speed-up the pairwise calculations of your simulation by 5-25% on a CPU.

The individual accelerator package doc pages explain:

- what hardware and software the accelerated package requires
- how to build LAMMPS with the accelerated package
- how to run with the accelerated package either via command-line switches or modifying the input script
- speed-ups to expect
- guidelines for best performance
- restrictions

5.4 Comparison of various accelerator packages

NOTE: this section still needs to be re-worked with additional KOKKOS and USER-INTEL information.

The next section compares and contrasts the various accelerator options, since there are multiple ways to perform OpenMP threading, run on GPUs, and run on Intel Xeon Phi coprocessors.

All 3 of these packages accelerate a LAMMPS calculation using NVIDIA hardware, but they do it in different ways.

As a consequence, for a particular simulation on specific hardware, one package may be faster than the other. We give guidelines below, but the best way to determine which package is faster for your input script is to try both of them on your machine. See the benchmarking section below for examples where this has been done.

Guidelines for using each package optimally:

- The GPU package allows you to assign multiple CPUs (cores) to a single GPU (a common configuration for "hybrid" nodes that contain multicore CPU(s) and GPU(s)) and works effectively in this mode. The USER-CUDA package does not allow this; you can only use one CPU per GPU.
- The GPU package moves per-atom data (coordinates, forces) back-and-forth between the CPU and GPU every timestep. The USER-CUDA package only does this on timesteps when a CPU calculation is required (e.g. to invoke a fix or compute that is non-GPU-ized). Hence, if you can formulate your input script to only use GPU-ized fixes and computes, and avoid doing I/O too often (thermo output, dump file snapshots, restart files), then the data transfer cost of the USER-CUDA package can be very low, causing it to run faster than the GPU package.
- The GPU package is often faster than the USER-CUDA package, if the number of atoms per GPU is smaller. The crossover point, in terms of atoms/GPU at which the USER-CUDA package becomes faster depends strongly on the pair style. For example, for a simple Lennard Jones system the crossover (in single precision) is often about 50K-100K atoms per GPU. When performing double precision calculations the crossover point can be significantly smaller.
- Both packages compute bonded interactions (bonds, angles, etc) on the CPU. This means a model with bonds will force the USER-CUDA package to transfer per-atom data back-and-forth between the CPU and GPU every timestep. If the GPU package is running with several MPI processes assigned to one GPU, the cost of computing the bonded interactions is spread across more CPUs and hence the GPU package can run faster.
- When using the GPU package with multiple CPUs assigned to one GPU, its performance depends to some extent on high bandwidth between the CPUs and the GPU. Hence its performance is affected if full 16 PCIe lanes are not available for each GPU. In HPC environments this can be the case if S2050/70 servers are used, where two devices generally share one PCIe 2.0 16x slot. Also many multi-GPU mainboards do not provide full 16 lanes to each of the PCIe 2.0 16x slots.

Differences between the two packages:

- The GPU package accelerates only pair force, neighbor list, and PPPM calculations. The USER-CUDA package currently supports a wider range of pair styles and can also accelerate many fix styles and some compute styles, as well as neighbor list and PPPM calculations.
- The USER-CUDA package does not support acceleration for minimization.
- The USER-CUDA package does not support hybrid pair styles.
- The USER-CUDA package can order atoms in the neighbor list differently from run to run resulting in a different order for force accumulation.
- The USER-CUDA package has a limit on the number of atom types that can be used in a simulation.
- The GPU package requires neighbor lists to be built on the CPU when using exclusion lists or a triclinic simulation box.
- The GPU package uses more GPU memory than the USER-CUDA package. This is generally not a problem since typical runs are computation-limited rather than memory-limited.

Examples:

The LAMMPS distribution has two directories with sample input scripts for the GPU and USER-CUDA

packages.

- lammps/examples/gpu = GPU package files
- lammps/examples/USER/cuda = USER-CUDA package files

These contain input scripts for identical systems, so they can be used to benchmark the performance of both packages on your system.

6. How-to discussions

This section describes how to perform common tasks using LAMMPS.

The example input scripts included in the LAMMPS distribution and highlighted in Section_example also show how to setup and run various kinds of simulations.

6.1 Restarting a simulation

There are 3 ways to continue a long LAMMPS simulation. Multiple run commands can be used in the same input script. Each run will continue from where the previous run left off. Or binary restart files can be saved to disk using the restart command. At a later time, these binary files can be read via a read_restart command in a new script. Or they can be converted to text data files using the -r command-line switch and read by a read_data command in a new script.

Here we give examples of 2 scripts that read either a binary restart file or a converted data file and then issue a new run command to continue where the previous run left off. They illustrate what settings must be made in the new script. Details are discussed in the documentation for the read_restart and read_data commands.

Look at the *in.chain* input script provided in the *bench* directory of the LAMMPS distribution to see the original script that these 2 scripts are based on. If that script had the line

```
restart         50 tmp.restart
```

added to it, it would produce 2 binary restart files (tmp.restart.50 and tmp.restart.100) as it ran.

This script could be used to read the 1st restart file and re-run the last 50 timesteps:

```
read_restart    tmp.restart.50

neighbor        0.4 bin
neigh_modify    every 1 delay 1

fix             1 all nve
fix             2 all langevin 1.0 1.0 10.0 904297

timestep        0.012

run             50
```

Note that the following commands do not need to be repeated because their settings are included in the restart file: *units, atom_style, special_bonds, pair_style, bond_style*. However these commands do need to be used, since their settings are not in the restart file: *neighbor, fix, timestep*.

If you actually use this script to perform a restarted run, you will notice that the thermodynamic data match at step 50 (if you also put a "thermo 50" command in the original script), but do not match at step 100. This is because the fix langevin command uses random numbers in a way that does not allow for perfect restarts.

As an alternate approach, the restart file could be converted to a data file as follows:

```
lmp_g++ -r tmp.restart.50 tmp.restart.data
```

Then, this script could be used to re-run the last 50 steps:

```
units           lj
atom_style      bond
pair_style      lj/cut 1.12
pair_modify     shift yes
bond_style      fene
special_bonds   0.0 1.0 1.0

read_data       tmp.restart.data

neighbor        0.4 bin
neigh_modify    every 1 delay 1

fix             1 all nve
fix             2 all langevin 1.0 1.0 10.0 904297

timestep        0.012

reset_timestep  50
run             50
```

Note that nearly all the settings specified in the original *in.chain* script must be repeated, except the *pair_coeff* and *bond_coeff* commands since the new data file lists the force field coefficients. Also, the reset_timestep

command is used to tell LAMMPS the current timestep. This value is stored in restart files, but not in data files.

6.2 2d simulations

Use the dimension command to specify a 2d simulation.

Make the simulation box periodic in z via the boundary command. This is the default.

If using the create box command to define a simulation box, set the z dimensions narrow, but finite, so that the create_atoms command will tile the 3d simulation box with a single z plane of atoms - e.g.

```
create box 1 -10 10 -10 10 -0.25 0.25
```

If using the read data command to read in a file of atom coordinates, set the "zlo zhi" values to be finite but narrow, similar to the create_box command settings just described. For each atom in the file, assign a z coordinate so it falls inside the z-boundaries of the box - e.g. 0.0.

Use the fix enforce2d command as the last defined fix to insure that the z-components of velocities and forces are zeroed out every timestep. The reason to make it the last fix is so that any forces induced by other fixes will be zeroed out.

Many of the example input scripts included in the LAMMPS distribution are for 2d models.

NOTE: Some models in LAMMPS treat particles as finite-size spheres, as opposed to point particles. In 2d, the particles will still be spheres, not disks, meaning their moment of inertia will be the same as in 3d.

6.3 CHARMM, AMBER, and DREIDING force fields

A force field has 2 parts: the formulas that define it and the coefficients used for a particular system. Here we only discuss formulas implemented in LAMMPS that correspond to formulas commonly used in the CHARMM, AMBER, and DREIDING force fields. Setting coefficients is done in the input data file via the read_data command or in the input script with commands like pair_coeff or bond_coeff. See Section_tools for additional tools that can use CHARMM or AMBER to assign force field coefficients and convert their output into LAMMPS input.

See (MacKerell) for a description of the CHARMM force field. See (Cornell) for a description of the AMBER force field.

These style choices compute force field formulas that are consistent with common options in CHARMM or AMBER. See each command's documentation for the formula it computes.

- bond_style harmonic
- angle_style charmm
- dihedral_style charmm
- pair_style lj/charmm/coul/charmm
- pair_style lj/charmm/coul/charmm/implicit
- pair_style lj/charmm/coul/long

- special_bonds charmm
- special_bonds amber

DREIDING is a generic force field developed by the Goddard group at Caltech and is useful for predicting structures and dynamics of organic, biological and main-group inorganic molecules. The philosophy in DREIDING is to use general force constants and geometry parameters based on simple hybridization considerations, rather than individual force constants and geometric parameters that depend on the particular combinations of atoms involved in the bond, angle, or torsion terms. DREIDING has an explicit hydrogen bond term to describe interactions involving a hydrogen atom on very electronegative atoms (N, O, F).

See (Mayo) for a description of the DREIDING force field

These style choices compute force field formulas that are consistent with the DREIDING force field. See each command's documentation for the formula it computes.

- bond_style harmonic
- bond_style morse

- angle_style harmonic
- angle_style cosine
- angle_style cosine/periodic

- dihedral_style charmm
- improper_style umbrella

- pair_style buck
- pair_style buck/coul/cut
- pair_style buck/coul/long
- pair_style lj/cut
- pair_style lj/cut/coul/cut
- pair_style lj/cut/coul/long

- pair_style hbond/dreiding/lj
- pair_style hbond/dreiding/morse

- special_bonds dreiding

6.4 Running multiple simulations from one input script

This can be done in several ways. See the documentation for individual commands for more details on how these examples work.

If "multiple simulations" means continue a previous simulation for more timesteps, then you simply use the run command multiple times. For example, this script

```
units lj
atom_style atomic
read_data data.lj
run 10000
run 10000
run 10000
run 10000
run 10000
```

would run 5 successive simulations of the same system for a total of 50,000 timesteps.

If you wish to run totally different simulations, one after the other, the clear command can be used in between them to re-initialize LAMMPS. For example, this script

```
units lj
atom_style atomic
read_data data.lj
run 10000
clear
units lj
atom_style atomic
read_data data.lj.new
run 10000
```

would run 2 independent simulations, one after the other.

For large numbers of independent simulations, you can use variables and the next and jump commands to loop over the same input script multiple times with different settings. For example, this script, named in.polymer

```
variable d index run1 run2 run3 run4 run5 run6 run7 run8
shell cd $d
read_data data.polymer
run 10000
shell cd ..
clear
next d
jump in.polymer
```

would run 8 simulations in different directories, using a data.polymer file in each directory. The same concept could be used to run the same system at 8 different temperatures, using a temperature variable and storing the output in different log and dump files, for example

```
variable a loop 8
variable t index 0.8 0.85 0.9 0.95 1.0 1.05 1.1 1.15
log log.$a
read data.polymer
velocity all create $t 352839
fix 1 all nvt $t $t 100.0
dump 1 all atom 1000 dump.$a
run 100000
clear
next t
next a
jump in.polymer
```

All of the above examples work whether you are running on 1 or multiple processors, but assumed you are running LAMMPS on a single partition of processors. LAMMPS can be run on multiple partitions via the "-partition" command-line switch as described in this section of the manual.

In the last 2 examples, if LAMMPS were run on 3 partitions, the same scripts could be used if the "index" and "loop" variables were replaced with *universe*-style variables, as described in the variable command. Also, the "next t" and "next a" commands would need to be replaced with a single "next a t" command. With these modifications, the 8 simulations of each script would run on the 3 partitions one after the other until all were finished. Initially, 3 simulations would be started simultaneously, one on each partition. When one finished, that partition would then start the 4th simulation, and so forth, until all 8 were completed.

6.5 Multi-replica simulations

Several commands in LAMMPS run mutli-replica simulations, meaning that multiple instances (replicas) of your simulation are run simultaneously, with small amounts of data exchanged between replicas periodically.

These are the relevant commands:

- neb for nudged elastic band calculations
- prd for parallel replica dynamics
- tad for temperature accelerated dynamics
- temper for parallel tempering
- fix pimd for path-integral molecular dynamics (PIMD)

NEB is a method for finding transition states and barrier energies. PRD and TAD are methods for performing accelerated dynamics to find and perform infrequent events. Parallel tempering or replica exchange runs different replicas at a series of temperature to facilitate rare-event sampling.

These commands can only be used if LAMMPS was built with the REPLICA package. See the Making LAMMPS section for more info on packages.

PIMD runs different replicas whose individual particles are coupled together by springs to model a system or ring-polymers.

This commands can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

In all these cases, you must run with one or more processors per replica. The processors assigned to each replica are determined at run-time by using the -partition command-line switch to launch LAMMPS on multiple partitions, which in this context are the same as replicas. E.g. these commands:

```
mpirun -np 16 lmp_linux -partition 8x2 -in in.temper
mpirun -np 8 lmp_linux -partition 8x1 -in in.neb
```

would each run 8 replicas, on either 16 or 8 processors. Note the use of the -in command-line switch to specify the input script which is required when running in multi-replica mode.

Also note that with MPI installed on a machine (e.g. your desktop), you can run on more (virtual) processors than you have physical processors. Thus the above commands could be run on a single-processor (or few-processor) desktop so that you can run a multi-replica simulation on more replicas than you have physical processors.

6.6 Granular models

Granular system are composed of spherical particles with a diameter, as opposed to point particles. This means they have an angular velocity and torque can be imparted to them to cause them to rotate.

To run a simulation of a granular model, you will want to use the following commands:

- atom_style sphere
- fix nve/sphere
- fix gravity

This compute

- compute erotate/sphere

calculates rotational kinetic energy which can be output with thermodynamic info.

Use one of these 3 pair potentials, which compute forces and torques between interacting pairs of particles:

- pair_style gran/history
- pair_style gran/no_history
- pair_style gran/hertzian

These commands implement fix options specific to granular systems:

- fix freeze
- fix pour
- fix viscous
- fix wall/gran

The fix style *freeze* zeroes both the force and torque of frozen atoms, and should be used for granular system instead of the fix style *setforce*.

For computational efficiency, you can eliminate needless pairwise computations between frozen atoms by using this command:

- neigh_modify exclude

6.7 TIP3P water model

The TIP3P water model as implemented in CHARMM (MacKerell) specifies a 3-site rigid water molecule with charges and Lennard-Jones parameters assigned to each of the 3 atoms. In LAMMPS the fix shake command can be used to hold the two O-H bonds and the H-O-H angle rigid. A bond style of *harmonic* and an angle style of *harmonic* or *charmm* should also be used.

These are the additional parameters (in real units) to set for O and H atoms and the water molecule to run a rigid TIP3P-CHARMM model with a cutoff. The K values can be used if a flexible TIP3P model (without fix shake) is desired. If the LJ epsilon and sigma for HH and OH are set to 0.0, it corresponds to the original 1983 TIP3P model (Jorgensen).

O mass = 15.9994
H mass = 1.008
O charge = -0.834
H charge = 0.417
LJ epsilon of OO = 0.1521
LJ sigma of OO = 3.1507
LJ epsilon of HH = 0.0460
LJ sigma of HH = 0.4000
LJ epsilon of OH = 0.0836
LJ sigma of OH = 1.7753
K of OH bond = 450
r0 of OH bond = 0.9572
K of HOH angle = 55
theta of HOH angle = 104.52

These are the parameters to use for TIP3P with a long-range Coulombic solver (e.g. Ewald or PPPM in LAMMPS), see (Price) for details:

O mass = 15.9994
H mass = 1.008
O charge = -0.830
H charge = 0.415
LJ epsilon of OO = 0.102
LJ sigma of OO = 3.188
LJ epsilon, sigma of OH, HH = 0.0
K of OH bond = 450
r0 of OH bond = 0.9572
K of HOH angle = 55
theta of HOH angle = 104.52

Wikipedia also has a nice article on water models.

6.8 TIP4P water model

The four-point TIP4P rigid water model extends the traditional three-point TIP3P model by adding an additional site, usually massless, where the charge associated with the oxygen atom is placed. This site M is located at a fixed distance away from the oxygen along the bisector of the HOH bond angle. A bond style of *harmonic* and an angle style of *harmonic* or *charmm* should also be used.

A TIP4P model is run with LAMMPS using either this command for a cutoff model:

pair_style lj/cut/tip4p/cut

or these two commands for a long-range model:

- pair_style lj/cut/tip4p/long
- kspace_style pppm/tip4p

For both models, the bond lengths and bond angles should be held fixed using the fix shake command.

These are the additional parameters (in real units) to set for O and H atoms and the water molecule to run a rigid TIP4P model with a cutoff (Jorgensen). Note that the OM distance is specified in the pair_style command, not as part of the pair coefficients.

O mass = 15.9994
H mass = 1.008
O charge = -1.040
H charge = 0.520
r0 of OH bond = 0.9572
theta of HOH angle = 104.52
OM distance = 0.15
LJ epsilon of O-O = 0.1550
LJ sigma of O-O = 3.1536
LJ epsilon, sigma of OH, HH = 0.0
Coulombic cutoff = 8.5

For the TIP4/Ice model (J Chem Phys, 122, 234511 (2005); http://dx.doi.org/10.1063/1.1931662) these values can be used:

O mass = 15.9994
H mass = 1.008
O charge = -1.1794
H charge = 0.5897
r0 of OH bond = 0.9572
theta of HOH angle = 104.52
OM distance = 0.1577
LJ epsilon of O-O = 0.21084
LJ sigma of O-O = 3.1668
LJ epsilon, sigma of OH, HH = 0.0
Coulombic cutoff = 8.5

For the TIP4P/2005 model (J Chem Phys, 123, 234505 (2005); http://dx.doi.org/10.1063/1.2121687), these values can be used:

O mass = 15.9994
H mass = 1.008
O charge = -1.1128
H charge = 0.5564
r0 of OH bond = 0.9572
theta of HOH angle = 104.52
OM distance = 0.1546
LJ epsilon of O-O = 0.1852
LJ sigma of O-O = 3.1589
LJ epsilon, sigma of OH, HH = 0.0
Coulombic cutoff = 8.5

These are the parameters to use for TIP4P with a long-range Coulombic solver (e.g. Ewald or PPPM in LAMMPS):

O mass = 15.9994
H mass = 1.008
O charge = -1.0484
H charge = 0.5242
r0 of OH bond = 0.9572
theta of HOH angle = 104.52
OM distance = 0.1250
LJ epsilon of O-O = 0.16275
LJ sigma of O-O = 3.16435
LJ epsilon, sigma of OH, HH = 0.0

Note that the when using the TIP4P pair style, the neighobr list cutoff for Coulomb interactions is effectively extended by a distance 2 * (OM distance), to account for the offset distance of the fictitious charges on O atoms in water molecules. Thus it is typically best in an efficiency sense to use a LJ cutoff >= Coulomb cutoff + 2*(OM distance), to shrink the size of the neighbor list. This leads to slightly larger cost for the long-range calculation, so you can test the trade-off for your model. The OM distance and the LJ and Coulombic cutoffs are set in the pair_style lj/cut/tip4p/long command.

Wikipedia also has a nice article on water models.

6.9 SPC water model

The SPC water model specifies a 3-site rigid water molecule with charges and Lennard-Jones parameters assigned to each of the 3 atoms. In LAMMPS the fix shake command can be used to hold the two O-H bonds and the H-O-H angle rigid. A bond style of *harmonic* and an angle style of *harmonic* or *charmm* should also be used.

These are the additional parameters (in real units) to set for O and H atoms and the water molecule to run a rigid SPC model.

O mass = 15.9994
H mass = 1.008
O charge = -0.820
H charge = 0.410
LJ epsilon of OO = 0.1553
LJ sigma of OO = 3.166
LJ epsilon, sigma of OH, HH = 0.0
r0 of OH bond = 1.0
theta of HOH angle = 109.47

Note that as originally proposed, the SPC model was run with a 9 Angstrom cutoff for both LJ and Coulommbic terms. It can also be used with long-range Coulombics (Ewald or PPPM in LAMMPS), without changing any of the parameters above, though it becomes a different model in that mode of usage.

The SPC/E (extended) water model is the same, except the partial charge assignemnts change:

O charge = -0.8476
H charge = 0.4238

See the (Berendsen) reference for more details on both the SPC and SPC/E models.

Wikipedia also has a nice article on water models.

6.10 Coupling LAMMPS to other codes

LAMMPS is designed to allow it to be coupled to other codes. For example, a quantum mechanics code might compute forces on a subset of atoms and pass those forces to LAMMPS. Or a continuum finite element (FE) simulation might use atom positions as boundary conditions on FE nodal points, compute a FE solution, and return interpolated forces on MD atoms.

LAMMPS can be coupled to other codes in at least 3 ways. Each has advantages and disadvantages, which you'll have to think about in the context of your application.

(1) Define a new fix command that calls the other code. In this scenario, LAMMPS is the driver code. During its timestepping, the fix is invoked, and can make library calls to the other code, which has been linked to LAMMPS as a library. This is the way the POEMS package that performs constrained rigid-body motion on groups of atoms is hooked to LAMMPS. See the fix_poems command for more details. See this section of the documentation for info on how to add a new fix to LAMMPS.

(2) Define a new LAMMPS command that calls the other code. This is conceptually similar to method (1), but in this case LAMMPS and the other code are on a more equal footing. Note that now the other code is not called during the timestepping of a LAMMPS run, but between runs. The LAMMPS input script can be used to alternate LAMMPS runs with calls to the other code, invoked via the new command. The run command facilitates this with its *every* option, which makes it easy to run a few steps, invoke the command, run a few steps, invoke the command, etc.

In this scenario, the other code can be called as a library, as in (1), or it could be a stand-alone code, invoked by a system() call made by the command (assuming your parallel machine allows one or more processors to start up another program). In the latter case the stand-alone code could communicate with LAMMPS thru files that the command writes and reads.

See Section_modify of the documentation for how to add a new command to LAMMPS.

(3) Use LAMMPS as a library called by another code. In this case the other code is the driver and calls LAMMPS as needed. Or a wrapper code could link and call both LAMMPS and another code as libraries. Again, the run command has options that allow it to be invoked with minimal overhead (no setup or clean-up) if you wish to do multiple short runs, driven by another program.

Examples of driver codes that call LAMMPS as a library are included in the examples/COUPLE directory of the LAMMPS distribution; see examples/COUPLE/README for more details:

- simple: simple driver programs in C++ and C which invoke LAMMPS as a library
- lammps_quest: coupling of LAMMPS and Quest, to run classical MD with quantum forces calculated by a density functional code
- lammps_spparks: coupling of LAMMPS and SPPARKS, to couple a kinetic Monte Carlo model for grain growth using MD to calculate strain induced across grain boundaries

This section of the documentation describes how to build LAMMPS as a library. Once this is done, you can interface with LAMMPS either via C++, C, Fortran, or Python (or any other language that supports a vanilla C-like interface). For example, from C++ you could create one (or more) "instances" of LAMMPS, pass it an input script to process, or execute individual commands, all by invoking the correct class methods in LAMMPS. From C or Fortran you can make function calls to do the same things. See Section_python of the manual for a description of the Python wrapper provided with LAMMPS that operates through the LAMMPS library interface.

The files src/library.cpp and library.h contain the C-style interface to LAMMPS. See Section_howto 19 of the manual for a description of the interface and how to extend it for your needs.

Note that the lammps_open() function that creates an instance of LAMMPS takes an MPI communicator as an argument. This means that instance of LAMMPS will run on the set of processors in the communicator. Thus the calling code can run LAMMPS on all or a subset of processors. For example, a wrapper script might decide to alternate between LAMMPS and another code, allowing them both to run on all the processors. Or it might allocate half the processors to LAMMPS and half to the other code and run both codes simultaneously before syncing them up periodically. Or it might instantiate multiple instances of LAMMPS to perform different calculations.

6.11 Visualizing LAMMPS snapshots

LAMMPS itself does not do visualization, but snapshots from LAMMPS simulations can be visualized (and analyzed) in a variety of ways.

LAMMPS snapshots are created by the dump command which can create files in several formats. The native LAMMPS dump format is a text file (see "dump atom" or "dump custom") which can be visualized by the xmovie program, included with the LAMMPS package. This produces simple, fast 2d projections of 3d systems, and can be useful for rapid debugging of simulation geometry and atom trajectories.

Several programs included with LAMMPS as auxiliary tools can convert native LAMMPS dump files to other formats. See the Section_tools doc page for details. The first is the ch2lmp tool, which contains a lammps2pdb Perl script which converts LAMMPS dump files into PDB files. The second is the lmp2arc tool which converts LAMMPS dump files into Accelrys' Insight MD program files. The third is the lmp2cfg tool which converts LAMMPS dump files into CFG files which can be read into the AtomEye visualizer.

A Python-based toolkit distributed by our group can read native LAMMPS dump files, including custom dump files with additional columns of user-specified atom information, and convert them to various formats or pipe them into visualization software directly. See the Pizza.py WWW site for details. Specifically, Pizza.py can convert LAMMPS dump files into PDB, XYZ, Ensight, and VTK formats. Pizza.py can pipe LAMMPS dump files directly into the Raster3d and RasMol visualization programs. Pizza.py has tools that do interactive 3d OpenGL visualization and one that creates SVG images of dump file snapshots.

LAMMPS can create XYZ files directly (via "dump xyz") which is a simple text-based file format used by many visualization programs including VMD.

LAMMPS can create DCD files directly (via "dump dcd") which can be read by VMD in conjunction with a CHARMM PSF file. Using this form of output avoids the need to convert LAMMPS snapshots to PDB files. See the dump command for more information on DCD files.

LAMMPS can create XTC files directly (via "dump xtc") which is GROMACS file format which can also be read by VMD for visualization. See the dump command for more information on XTC files.

6.12 Triclinic (non-orthogonal) simulation boxes

By default, LAMMPS uses an orthogonal simulation box to encompass the particles. The boundary command sets the boundary conditions of the box (periodic, non-periodic, etc). The orthogonal box has its "origin" at (xlo,ylo,zlo) and is defined by 3 edge vectors starting from the origin given by **a** = (xhi-xlo,0,0); **b** = (0,yhi-ylo,0); **c** = (0,0,zhi-zlo). The 6 parameters (xlo,xhi,ylo,yhi,zlo,zhi) are defined at the time the simulation box is created, e.g. by the create_box or read_data or read_restart commands. Additionally, LAMMPS defines box size parameters lx,ly,lz where lx = xhi-xlo, and similarly in the y and z dimensions. The 6 parameters, as well as lx,ly,lz, can be output via the thermo_style custom command.

LAMMPS also allows simulations to be performed in triclinic (non-orthogonal) simulation boxes shaped as a parallelepiped with triclinic symmetry. The parallelepiped has its "origin" at (xlo,ylo,zlo) and is defined by 3 edge vectors starting from the origin given by **a** = (xhi-xlo,0,0); **b** = (xy,yhi-ylo,0); **c** = (xz,yz,zhi-zlo). *xy,xz,yz* can be 0.0 or positive or negative values and are called "tilt factors" because they are the amount of displacement applied to faces of an originally orthogonal box to transform it into the parallelepiped. In LAMMPS the triclinic simulation box edge vectors **a**, **b**, and **c** cannot be arbitrary vectors. As indicated, **a** must lie on the positive x axis. **b** must lie in the xy plane, with strictly positive y component. **c** may have any orientation with strictly positive z component. The requirement that **a**, **b**, and **c** have strictly positive x, y, and z components, respectively, ensures that **a**, **b**, and **c** form a complete right-handed basis. These restrictions impose no loss of generality, since it is possible to rotate/invert any set of 3 crystal basis vectors so that they conform to the restrictions.

For example, assume that the 3 vectors **A**,**B**,**C** are the edge vectors of a general parallelepiped, where there is no restriction on **A**,**B**,**C** other than they form a complete right-handed basis i.e. **A** x **B** . **C** > 0. The equivalent

LAMMPS **a**,**b**,**c** are a linear rotation of **A**, **B**, and **C** and can be computed as follows:

$$
\begin{aligned}
(\mathbf{a} \quad \mathbf{b} \quad \mathbf{c}) &= \begin{pmatrix} a_x & b_x & c_x \\ 0 & b_y & c_y \\ 0 & 0 & c_z \end{pmatrix} \\
a_x &= A \\
b_x &= \mathbf{B} \cdot \hat{\mathbf{A}} = B \cos\gamma \\
b_y &= |\hat{\mathbf{A}} \times \mathbf{B}| = B \sin\gamma = \sqrt{B^2 - {b_x}^2} \\
c_x &= \mathbf{C} \cdot \hat{\mathbf{A}} = C \cos\beta \\
c_y &= \mathbf{C} \cdot \widehat{(\mathbf{A} \times \mathbf{B})} \times \hat{\mathbf{A}} = \frac{\mathbf{B} \cdot \mathbf{C} - b_x c_x}{b_y} \\
c_z &= |\mathbf{C} \cdot \widehat{(\mathbf{A} \times \mathbf{B})}| = \sqrt{C^2 - {c_x}^2 - {c_y}^2}
\end{aligned}
$$

where A = |**A**| indicates the scalar length of **A**. The ^ hat symbol indicates the corresponding unit vector. *beta* and *gamma* are angles between the vectors described below. Note that by construction, **a**, **b**, and **c** have strictly positive x, y, and z components, respectively. If it should happen that **A**, **B**, and **C** form a left-handed basis, then the above equations are not valid for **c**. In this case, it is necessary to first apply an inversion. This can be achieved by interchanging two basis vectors or by changing the sign of one of them.

For consistency, the same rotation/inversion applied to the basis vectors must also be applied to atom positions, velocities, and any other vector quantities. This can be conveniently achieved by first converting to fractional coordinates in the old basis and then converting to distance coordinates in the new basis. The transformation is given by the following equation:

$$
\mathbf{x} = (\mathbf{a} \quad \mathbf{b} \quad \mathbf{c}) \cdot \frac{1}{V} \begin{pmatrix} \mathbf{B} \times \mathbf{C} \\ \mathbf{C} \times \mathbf{A} \\ \mathbf{A} \times \mathbf{B} \end{pmatrix} \cdot \mathbf{X}
$$

where *V* is the volume of the box, **X** is the original vector quantity and **x** is the vector in the LAMMPS basis.

There is no requirement that a triclinic box be periodic in any dimension, though it typically should be in at least the 2nd dimension of the tilt (y in xy) if you want to enforce a shift in periodic boundary conditions across that boundary. Some commands that work with triclinic boxes, e.g. the fix deform and fix npt commands, require periodicity or non-shrink-wrap boundary conditions in specific dimensions. See the command doc pages for details.

The 9 parameters (xlo,xhi,ylo,yhi,zlo,zhi,xy,xz,yz) are defined at the time the simluation box is created. This happens in one of 3 ways. If the create_box command is used with a region of style *prism*, then a triclinic box is setup. See the region command for details. If the read_data command is used to define the simulation box, and the header of the data file contains a line with the "xy xz yz" keyword, then a triclinic box is setup. See the read_data command for details. Finally, if the read_restart command reads a restart file which was written from a simulation using a triclinic box, then a triclinic box will be setup for the restarted simulation.

Note that you can define a triclinic box with all 3 tilt factors = 0.0, so that it is initially orthogonal. This is necessary if the box will become non-orthogonal, e.g. due to the fix npt or fix deform commands. Alternatively, you can use the change_box command to convert a simulation box from orthogonal to triclinic and vice versa.

As with orthogonal boxes, LAMMPS defines triclinic box size parameters lx,ly,lz where lx = xhi-xlo, and similarly in the y and z dimensions. The 9 parameters, as well as lx,ly,lz, can be output via the thermo_style custom command.

To avoid extremely tilted boxes (which would be computationally inefficient), LAMMPS normally requires that no tilt factor can skew the box more than half the distance of the parallel box length, which is the 1st dimension in the tilt factor (x for xz). This is required both when the simulation box is created, e.g. via the create_box or read_data commands, as well as when the box shape changes dynamically during a simulation, e.g. via the fix deform or fix npt commands.

For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = ..., -15, -5, 5, 15, 25, ... are geometrically all equivalent. If the box tilt exceeds this limit during a dynamics run (e.g. via the fix deform command), then the box is "flipped" to an equivalent shape with a tilt factor within the bounds, so the run can continue. See the fix deform doc page for further details.

One exception to this rule is if the 1st dimension in the tilt factor (x for xy) is non-periodic. In that case, the limits on the tilt factor are not enforced, since flipping the box in that dimension does not change the atom positions due to non-periodicity. In this mode, if you tilt the system to extreme angles, the simulation will simply become inefficient, due to the highly skewed simulation box.

The limitation on not creating a simulation box with a tilt factor skewing the box more than half the distance of the parallel box length can be overridden via the box command. Setting the *tilt* keyword to *large* allows any tilt factors to be specified.

Box flips that may occur using the fix deform or fix npt commands can be turned off using the *flip no* option with either of the commands.

Note that if a simulation box has a large tilt factor, LAMMPS will run less efficiently, due to the large volume of communication needed to acquire ghost atoms around a processor's irregular-shaped sub-domain. For extreme values of tilt, LAMMPS may also lose atoms and generate an error.

Triclinic crystal structures are often defined using three lattice constants *a*, *b*, and *c*, and three angles *alpha*, *beta* and *gamma*. Note that in this nomenclature, the a, b, and c lattice constants are the scalar lengths of the edge

vectors **a**, **b**, and **c** defined above. The relationship between these 6 quantities (a,b,c,alpha,beta,gamma) and the LAMMPS box sizes (lx,ly,lz) = (xhi-xlo,yhi-ylo,zhi-zlo) and tilt factors (xy,xz,yz) is as follows:

$$
\begin{aligned}
a &= \mathrm{lx} \\
b^2 &= \mathrm{ly}^2 + \mathrm{xy}^2 \\
c^2 &= \mathrm{lz}^2 + \mathrm{xz}^2 + \mathrm{yz}^2 \\
\cos\alpha &= \frac{\mathrm{xy} * \mathrm{xz} + \mathrm{ly} * \mathrm{yz}}{b * c} \\
\cos\beta &= \frac{\mathrm{xz}}{c} \\
\cos\gamma &= \frac{\mathrm{xy}}{b}
\end{aligned}
$$

The inverse relationship can be written as follows:

$$
\begin{aligned}
\mathrm{lx} &= a \\
\mathrm{xy} &= b\cos\gamma \\
\mathrm{xz} &= c\cos\beta \\
\mathrm{ly}^2 &= b^2 - \mathrm{xy}^2 \\
\mathrm{yz} &= \frac{b * c\cos\alpha - \mathrm{xy} * \mathrm{xz}}{\mathrm{ly}} \\
\mathrm{lz}^2 &= c^2 - \mathrm{xz}^2 - \mathrm{yz}^2
\end{aligned}
$$

The values of *a*, *b*, *c* , *alpha*, *beta* , and *gamma* can be printed out or accessed by computes using the thermo_style custom keywords *cella*, *cellb*, *cellc*, *cellalpha*, *cellbeta*, *cellgamma*, respectively.

As discussed on the dump command doc page, when the BOX BOUNDS for a snapshot is written to a dump file for a triclinic box, an orthogonal bounding box which encloses the triclinic simulation box is output, along with the 3 tilt factors (xy, xz, yz) of the triclinic box, formatted as follows:

```
ITEM: BOX BOUNDS xy xz yz
xlo_bound xhi_bound xy
ylo_bound yhi_bound xz
zlo_bound zhi_bound yz
```

This bounding box is convenient for many visualization programs and is calculated from the 9 triclinic box parameters (xlo,xhi,ylo,yhi,zlo,zhi,xy,xz,yz) as follows:

```
xlo_bound = xlo + MIN(0.0,xy,xz,xy+xz)
xhi_bound = xhi + MAX(0.0,xy,xz,xy+xz)
ylo_bound = ylo + MIN(0.0,yz)
yhi_bound = yhi + MAX(0.0,yz)
zlo_bound = zlo
zhi_bound = zhi
```

These formulas can be inverted if you need to convert the bounding box back into the triclinic box parameters, e.g. xlo = xlo_bound - MIN(0.0,xy,xz,xy+xz).

One use of triclinic simulation boxes is to model solid-state crystals with triclinic symmetry. The lattice command can be used with non-orthogonal basis vectors to define a lattice that will tile a triclinic simulation box via the create_atoms command.

A second use is to run Parinello-Rahman dyanamics via the fix npt command, which will adjust the xy, xz, yz tilt factors to compensate for off-diagonal components of the pressure tensor. The analalog for an energy minimization is the fix box/relax command.

A third use is to shear a bulk solid to study the response of the material. The fix deform command can be used for this purpose. It allows dynamic control of the xy, xz, yz tilt factors as a simulation runs. This is discussed in the next section on non-equilibrium MD (NEMD) simulations.

6.13 NEMD simulations

Non-equilibrium molecular dynamics or NEMD simulations are typically used to measure a fluid's rheological properties such as viscosity. In LAMMPS, such simulations can be performed by first setting up a non-orthogonal simulation box (see the preceding Howto section).

A shear strain can be applied to the simulation box at a desired strain rate by using the fix deform command. The fix nvt/sllod command can be used to thermostat the sheared fluid and integrate the SLLOD equations of motion for the system. Fix nvt/sllod uses compute temp/deform to compute a thermal temperature by subtracting out the streaming velocity of the shearing atoms. The velocity profile or other properties of the fluid can be monitored via the fix ave/spatial command.

As discussed in the previous section on non-orthogonal simulation boxes, the amount of tilt or skew that can be applied is limited by LAMMPS for computational efficiency to be 1/2 of the parallel box length. However, fix deform can continuously strain a box by an arbitrary amount. As discussed in the fix deform command, when the tilt value reaches a limit, the box is flipped to the opposite limit which is an equivalent tiling of periodic space. The strain rate can then continue to change as before. In a long NEMD simulation these box re-shaping events may occur many times.

In a NEMD simulation, the "remap" option of fix deform should be set to "remap v", since that is what fix nvt/sllod assumes to generate a velocity profile consistent with the applied shear strain rate.

An alternative method for calculating viscosities is provided via the fix viscosity command.

6.14 Finite-size spherical and aspherical particles

Typical MD models treat atoms or particles as point masses. Sometimes it is desirable to have a model with finite-size particles such as spheroids or ellipsoids or generalized aspherical bodies. The difference is that such particles have a moment of inertia, rotational energy, and angular momentum. Rotation is induced by torque

coming from interactions with other particles.

LAMMPS has several options for running simulations with these kinds of particles. The following aspects are discussed in turn:

- atom styles
- pair potentials
- time integration
- computes, thermodynamics, and dump output
- rigid bodies composed of finite-size particles

Example input scripts for these kinds of models are in the body, colloid, dipole, ellipse, line, peri, pour, and tri directories of the examples directory in the LAMMPS distribution.

Atom styles

There are several atom styles that allow for definition of finite-size particles: sphere, dipole, ellipsoid, line, tri, peri, and body.

The sphere style defines particles that are spheriods and each particle can have a unique diameter and mass (or density). These particles store an angular velocity (omega) and can be acted upon by torque. The "set" command can be used to modify the diameter and mass of individual particles, after then are created.

The dipole style does not actually define finite-size particles, but is often used in conjunction with spherical particles, via a command like

```
atom_style hybrid sphere dipole
```

This is because when dipoles interact with each other, they induce torques, and a particle must be finite-size (i.e. have a moment of inertia) in order to respond and rotate. See the atom_style dipole command for details. The "set" command can be used to modify the orientation and length of the dipole moment of individual particles, after then are created.

The ellipsoid style defines particles that are ellipsoids and thus can be aspherical. Each particle has a shape, specified by 3 diameters, and mass (or density). These particles store an angular momentum and their orientation (quaternion), and can be acted upon by torque. They do not store an angular velocity (omega), which can be in a different direction than angular momentum, rather they compute it as needed. The "set" command can be used to modify the diameter, orientation, and mass of individual particles, after then are created. It also has a brief explanation of what quaternions are.

The line style defines line segment particles with two end points and a mass (or density). They can be used in 2d simulations, and they can be joined together to form rigid bodies which represent arbitrary polygons.

The tri style defines triangular particles with three corner points and a mass (or density). They can be used in 3d simulations, and they can be joined together to form rigid bodies which represent arbitrary particles with a triangulated surface.

The peri style is used with Peridynamic models and defines particles as having a volume, that is used internally in the pair_style peri potentials.

The body style allows for definition of particles which can represent complex entities, such as surface meshes of discrete points, collections of sub-particles, deformable objects, etc. The body style is discussed in more detail on the body doc page.

Note that if one of these atom styles is used (or multiple styles via the atom_style hybrid command), not all particles in the system are required to be finite-size or aspherical.

For example, in the ellipsoid style, if the 3 shape parameters are set to the same value, the particle will be a sphere rather than an ellipsoid. If the 3 shape parameters are all set to 0.0 or if the diameter is set to 0.0, it will be a point particle. In the line or tri style, if the lineflag or triflag is specified as 0, then it will be a point particle.

Some of the pair styles used to compute pairwise interactions between finite-size particles also compute the correct interaction with point particles as well, e.g. the interaction between a point particle and a finite-size particle or between two point particles. If necessary, pair_style hybrid can be used to insure the correct interactions are computed for the appropriate style of interactions. Likewise, using groups to partition particles (ellipsoids versus spheres versus point particles) will allow you to use the appropriate time integrators and temperature computations for each class of particles. See the doc pages for various commands for details.

Also note that for 2d simulations, atom styles sphere and ellipsoid still use 3d particles, rather than as circular disks or ellipses. This means they have the same moment of inertia as the 3d object. When temperature is computed, the correct degrees of freedom are used for rotation in a 2d versus 3d system.

Pair potentials

When a system with finite-size particles is defined, the particles will only rotate and experience torque if the force field computes such interactions. These are the various pair styles that generate torque:

- pair_style gran/history
- pair_style gran/hertzian
- pair_style gran/no_history
- pair_style dipole/cut
- pair_style gayberne
- pair_style resquared
- pair_style brownian
- pair_style lubricate
- pair_style line/lj
- pair_style tri/lj
- pair_style body

The granular pair styles are used with spherical particles. The dipole pair style is used with the dipole atom style, which could be applied to spherical or ellipsoidal particles. The GayBerne and REsquared potentials require ellipsoidal particles, though they will also work if the 3 shape parameters are the same (a sphere). The Brownian and lubrication potentials are used with spherical particles. The line, tri, and body potentials are used with line segment, triangular, and body particles respectively.

Time integration

There are several fixes that perform time integration on finite-size spherical particles, meaning the integrators update the rotational orientation and angular velocity or angular momentum of the particles:

- fix nve/sphere
- fix nvt/sphere
- fix npt/sphere

Likewise, there are 3 fixes that perform time integration on ellipsoidal particles:

- fix nve/asphere

- fix nvt/asphere
- fix npt/asphere

The advantage of these fixes is that those which thermostat the particles include the rotational degrees of freedom in the temperature calculation and thermostatting. The fix langevin command can also be used with its *omgea* or *angmom* options to thermostat the rotational degrees of freedom for spherical or ellipsoidal particles. Other thermostatting fixes only operate on the translational kinetic energy of finite-size particles.

These fixes perform constant NVE time integration on line segment, triangular, and body particles:

- fix nve/line
- fix nve/tri
- fix nve/body

Note that for mixtures of point and finite-size particles, these integration fixes can only be used with groups which contain finite-size particles.

Computes, thermodynamics, and dump output

There are several computes that calculate the temperature or rotational energy of spherical or ellipsoidal particles:

- compute temp/sphere
- compute temp/asphere
- compute erotate/sphere
- compute erotate/asphere

These include rotational degrees of freedom in their computation. If you wish the thermodynamic output of temperature or pressure to use one of these computes (e.g. for a system entirely composed of finite-size particles), then the compute can be defined and the thermo_modify command used. Note that by default thermodynamic quantities will be calculated with a temperature that only includes translational degrees of freedom. See the thermo_style command for details.

These commands can be used to output various attributes of finite-size particles:

- dump custom
- compute property/atom
- dump local
- compute body/local

Attributes include the dipole moment, the angular velocity, the angular momentum, the quaternion, the torque, the end-point and corner-point coordinates (for line and tri particles), and sub-particle attributes of body particles.

Rigid bodies composed of finite-size particles

The fix rigid command treats a collection of particles as a rigid body, computes its inertia tensor, sums the total force and torque on the rigid body each timestep due to forces on its constituent particles, and integrates the motion of the rigid body.

If any of the constituent particles of a rigid body are finite-size particles (spheres or ellipsoids or line segments or triangles), then their contribution to the inertia tensor of the body is different than if they were point particles. This means the rotational dynamics of the rigid body will be different. Thus a model of a dimer is different if the dimer consists of two point masses versus two spheroids, even if the two particles have the same mass. Finite-size particles that experience torque due to their interaction with other particles will also impart that torque to a rigid

body they are part of.

See the "fix rigid" command for example of complex rigid-body models it is possible to define in LAMMPS.

Note that the fix shake command can also be used to treat 2, 3, or 4 particles as a rigid body, but it always assumes the particles are point masses.

Also note that body particles cannot be modeled with the fix rigid command. Body particles are treated by LAMMPS as single particles, though they can store internal state, such as a list of sub-particles. Individual body partices are typically treated as rigid bodies, and their motion integrated with a command like fix nve/body. Interactions between pairs of body particles are computed via a command like pair_style body.

6.15 Output from LAMMPS (thermo, dumps, computes, fixes, variables)

There are four basic kinds of LAMMPS output:

- Thermodynamic output, which is a list of quantities printed every few timesteps to the screen and logfile.
- Dump files, which contain snapshots of atoms and various per-atom values and are written at a specified frequency.
- Certain fixes can output user-specified quantities to files: fix ave/time for time averaging, fix ave/spatial for spatial averaging, and fix print for single-line output of variables. Fix print can also output to the screen.
- Restart files.

A simulation prints one set of thermodynamic output and (optionally) restart files. It can generate any number of dump files and fix output files, depending on what dump and fix commands you specify.

As discussed below, LAMMPS gives you a variety of ways to determine what quantities are computed and printed when the thermodynamics, dump, or fix commands listed above perform output. Throughout this discussion, note that users can also add their own computes and fixes to LAMMPS which can then generate values that can then be output with these commands.

The following sub-sections discuss different LAMMPS command related to output and the kind of data they operate on and produce:

- Global/per-atom/local data
- Scalar/vector/array data
- Thermodynamic output
- Dump file output
- Fixes that write output files
- Computes that process output quantities
- Fixes that process output quantities
- Computes that generate values to output
- Fixes that generate values to output
- Variables that generate values to output
- Summary table of output options and data flow between commands

Global/per-atom/local data

Various output-related commands work with three different styles of data: global, per-atom, or local. A global datum is one or more system-wide values, e.g. the temperature of the system. A per-atom datum is one or more

values per atom, e.g. the kinetic energy of each atom. Local datums are calculated by each processor based on the atoms it owns, but there may be zero or more per atom, e.g. a list of bond distances.

Scalar/vector/array data

Global, per-atom, and local datums can each come in three kinds: a single scalar value, a vector of values, or a 2d array of values. The doc page for a "compute" or "fix" or "variable" that generates data will specify both the style and kind of data it produces, e.g. a per-atom vector.

When a quantity is accessed, as in many of the output commands discussed below, it can be referenced via the following bracket notation, where ID in this case is the ID of a compute. The leading "c_" would be replaced by "f_" for a fix, or "v_" for a variable:

c_ID	entire scalar, vector, or array
c_ID[I]	one element of vector, one column of array
c_ID[I][J]	one element of array

In other words, using one bracket reduces the dimension of the data once (vector -> scalar, array -> vector). Using two brackets reduces the dimension twice (array -> scalar). Thus a command that uses scalar values as input can typically also process elements of a vector or array.

Thermodynamic output

The frequency and format of thermodynamic output is set by the thermo, thermo_style, and thermo_modify commands. The thermo_style command also specifies what values are calculated and written out. Pre-defined keywords can be specified (e.g. press, etotal, etc). Three additional kinds of keywords can also be specified (c_ID, f_ID, v_name), where a compute or fix or variable provides the value to be output. In each case, the compute, fix, or variable must generate global values for input to the thermo_style custom command.

Note that thermodynamic output values can be "extensive" or "intensive". The former scale with the number of atoms in the system (e.g. total energy), the latter do not (e.g. temperature). The setting for thermo_modify norm determines whether extensive quantities are normalized or not. Computes and fixes produce either extensive or intensive values; see their individual doc pages for details. Equal-style variables produce only intensive values; you can include a division by "natoms" in the formula if desired, to make an extensive calculation produce an intensive result.

Dump file output

Dump file output is specified by the dump and dump_modify commands. There are several pre-defined formats (dump atom, dump xtc, etc).

There is also a dump custom format where the user specifies what values are output with each atom. Pre-defined atom attributes can be specified (id, x, fx, etc). Three additional kinds of keywords can also be specified (c_ID, f_ID, v_name), where a compute or fix or variable provides the values to be output. In each case, the compute, fix, or variable must generate per-atom values for input to the dump custom command.

There is also a dump local format where the user specifies what local values to output. A pre-defined index keyword can be specified to enumuerate the local values. Two additional kinds of keywords can also be specified (c_ID, f_ID), where a compute or fix or variable provides the values to be output. In each case, the compute or fix must generate local values for input to the dump local command.

Fixes that write output files

Several fixes take various quantities as input and can write output files: fix ave/time, fix ave/spatial, fix ave/histo, fix ave/correlate, and fix print.

The fix ave/time command enables direct output to a file and/or time-averaging of global scalars or vectors. The user specifies one or more quantities as input. These can be global compute values, global fix values, or variables of any style except the atom style which produces per-atom values. Since a variable can refer to keywords used by the thermo_style custom command (like temp or press) and individual per-atom values, a wide variety of quantities can be time averaged and/or output in this way. If the inputs are one or more scalar values, then the fix generate a global scalar or vector of output. If the inputs are one or more vector values, then the fix generates a global vector or array of output. The time-averaged output of this fix can also be used as input to other output commands.

The fix ave/spatial command enables direct output to a file of spatial-averaged per-atom quantities like those output in dump files, within 1d layers of the simulation box. The per-atom quantities can be atom density (mass or number) or atom attributes such as position, velocity, force. They can also be per-atom quantities calculated by a compute, by a fix, or by an atom-style variable. The spatial-averaged output of this fix can also be used as input to other output commands.

The fix ave/histo command enables direct output to a file of histogrammed quantities, which can be global or per-atom or local quantities. The histogram output of this fix can also be used as input to other output commands.

The fix ave/correlate command enables direct output to a file of time-correlated quantities, which can be global scalars. The correlation matrix output of this fix can also be used as input to other output commands.

The fix print command can generate a line of output written to the screen and log file or to a separate file, periodically during a running simulation. The line can contain one or more variable values for any style variable except the atom style). As explained above, variables themselves can contain references to global values generated by thermodynamic keywords, computes, fixes, or other variables, or to per-atom values for a specific atom. Thus the fix print command is a means to output a wide variety of quantities separate from normal thermodynamic or dump file output.

Computes that process output quantities

The compute reduce and compute reduce/region commands take one or more per-atom or local vector quantities as inputs and "reduce" them (sum, min, max, ave) to scalar quantities. These are produced as output values which can be used as input to other output commands.

The compute slice command take one or more global vector or array quantities as inputs and extracts a subset of their values to create a new vector or array. These are produced as output values which can be used as input to other output commands.

The compute property/atom command takes a list of one or more pre-defined atom attributes (id, x, fx, etc) and stores the values in a per-atom vector or array. These are produced as output values which can be used as input to other output commands. The list of atom attributes is the same as for the dump custom command.

The compute property/local command takes a list of one or more pre-defined local attributes (bond info, angle info, etc) and stores the values in a local vector or array. These are produced as output values which can be used as input to other output commands.

Fixes that process output quantities

The fix vector command can create global vectors as output from global scalars as input, accumulating them one element at a time.

The fix ave/atom command performs time-averaging of per-atom vectors. The per-atom quantities can be atom attributes such as position, velocity, force. They can also be per-atom quantities calculated by a compute, by a fix, or by an atom-style variable. The time-averaged per-atom output of this fix can be used as input to other output commands.

The fix store/state command can archive one or more per-atom attributes at a particular time, so that the old values can be used in a future calculation or output. The list of atom attributes is the same as for the dump custom command, including per-atom quantities calculated by a compute, by a fix, or by an atom-style variable. The output of this fix can be used as input to other output commands.

Computes that generate values to output

Every compute in LAMMPS produces either global or per-atom or local values. The values can be scalars or vectors or arrays of data. These values can be output using the other commands described in this section. The doc page for each compute command describes what it produces. Computes that produce per-atom or local values have the word "atom" or "local" in their style name. Computes without the word "atom" or "local" produce global values.

Fixes that generate values to output

Some fixes in LAMMPS produces either global or per-atom or local values which can be accessed by other commands. The values can be scalars or vectors or arrays of data. These values can be output using the other commands described in this section. The doc page for each fix command tells whether it produces any output quantities and describes them.

Variables that generate values to output

Every variables defined in an input script generates either a global scalar value or a per-atom vector (only atom-style variables) when it is accessed. The formulas used to define equal- and atom-style variables can contain references to the thermodynamic keywords and to global and per-atom data generated by computes, fixes, and other variables. The values generated by variables can be output using the other commands described in this section.

Summary table of output options and data flow between commands

This table summarizes the various commands that can be used for generating output from LAMMPS. Each command produces output data of some kind and/or writes data to a file. Most of the commands can take data from other commands as input. Thus you can link many of these commands together in pipeline form, where data produced by one command is used as input to another command and eventually written to the screen or to a file. Note that to hook two commands together the output and input data types must match, e.g. global/per-atom/local data and scalar/vector/array data.

Also note that, as described above, when a command takes a scalar as input, that could be an element of a vector or array. Likewise a vector input could be a column of an array.

Command	Input	Output
thermo_style custom	global scalars	screen, log file
dump custom	per-atom vectors	dump file

dump local	local vectors	dump file
fix print	global scalar from variable	screen, file
print	global scalar from variable	screen
computes	N/A	global/per-atom/local scalar/vector/array
fixes	N/A	global/per-atom/local scalar/vector/array
variables	global scalars, per-atom vectors	global scalar, per-atom vector
compute reduce	per-atom/local vectors	global scalar/vector
compute slice	global vectors/arrays	global vector/array
compute property/atom	per-atom vectors	per-atom vector/array
compute property/local	local vectors	local vector/array
fix vector	global scalars	global vector
fix ave/atom	per-atom vectors	per-atom vector/array
fix ave/time	global scalars/vectors	global scalar/vector/array, file
fix ave/spatial	per-atom vectors	global array, file
fix ave/histo	global/per-atom/local scalars and vectors	global array, file
fix ave/correlate	global scalars	global array, file
fix store/state	per-atom vectors	per-atom vector/array

6.16 Thermostatting, barostatting, and computing temperature

Thermostatting means controlling the temperature of particles in an MD simulation. Barostatting means controlling the pressure. Since the pressure includes a kinetic component due to particle velocities, both these operations require calculation of the temperature. Typically a target temperature (T) and/or pressure (P) is specified by the user, and the thermostat or barostat attempts to equilibrate the system to the requested T and/or P.

Temperature is computed as kinetic energy divided by some number of degrees of freedom (and the Boltzmann constant). Since kinetic energy is a function of particle velocity, there is often a need to distinguish between a particle's advection velocity (due to some aggregate motiion of particles) and its thermal velocity. The sum of the two is the particle's total velocity, but the latter is often what is wanted to compute a temperature.

LAMMPS has several options for computing temperatures, any of which can be used in thermostatting and barostatting. These compute commands calculate temperature, and the compute pressure command calculates pressure.

- compute temp
- compute temp/sphere
- compute temp/asphere
- compute temp/com
- compute temp/deform
- compute temp/partial
- compute temp/profile
- compute temp/ramp
- compute temp/region

All but the first 3 calculate velocity biases directly (e.g. advection velocities) that are removed when computing the thermal temperature. Compute temp/sphere and compute temp/asphere compute kinetic energy for finite-size particles that includes rotational degrees of freedom. They both allow for velocity biases indirectly, via an

optional extra argument, another temperature compute that subtracts a velocity bias. This allows the translational velocity of spherical or aspherical particles to be adjusted in prescribed ways.

Thermostatting in LAMMPS is performed by fixes, or in one case by a pair style. Several thermostatting fixes are available: Nose-Hoover (nvt), Berendsen, CSVR, Langevin, and direct rescaling (temp/rescale). Dissipative particle dynamics (DPD) thermostatting can be invoked via the *dpd/tstat* pair style:

- fix nvt
- fix nvt/sphere
- fix nvt/asphere
- fix nvt/sllod
- fix temp/berendsen
- fix temp/csvr
- fix langevin
- fix temp/rescale
- pair_style dpd/tstat

Fix nvt only thermostats the translational velocity of particles. Fix nvt/sllod also does this, except that it subtracts out a velocity bias due to a deforming box and integrates the SLLOD equations of motion. See the NEMD simulations section of this page for further details. Fix nvt/sphere and fix nvt/asphere thermostat not only translation velocities but also rotational velocities for spherical and aspherical particles.

DPD thermostatting alters pairwise interactions in a manner analagous to the per-particle thermostatting of fix langevin.

Any of the thermostatting fixes can use temperature computes that remove bias which has two effects. First, the current calculated temperature, which is compared to the requested target temperature, is caluclated with the velocity bias removed. Second, the thermostat adjusts only the thermal temperature component of the particle's velocities, which are the velocities with the bias removed. The removed bias is then added back to the adjusted velocities. See the doc pages for the individual fixes and for the fix_modify command for instructions on how to assign a temperature compute to a thermostatting fix. For example, you can apply a thermostat to only the x and z components of velocity by using it in conjunction with compute temp/partial. Of you could thermostat only the thermal temperature of a streaming flow of particles without affecting the streaming velocity, by using compute temp/profile.

NOTE: Only the nvt fixes perform time integration, meaning they update the velocities and positions of particles due to forces and velocities respectively. The other thermostat fixes only adjust velocities; they do NOT perform time integration updates. Thus they should be used in conjunction with a constant NVE integration fix such as these:

- fix nve
- fix nve/sphere
- fix nve/asphere

Barostatting in LAMMPS is also performed by fixes. Two barosttating methods are currently available: Nose-Hoover (npt and nph) and Berendsen:

- fix npt
- fix npt/sphere
- fix npt/asphere
- fix nph
- fix press/berendsen

The fix npt commands include a Nose-Hoover thermostat and barostat. Fix nph is just a Nose/Hoover barostat; it does no thermostatting. Both fix nph and fix press/bernendsen can be used in conjunction with any of the thermostatting fixes.

As with the thermostats, fix npt and fix nph only use translational motion of the particles in computing T and P and performing thermo/barostatting. Fix npt/sphere and fix npt/asphere thermo/barostat using not only translation velocities but also rotational velocities for spherical and aspherical particles.

All of the barostatting fixes use the compute pressure compute to calculate a current pressure. By default, this compute is created with a simple compute temp (see the last argument of the compute pressure command), which is used to calculated the kinetic componenet of the pressure. The barostatting fixes can also use temperature computes that remove bias for the purpose of computing the kinetic componenet which contributes to the current pressure. See the doc pages for the individual fixes and for the fix_modify command for instructions on how to assign a temperature or pressure compute to a barostatting fix.

NOTE: As with the thermostats, the Nose/Hoover methods (fix npt and fix nph) perform time integration. Fix press/berendsen does NOT, so it should be used with one of the constant NVE fixes or with one of the NVT fixes.

Finally, thermodynamic output, which can be setup via the thermo_style command, often includes temperature and pressure values. As explained on the doc page for the thermo_style command, the default T and P are setup by the thermo command itself. They are NOT the ones associated with any thermostatting or barostatting fix you have defined or with any compute that calculates a temperature or pressure. Thus if you want to view these values of T and P, you need to specify them explicitly via a thermo_style custom command. Or you can use the thermo_modify command to re-define what temperature or pressure compute is used for default thermodynamic output.

6.17 Walls

Walls in an MD simulation are typically used to bound particle motion, i.e. to serve as a boundary condition.

Walls in LAMMPS can be of rough (made of particles) or idealized surfaces. Ideal walls can be smooth, generating forces only in the normal direction, or frictional, generating forces also in the tangential direction.

Rough walls, built of particles, can be created in various ways. The particles themselves can be generated like any other particle, via the lattice and create_atoms commands, or read in via the read_data command.

Their motion can be constrained by many different commands, so that they do not move at all, move together as a group at constant velocity or in response to a net force acting on them, move in a prescribed fashion (e.g. rotate around a point), etc. Note that if a time integration fix like fix nve or fix nvt is not used with the group that contains wall particles, their positions and velocities will not be updated.

- fix aveforce - set force on particles to average value, so they move together
- fix setforce - set force on particles to a value, e.g. 0.0
- fix freeze - freeze particles for use as granular walls
- fix nve/noforce - advect particles by their velocity, but without force
- fix move - prescribe motion of particles by a linear velocity, oscillation, rotation, variable

The fix move command offers the most generality, since the motion of individual particles can be specified with variable formula which depends on time and/or the particle position.

For rough walls, it may be useful to turn off pairwise interactions between wall particles via the neigh_modify exclude command.

Rough walls can also be created by specifying frozen particles that do not move and do not interact with mobile particles, and then tethering other particles to the fixed particles, via a bond. The bonded particles do interact with other mobile particles.

Idealized walls can be specified via several fix commands. Fix wall/gran creates frictional walls for use with granular particles; all the other commands create smooth walls.

- fix wall/reflect - reflective flat walls
- fix wall/lj93 - flat walls, with Lennard-Jones 9/3 potential
- fix wall/lj126 - flat walls, with Lennard-Jones 12/6 potential
- fix wall/colloid - flat walls, with pair_style colloid potential
- fix wall/harmonic - flat walls, with repulsive harmonic spring potential
- fix wall/region - use region surface as wall
- fix wall/gran - flat or curved walls with pair_style granular potential

The *lj93*, *lj126*, *colloid*, and *harmonic* styles all allow the flat walls to move with a constant velocity, or oscillate in time. The fix wall/region command offers the most generality, since the region surface is treated as a wall, and the geometry of the region can be a simple primitive volume (e.g. a sphere, or cube, or plane), or a complex volume made from the union and intersection of primitive volumes. Regions can also specify a volume "interior" or "exterior" to the specified primitive shape or *union* or *intersection*. Regions can also be "dynamic" meaning they move with constant velocity, oscillate, or rotate.

The only frictional idealized walls currently in LAMMPS are flat or curved surfaces specified by the fix wall/gran command. At some point we plan to allow regoin surfaces to be used as frictional walls, as well as triangulated surfaces.

6.18 Elastic constants

Elastic constants characterize the stiffness of a material. The formal definition is provided by the linear relation that holds between the stress and strain tensors in the limit of infinitesimal deformation. In tensor notation, this is expressed as s_ij = C_ijkl * e_kl, where the repeated indices imply summation. s_ij are the elements of the symmetric stress tensor. e_kl are the elements of the symmetric strain tensor. C_ijkl are the elements of the fourth rank tensor of elastic constants. In three dimensions, this tensor has 3^4=81 elements. Using Voigt notation, the tensor can be written as a 6x6 matrix, where C_ij is now the derivative of s_i w.r.t. e_j. Because s_i is itself a derivative w.r.t. e_i, it follows that C_ij is also symmetric, with at most 7*6/2 = 21 distinct elements.

At zero temperature, it is easy to estimate these derivatives by deforming the simulation box in one of the six directions using the change_box command and measuring the change in the stress tensor. A general-purpose script that does this is given in the examples/elastic directory described in this section.

Calculating elastic constants at finite temperature is more challenging, because it is necessary to run a simulation that perfoms time averages of differential properties. One way to do this is to measure the change in average stress tensor in an NVT simulations when the cell volume undergoes a finite deformation. In order to balance the systematic and statistical errors in this method, the magnitude of the deformation must be chosen judiciously, and care must be taken to fully equilibrate the deformed cell before sampling the stress tensor. Another approach is to sample the triclinic cell fluctuations that occur in an NPT simulation. This method can also be slow to converge and requires careful post-processing (Shinoda)

6.19 Library interface to LAMMPS

As described in Section_start 5, LAMMPS can be built as a library, so that it can be called by another code, used in a coupled manner with other codes, or driven through a Python interface.

All of these methodologies use a C-style interface to LAMMPS that is provided in the files src/library.cpp and src/library.h. The functions therein have a C-style argument list, but contain C++ code you could write yourself in a C++ application that was invoking LAMMPS directly. The C++ code in the functions illustrates how to invoke internal LAMMPS operations. Note that LAMMPS classes are defined within a LAMMPS namespace (LAMMPS_NS) if you use them from another C++ application.

Library.cpp contains these 5 basic functions:

```
void lammps_open(int, char **, MPI_Comm, void **)
void lammps_close(void *)
int lammps_version(void *)
void lammps_file(void *, char *)
char *lammps_command(void *, char *)
```

The lammps_open() function is used to initialize LAMMPS, passing in a list of strings as if they were command-line arguments when LAMMPS is run in stand-alone mode from the command line, and a MPI communicator for LAMMPS to run under. It returns a ptr to the LAMMPS object that is created, and which is used in subsequent library calls. The lammps_open() function can be called multiple times, to create multiple instances of LAMMPS.

LAMMPS will run on the set of processors in the communicator. This means the calling code can run LAMMPS on all or a subset of processors. For example, a wrapper script might decide to alternate between LAMMPS and another code, allowing them both to run on all the processors. Or it might allocate half the processors to LAMMPS and half to the other code and run both codes simultaneously before syncing them up periodically. Or it might instantiate multiple instances of LAMMPS to perform different calculations.

The lammps_close() function is used to shut down an instance of LAMMPS and free all its memory.

The lammps_version() function can be used to determined the specific version of the underlying LAMMPS code. This is particularly useful when loading LAMMPS as a shared library via dlopen(). The code using the library interface can than use this information to adapt to changes to the LAMMPS command syntax between versions. The returned LAMMPS version code is an integer (e.g. 2 Sep 2015 results in 20150902) that grows with every new LAMMPS version.

The lammps_file() and lammps_command() functions are used to pass a file or string to LAMMPS as if it were an input script or single command in an input script. Thus the calling code can read or generate a series of LAMMPS commands one line at a time and pass it thru the library interface to setup a problem and then run it, interleaving the lammps_command() calls with other calls to extract information from LAMMPS, perform its own operations, or call another code's library.

Other useful functions are also included in library.cpp. For example:

```
void *lammps_extract_global(void *, char *)
void *lammps_extract_atom(void *, char *)
void *lammps_extract_compute(void *, char *, int, int)
void *lammps_extract_fix(void *, char *, int, int, int, int)
void *lammps_extract_variable(void *, char *, char *)
int lammps_set_variable(void *, char *, char *)
int lammps_get_natoms(void *)
void lammps_get_coords(void *, double *)
```

```
void lammps_put_coords(void *, double *)
```

These can extract various global or per-atom quantities from LAMMPS as well as values calculated by a compute, fix, or variable. The "set_variable" function can set an existing string-style variable to a new value, so that subsequent LAMMPS commands can access the variable. The "get" and "put" operations can retrieve and reset atom coordinates. See the library.cpp file and its associated header file library.h for details.

The key idea of the library interface is that you can write any functions you wish to define how your code talks to LAMMPS and add them to src/library.cpp and src/library.h, as well as to the Python interface. The routines you add can access or change any LAMMPS data you wish. The examples/COUPLE and python directories have example C++ and C and Python codes which show how a driver code can link to LAMMPS as a library, run LAMMPS on a subset of processors, grab data from LAMMPS, change it, and put it back into LAMMPS.

6.20 Calculating thermal conductivity

The thermal conductivity kappa of a material can be measured in at least 4 ways using various options in LAMMPS. See the examples/KAPPA directory for scripts that implement the 4 methods discussed here for a simple Lennard-Jones fluid model. Also, see this section of the manual for an analogous discussion for viscosity.

The thermal conducitivity tensor kappa is a measure of the propensity of a material to transmit heat energy in a diffusive manner as given by Fourier's law

J = -kappa grad(T)

where J is the heat flux in units of energy per area per time and grad(T) is the spatial gradient of temperature. The thermal conductivity thus has units of energy per distance per time per degree K and is often approximated as an isotropic quantity, i.e. as a scalar.

The first method is to setup two thermostatted regions at opposite ends of a simulation box, or one in the middle and one at the end of a periodic box. By holding the two regions at different temperatures with a thermostatting fix, the energy added to the hot region should equal the energy subtracted from the cold region and be proportional to the heat flux moving between the regions. See the paper by Ikeshoji and Hafskjold for details of this idea. Note that thermostatting fixes such as fix nvt, fix langevin, and fix temp/rescale store the cumulative energy they add/subtract.

Alternatively, as a second method, the fix heat command can used in place of thermostats on each of two regions to add/subtract specified amounts of energy to both regions. In both cases, the resulting temperatures of the two regions can be monitored with the "compute temp/region" command and the temperature profile of the intermediate region can be monitored with the fix ave/spatial and compute ke/atom commands.

The third method is to perform a reverse non-equilibrium MD simulation using the fix thermal/conductivity command which implements the rNEMD algorithm of Muller-Plathe. Kinetic energy is swapped between atoms in two different layers of the simulation box. This induces a temperature gradient between the two layers which can be monitored with the fix ave/spatial and compute ke/atom commands. The fix tallies the cumulative energy transfer that it performs. See the fix thermal/conductivity command for details.

The fourth method is based on the Green-Kubo (GK) formula which relates the ensemble average of the auto-correlation of the heat flux to kappa. The heat flux can be calculated from the fluctuations of per-atom potential and kinetic energies and per-atom stress tensor in a steady-state equilibrated simulation. This is in contrast to the two preceding non-equilibrium methods, where energy flows continuously between hot and cold regions of the simulation box.

The compute heat/flux command can calculate the needed heat flux and describes how to implement the Green_Kubo formalism using additional LAMMPS commands, such as the fix ave/correlate command to calculate the needed auto-correlation. See the doc page for the compute heat/flux command for an example input script that calculates the thermal conductivity of solid Ar via the GK formalism.

6.21 Calculating viscosity

The shear viscosity eta of a fluid can be measured in at least 4 ways using various options in LAMMPS. See the examples/VISCOSITY directory for scripts that implement the 4 methods discussed here for a simple Lennard-Jones fluid model. Also, see this section of the manual for an analogous discussion for thermal conductivity.

Eta is a measure of the propensity of a fluid to transmit momentum in a direction perpendicular to the direction of velocity or momentum flow. Alternatively it is the resistance the fluid has to being sheared. It is given by

J = -eta grad(Vstream)

where J is the momentum flux in units of momentum per area per time. and grad(Vstream) is the spatial gradient of the velocity of the fluid moving in another direction, normal to the area through which the momentum flows. Viscosity thus has units of pressure-time.

The first method is to perform a non-equlibrium MD (NEMD) simulation by shearing the simulation box via the fix deform command, and using the fix nvt/sllod command to thermostat the fluid via the SLLOD equations of motion. Alternatively, as a second method, one or more moving walls can be used to shear the fluid in between them, again with some kind of thermostat that modifies only the thermal (non-shearing) components of velocity to prevent the fluid from heating up.

In both cases, the velocity profile setup in the fluid by this procedure can be monitored by the fix ave/spatial command, which determines grad(Vstream) in the equation above. E.g. the derivative in the y-direction of the Vx component of fluid motion or grad(Vstream) = dVx/dy. The Pxy off-diagonal component of the pressure or stress tensor, as calculated by the compute pressure command, can also be monitored, which is the J term in the equation above. See this section of the manual for details on NEMD simulations.

The third method is to perform a reverse non-equilibrium MD simulation using the fix viscosity command which implements the rNEMD algorithm of Muller-Plathe. Momentum in one dimension is swapped between atoms in two different layers of the simulation box in a different dimension. This induces a velocity gradient which can be monitored with the fix ave/spatial command. The fix tallies the cummulative momentum transfer that it performs. See the fix viscosity command for details.

The fourth method is based on the Green-Kubo (GK) formula which relates the ensemble average of the auto-correlation of the stress/pressure tensor to eta. This can be done in a steady-state equilibrated simulation which is in contrast to the two preceding non-equilibrium methods, where momentum flows continuously through the simulation box.

Here is an example input script that calculates the viscosity of liquid Ar via the GK formalism:

```
# Sample LAMMPS input script for viscosity of liquid Ar

units       real
variable    T equal 86.4956
variable    V equal vol
variable    dt equal 4.0
```

```
variable    p equal 400     # correlation length
variable    s equal 5       # sample interval
variable    d equal $p*$s   # dump interval

# convert from LAMMPS real units to SI

variable    kB equal 1.3806504e-23    # [J/K/ Boltzmann
variable    atm2Pa equal 101325.0
variable    A2m equal 1.0e-10
variable    fs2s equal 1.0e-15
variable    convert equal ${atm2Pa}*${atm2Pa}*${fs2s}*${A2m}*${A2m}*${A2m}

# setup problem

dimension    3
boundary     p p p
lattice      fcc 5.376 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
region       box block 0 4 0 4 0 4
create_box   1 box
create_atoms 1 box
mass         1 39.948
pair_style   lj/cut 13.0
pair_coeff   * * 0.2381 3.405
timestep     ${dt}
thermo       $d

# equilibration and thermalization

velocity     all create $T 102486 mom yes rot yes dist gaussian
fix          NVT all nvt temp $T $T 10 drag 0.2
run          8000

# viscosity calculation, switch to NVE if desired

#unfix       NVT
#fix         NVE all nve

reset_timestep 0
variable     pxy equal pxy
variable     pxz equal pxz
variable     pyz equal pyz
fix          SS all ave/correlate $s $p $d &
             v_pxy v_pxz v_pyz type auto file S0St.dat ave running
variable     scale equal ${convert}/(${kB}*$T)*$V*$s*${dt}
variable     v11 equal trap(f_SS[3])*${scale}
variable     v22 equal trap(f_SS[4])*${scale}
variable     v33 equal trap(f_SS[5])*${scale}
thermo_style custom step temp press v_pxy v_pxz v_pyz v_v11 v_v22 v_v33
run          100000
variable     v equal (v_v11+v_v22+v_v33)/3.0
variable     ndens equal count(all)/vol
print        "average viscosity: $v [Pa.s/ @ $T K, ${ndens} /A^3"
```

6.22 Calculating a diffusion coefficient

The diffusion coefficient D of a material can be measured in at least 2 ways using various options in LAMMPS. See the examples/DIFFUSE directory for scripts that implement the 2 methods discussed here for a simple Lennard-Jones fluid model.

The first method is to measure the mean-squared displacement (MSD) of the system, via the compute msd command. The slope of the MSD versus time is proportional to the diffusion coefficient. The instantaneous MSD values can be accumulated in a vector via the fix vector command, and a line fit to the vector to compute its slope via the variable slope function, and thus extract D.

The second method is to measure the velocity auto-correlation function (VACF) of the system, via the compute vacf command. The time-integral of the VACF is proportional to the diffusion coefficient. The instantaneous VACF values can be accumulated in a vector via the fix vector command, and time integrated via the variable trap function, and thus extract D.

6.23 Using chunks to calculate system properties

In LAMMS, "chunks" are collections of atoms, as defined by the compute chunk/atom command, which assigns each atom to a chunk ID (or to no chunk at all). The number of chunks and the assignment of chunk IDs to atoms can be static or change over time. Examples of "chunks" are molecules or spatial bins or atoms with similar values (e.g. coordination number or potential energy).

The per-atom chunk IDs can be used as input to two other kinds of commands, to calculate various properties of a system:

- fix ave/chunk
- any of the compute */chunk commands

Here, each of the 3 kinds of chunk-related commands is briefly overviewed. Then some examples are given of how to compute different properties with chunk commands.

Compute chunk/atom command:

This compute can assign atoms to chunks of various styles. Only atoms in the specified group and optional specified region are assigned to a chunk. Here are some possible chunk definitions:

atoms in same molecule	chunk ID = molecule ID
atoms of same atom type	chunk ID = atom type
all atoms with same atom property (charge, radius, etc)	chunk ID = output of compute property/atom
atoms in same cluster	chunk ID = output of compute cluster/atom command
atoms in same spatial bin	chunk ID = bin ID
atoms in same rigid body	chunk ID = molecule ID used to define rigid bodies
atoms with similar potential energy	chunk ID = output of compute pe/atom
atoms with same local defect structure	chunk ID = output of compute centro/atom or compute coord/atom command

Note that chunk IDs are integer values, so for atom properties or computes that produce a floating point value, they will be truncated to an integer. You could also use the compute in a variable that scales the floating point value to spread it across multiple intergers.

Spatial bins can be of various kinds, e.g. 1d bins = slabs, 2d bins = pencils, 3d bins = boxes, spherical bins, cylindrical bins.

This compute also calculates the number of chunks *Nchunk*, which is used by other commands to tally per-chunk data. *Nchunk* can be a static value or change over time (e.g. the number of clusters). The chunk ID for an

individual atom can also be static (e.g. a molecule ID), or dynamic (e.g. what spatial bin an atom is in as it moves).

Note that this compute allows the per-atom output of other computes, fixes, and variables to be used to define chunk IDs for each atom. This means you can write your own compute or fix to output a per-atom quantity to use as chunk ID. See Section_modify of the documentation for how to do this. You can also define a per-atom variable in the input script that uses a formula to generate a chunk ID for each atom.

Fix ave/chunk command:

This fix takes the ID of a compute chunk/atom command as input. For each chunk, it then sums one or more specified per-atom values over the atoms in each chunk. The per-atom values can be any atom property, such as velocity, force, charge, potential energy, kinetic energy, stress, etc. Additional keywords are defined for per-chunk properties like density and temperature. More generally any per-atom value generated by other computes, fixes, and per-atom variables, can be summed over atoms in each chunk.

Similar to other averaging fixes, this fix allows the summed per-chunk values to be time-averaged in various ways, and output to a file. The fix produces a global array as output with one row of values per chunk.

Compute */chunk commands:

Currently the following computes operate on chunks of atoms to produce per-chunk values.

- compute com/chunk
- compute gyration/chunk
- compute inertia/chunk
- compute msd/chunk
- compute property/chunk
- compute temp/chunk
- compute torque/chunk
- compute vcm/chunk

They each take the ID of a compute chunk/atom command as input. As their names indicate, they calculate the center-of-mass, radius of gyration, moments of inertia, mean-squared displacement, temperature, torque, and velocity of center-of-mass for each chunk of atoms. The compute property/chunk command can tally the count of atoms in each chunk and extract other per-chunk properties.

The reason these various calculations are not part of the fix ave/chunk command, is that each requires a more complicated operation than simply summing and averaging over per-atom values in each chunk. For example, many of them require calculation of a center of mass, which requires summing mass*position over the atoms and then dividing by summed mass.

All of these computes produce a global vector or global array as output, wih one or more values per chunk. They can be used in various ways:

- As input to the fix ave/time command, which can write the values to a file and optionally time average them.
- As input to the fix ave/histo command to histogram values across chunks. E.g. a histogram of cluster sizes or molecule diffusion rates.
- As input to special functions of equal-style variables, like sum() and max(). E.g. to find the largest cluster or fastest diffusing molecule.

Example calculations with chunks

Here are eaxmples using chunk commands to calculate various properties:

(1) Average velocity in each of 1000 2d spatial bins:

```
compute cc1 all chunk/atom bin/2d x 0.0 0.1 y lower 0.01 units reduced
fix 1 all ave/chunk 100 10 1000 cc1 vx vy file tmp.out
```

(2) Temperature in each spatial bin, after subtracting a flow velocity:

```
compute cc1 all chunk/atom bin/2d x 0.0 0.1 y lower 0.1 units reduced
compute vbias all temp/profile 1 0 0 y 10
fix 1 all ave/chunk 100 10 1000 cc1 temp bias vbias file tmp.out
```

(3) Center of mass of each molecule:

```
compute cc1 all chunk/atom molecule
compute myChunk all com/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk file tmp.out mode vector
```

(4) Total force on each molecule and ave/max across all molecules:

```
compute cc1 all chunk/atom molecule
fix 1 all ave/chunk 1000 1 1000 cc1 fx fy fz file tmp.out
variable xave equal ave(f_12)
variable xmax equal max(f_12)
thermo 1000
thermo_style custom step temp v_xave v_xmax
```

(5) Histogram of cluster sizes:

```
compute cluster all cluster/atom 1.0
compute cc1 all chunk/atom c_cluster compress yes
compute size all property/chunk cc1 count
fix 1 all ave/histo 100 1 100 0 20 20 c_size mode vector ave running beyond ignore file tmp.histo
```

6.24 Setting parameters for the kspace_style pppm/disp command

The PPPM method computes interactions by splitting the pair potential into two parts, one of which is computed in a normal pairwise fashion, the so-called real-space part, and one of which is computed using the Fourier transform, the so called reciprocal-space or kspace part. For both parts, the potential is not computed exactly but is approximated. Thus, there is an error in both parts of the computation, the real-space and the kspace error. The just mentioned facts are true both for the PPPM for Coulomb as well as dispersion interactions. The deciding difference - and also the reason why the parameters for pppm/disp have to be selected with more care - is the impact of the errors on the results: The kspace error of the PPPM for Coulomb and dispersion interaction and the real-space error of the PPPM for Coulomb interaction have the character of noise. In contrast, the real-space error of the PPPM for dispersion has a clear physical interpretation: the underprediction of cohesion. As a consequence, the real-space error has a much stronger effect than the kspace error on simulation results for pppm/disp. Parameters must thus be chosen in a way that this error is much smaller than the kspace error.

When using pppm/disp and not making any specifications on the PPPM parameters via the kspace modify command, parameters will be tuned such that the real-space error and the kspace error are equal. This will result in simulations that are either inaccurate or slow, both of which is not desirable. For selecting parameters for the pppm/disp that provide fast and accurate simulations, there are two approaches, which both have their up- and

downsides.

The first approach is to set desired real-space an kspace accuracies via the *kspace_modify force/disp/real* and *kspace_modify force/disp/kspace* commands. Note that the accuracies have to be specified in force units and are thus dependend on the chosen unit settings. For real units, 0.0001 and 0.002 seem to provide reasonable accurate and efficient computations for the real-space and kspace accuracies. 0.002 and 0.05 work well for most systems using lj units. PPPM parameters will be generated based on the desired accuracies. The upside of this approach is that it usually provides a good set of parameters and will work for both the *kspace_modify diff ad* and *kspace_modify diff ik* options. The downside of the method is that setting the PPPM parameters will take some time during the initialization of the simulation.

The second approach is to set the parameters for the pppm/disp explicitly using the *kspace_modify mesh/disp*, *kspace_modify order/disp*, and *kspace_modify gewald/disp* commands. This approach requires a more experienced user who understands well the impact of the choice of parameters on the simulation accuracy and performance. This approach provides a fast initialization of the simulation. However, it is sensitive to errors: A combination of parameters that will perform well for one system might result in far-from-optimal conditions for other simulations. For example, parametes that provide accurate and fast computations for all-atomistic force fields can provide insufficient accuracy or united-atomistic force fields (which is related to that the latter typically have larger dispersion coefficients).

To avoid inaccurate or inefficient simulations, the pppm/disp stops simulations with an error message if no action is taken to control the PPPM parameters. If the automatic parameter generation is desired and real-space and kspace accuracies are desired to be equal, this error message can be suppressed using the *kspace_modify disp/auto yes* command.

A reasonable approach that combines the upsides of both methods is to make the first run using the *kspace_modify force/disp/real* and *kspace_modify force/disp/kspace* commands, write down the PPPM parameters from the outut, and specify these parameters using the second approach in subsequent runs (which have the same composition, force field, and approximately the same volume).

Concerning the performance of the pppm/disp there are two more things to consider. The first is that when using the pppm/disp, the cutoff parameter does no longer affect the accuracy of the simulation (subject to that gewald/disp is adjusted when changing the cutoff). The performance can thus be increased by examining different values for the cutoff parameter. A lower bound for the cutoff is only set by the truncation error of the repulsive term of pair potentials.

The second is that the mixing rule of the pair style has an impact on the computation time when using the pppm/disp. Fastest computations are achieved when using the geometric mixing rule. Using the arithmetic mixing rule substantially increases the computational cost. The computational overhead can be reduced using the *kspace_modify mix/disp geom* and *kspace_modify splittol* commands. The first command simply enforces geometric mixing of the dispersion coeffiecients in kspace computations. This introduces some error in the computations but will also significantly speed-up the simulations. The second keyword sets the accuracy with which the dispersion coefficients are approximated using a matrix factorization approach. This may result in better accuracy then using the first command, but will usually also not provide an equally good increase of efficiency.

Finally, pppm/disp can also be used when no mixing rules apply. This can be achieved using the *kspace_modify mix/disp none* command. Note that the code does not check automatically whether any mixing rule is fulfilled. If mixing rules do not apply, the user will have to specify this command explicitly.

6.25 Polarizable models

In polarizable force fields the charge distributions in molecules and materials respond to their electrostatic environements. Polarizable systems can be simulated in LAMMPS using three methods:

- the fluctuating charge method, implemented in the QEQ package,
- the adiabatic core-shell method, implemented in the CORESHELL package,
- the thermalized Drude dipole method, implemented in the USER-DRUDE package.

The fluctuating charge method calculates instantaneous charges on interacting atoms based on the electronegativity equalization principle. It is implemented in the fix qeq which is available in several variants. It is a relatively efficient technique since no additional particles are introduced. This method allows for charge transfer between molecules or atom groups. However, because the charges are located at the interaction sites, off-plane components of polarization cannot be represented in planar molecules or atom groups.

The two other methods share the same basic idea: polarizable atoms are split into one core atom and one satellite particle (called shell or Drude particle) attached to it by a harmonic spring. Both atoms bear a charge and they represent collectively an induced electric dipole. These techniques are computationally more expensive than the QEq method because of additional particles and bonds. These two charge-on-spring methods differ in certain features, with the core-shell model being normally used for ionic/crystalline materials, whereas the so-called Drude model is normally used for molecular systems and fluid states.

The core-shell model is applicable to crystalline materials where the high symmetry around each site leads to stable trajectories of the core-shell pairs. However, bonded atoms in molecules can be so close that a core would interact too strongly or even capture the Drude particle of a neighbor. The Drude dipole model is relatively more complex in order to remediate this and other issues. Specifically, the Drude model includes specific thermostating of the core-Drude pairs and short-range damping of the induced dipoles.

The three polarization methods can be implemented through a self-consistent calculation of charges or induced dipoles at each timestep. In the fluctuating charge scheme this is done by the matrix inversion method in fix qeq/point, but for core-shell or Drude-dipoles the relaxed-dipoles technique would require an slow iterative procedure. These self-consistent solutions yield accurate trajectories since the additional degrees of freedom representing polarization are massless. An alternative is to attribute a mass to the additional degrees of freedom and perform time integration using an extended Lagrangian technique. For the fluctuating charge scheme this is done by fix qeq/dynamic, and for the charge-on-spring models by the methods outlined in the next two sections. The assignment of masses to the additional degrees of freedom can lead to unphysical trajectories if care is not exerted in choosing the parameters of the poarizable models and the simulation conditions.

In the core-shell model the vibration of the shells is kept faster than the ionic vibrations to mimic the fast response of the polarizable electrons. But in molecular systems thermalizing the core-Drude pairs at temperatures comparable to the rest of the simulation leads to several problems (kinetic energy transfer, too short a timestep, etc.) In order to avoid these problems the relative motion of the Drude particles with respect to their cores is kept "cold" so the vibration of the core-Drude pairs is very slow, approaching the self-consistent regime. In both models the temperature is regulated using the velocities of the center of mass of core+shell (or Drude) pairs, but in the Drude model the actual relative core-Drude particle motion is thermostated separately as well.

6.26 Adiabatic core/shell model

The adiabatic core-shell model by Mitchell and Finchham is a simple method for adding polarizability to a system. In order to mimic the electron shell of an ion, a satellite particle is attached to it. This way the ions are split into a core and a shell where the latter is meant to react to the electrostatic environment inducing

polarizability.

Technically, shells are attached to the cores by a spring force f = k*r where k is a parametrized spring constant and r is the distance between the core and the shell. The charges of the core and the shell add up to the ion charge, thus q(ion) = q(core) + q(shell). This setup introduces the ion polarizability (alpha) given by alpha = q(shell)^2 / k. In a similar fashion the mass of the ion is distributed on the core and the shell with the core having the larger mass.

To run this model in LAMMPS, atom_style *full* can be used since atom charge and bonds are needed. Each kind of core/shell pair requires two atom types and a bond type. The core and shell of a core/shell pair should be bonded to each other with a harmonic bond that provides the spring force. For example, a data file for NaCl, as found in examples/coreshell, has this format:

```
432   atoms  # core and shell atoms
216   bonds  # number of core/shell springs

4     atom types  # 2 cores and 2 shells for Na and Cl
2     bond types

0.0 24.09597 xlo xhi
0.0 24.09597 ylo yhi
0.0 24.09597 zlo zhi

Masses       # core/shell mass ratio = 0.1

1 20.690784  # Na core
2 31.90500   # Cl core
3 2.298976   # Na shell
4 3.54500    # Cl shell

Atoms

1    1    2   1.5005    0.00000000   0.00000000   0.00000000 # core of core/shell pair 1
2    1    4  -2.5005    0.00000000   0.00000000   0.00000000 # shell of core/shell pair 1
3    2    1   1.5056    4.01599500   4.01599500   4.01599500 # core of core/shell pair 2
4    2    3  -0.5056    4.01599500   4.01599500   4.01599500 # shell of core/shell pair 2
(...)

Bonds   # Bond topology for spring forces

1     2     1     2   # spring for core/shell pair 1
2     2     3     4   # spring for core/shell pair 2
(...)
```

Non-Coulombic (e.g. Lennard-Jones) pairwise interactions are only defined between the shells. Coulombic interactions are defined between all cores and shells. If desired, additional bonds can be specified between cores.

The special_bonds command should be used to turn-off the Coulombic interaction within core/shell pairs, since that interaction is set by the bond spring. This is done using the special_bonds command with a 1-2 weight = 0.0, which is the default value. It needs to be considered whether one has to adjust the special_bonds weighting according to the molecular topology since the interactions of the shells are bypassed over an extra bond.

Note that this core/shell implementation does not require all ions to be polarized. One can mix core/shell pairs and ions without a satellite particle if desired.

Since the core/shell model permits distances of r = 0.0 between the core and shell, a pair style with a "cs" suffix

needs to be used to implement a valid long-range Coulombic correction. Several such pair styles are provided in the CORESHELL package. See this doc page for details. All of the core/shell enabled pair styles require the use of a long-range Coulombic solver, as specified by the kspace_style command. Either the PPPM or Ewald solvers can be used.

For the NaCL example problem, these pair style and bond style settings are used:

```
pair_style      born/coul/long/cs 20.0 20.0
pair_coeff      * *      0.0 1.000   0.00  0.00   0.00
pair_coeff      3 3    487.0 0.23768 0.00  1.05   0.50 #Na-Na
pair_coeff      3 4 145134.0 0.23768 0.00  6.99   8.70 #Na-Cl
pair_coeff      4 4 405774.0 0.23768 0.00 72.40 145.40 #Cl-Cl

bond_style      harmonic
bond_coeff      1 63.014 0.0
bond_coeff      2 25.724 0.0
```

When running dynamics with the adiabatic core/shell model, the following issues should be considered. Since the relative motion of the core and shell particles corresponds to the polarization, typical thermostats can alter the polarization behaviour, meaning the shell will not react freely to its electrostatic environment. This is critical during the equilibration of the system. Therefore it's typically desirable to decouple the relative motion of the core/shell pair, which is an imaginary degree of freedom, from the real physical system. To do that, the compute temp/cs command can be used, in conjunction with any of the thermostat fixes, such as fix nvt or fix langevin. This compute uses the center-of-mass velocity of the core/shell pairs to calculate a temperature, and insures that velocity is what is rescaled for thermostatting purposes. This compute also works for a system with both core/shell pairs and non-polarized ions (ions without an attached satellite particle). The compute temp/cs command requires input of two groups, one for the core atoms, another for the shell atoms. Non-polarized ions which might also be included in the treated system should not be included into either of these groups, they are taken into account by the *group-ID* (2nd argument) of the compute. The groups can be defined using the group *type* command. Note that to perform thermostatting using this definition of temperature, the fix modify temp command should be used to assign the compute to the thermostat fix. Likewise the thermo_modify temp command can be used to make this temperature be output for the overall system.

For the NaCl example, this can be done as follows:

```
group cores type 1 2
group shells type 3 4
compute CSequ all temp/cs cores shells
fix thermoberendsen all temp/berendsen 1427 1427 0.4    # thermostat for the true physical system
fix thermostatequ all nve                               # integrator as needed for the berendsen the
fix_modify thermoberendsen temp CSequ
thermo_modify temp CSequ                                # output of center-of-mass derived temperatu
```

If compute temp/cs is used, the decoupled relative motion of the core and the shell should in theory be stable. However numerical fluctuation can introduce a small momentum to the system, which is noticable over long trajectories. Therefore it is recomendable to use the fix momentum command in combination with compute temp/cs when equilibrating the system to prevent any drift.

When intializing the velocities of a system with core/shell pairs, it is also desirable to not introduce energy into the relative motion of the core/shell particles, but only assign a center-of-mass velocity to the pairs. This can be done by using the *bias* keyword of the velocity create command and assigning the compute temp/cs command to the *temp* keyword of the velocity commmand, e.g.

```
velocity all create 1427 134 bias yes temp CSequ
velocity all scale 1427 temp CSequ
```

It is important to note that the polarizability of the core/shell pairs is based on their relative motion. Therefore the choice of spring force and mass ratio need to ensure much faster relative motion of the 2 atoms within the core/shell pair than their center-of-mass velocity. This allow the shells to effectively react instantaneously to the electrostatic environment. This fast movement also limits the timestep size that can be used.

The primary literature of the adiabatic core/shell model suggests that the fast relative motion of the core/shell pairs only allows negligible energy transfer to the environment. Therefore it is not intended to decouple the core/shell degree of freedom from the physical system during production runs. In other words, the compute temp/cs command should not be used during production runs and is only required during equilibration. This way one is consistent with literature (based on the code packages DL_POLY or GULP for instance).

The mentioned energy transfer will typically lead to a a small drift in total energy over time. This internal energy can be monitored using the compute chunk/atom and compute temp/chunk commands. The internal kinetic energies of each core/shell pair can then be summed using the sum() special function of the variable command. Or they can be time/averaged and output using the fix ave/time command. To use these commands, each core/shell pair must be defined as a "chunk". If each core/shell pair is defined as its own molecule, the molecule ID can be used to define the chunks. If cores are bonded to each other to form larger molecules, the chunks can be identified by the fix property/atom via assigning a core/shell ID to each atom using a special field in the data file read by the read_data command. This field can then be accessed by the compute property/atom command, to use as input to the compute chunk/atom command to define the core/shell pairs as chunks.

For example,

```
fix csinfo all property/atom i_CSID                          # property/atom command
read_data NaCl_CS_x0.1_prop.data fix csinfo NULL CS-Info  # atom property added in the data-file
compute prop all property/atom i_CSID
compute cs_chunk all chunk/atom c_prop
compute cstherm all temp/chunk cs_chunk temp internal com yes cdof 3.0     # note the chosen degrees
fix ave_chunk all ave/time 10 1 10 c_cstherm file chunk.dump mode vector
```

The additional section in the date file would be formatted like this:

```
CS-Info          # header of additional section

1   1            # column 1 = atom ID, column 2 = core/shell ID
2   1
3   2
4   2
5   3
6   3
7   4
8   4
(...)
```

6.27 Drude induced dipoles

The thermalized Drude model, similarly to the core-shell model, representes induced dipoles by a pair of charges (the core atom and the Drude particle) connected by a harmonic spring. The Drude model has a number of features aimed at its use in molecular systems (Lamoureux and Roux):

- Thermostating of the additional degrees of freedom associated with the induced dipoles at very low temperature, in terms of the reduced coordinates of the Drude particles with respect to their cores. This makes the trajectory close to that of relaxed induced dipoles.

- Consistent definition of 1-2 to 1-4 neighbors. A core-Drude particle pair represents a single (polarizable) atom, so the special screening factors in a covalent structure should be the same for the core and the Drude particle. Drude particles have to inherit the 1-2, 1-3, 1-4 special neighbor relations from their respective cores.
- Stabilization of the interactions between induced dipoles. Drude dipoles on covalently bonded atoms interact too strongly due to the short distances, so an atom may capture the Drude particle of a neighbor, or the induced dipoles within the same molecule may align too much. To avoid this, damping at short range can be done by Thole functions (for which there are physical grounds). This Thole damping is applied to the point charges composing the induced dipole (the charge of the Drude particle and the opposite charge on the core, not to the total charge of the core atom).

A detailed tutorial covering the usage of Drude induced dipoles in LAMMPS is available here.

As with the core-shell model, the cores and Drude particles should appear in the data file as standard atoms. The same holds for the springs between them, which are described by standard harmonic bonds. The nature of the atoms (core, Drude particle or non-polarizable) is specified via the fix drude command. The special list of neighbors is automatically refactored to account for the equivalence of core and Drude particles as regards special 1-2 to 1-4 screening. It may be necessary to use the *extra* keyword of the special_bonds command. If using fix shake, make sure no Drude particle is in this fix group.

There are two ways to thermostat the Drude particles at a low temperature: use either fix langevin/drude for a Langevin thermostat, or fix drude/transform/* for a Nose-Hoover thermostat. The former requires use of the command comm_modify vel yes. The latter requires two separate integration fixes like *nvt* or *npt*. The correct temperatures of the reduced degrees of freedom can be calculated using the compute temp/drude. This requires also to use the command *comm_modify vel yes*.

Short-range damping of the induced dipole interactions can be achieved using Thole functions through the the pair style thole in pair_style hybrid/overlay with a Coulomb pair style. It may be useful to use *coul/long/cs* or similar from the CORESHELL package if the core and Drude particle come too close, which can cause numerical issues.

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(Mitchell and Finchham) Mitchell, Finchham, J Phys Condensed Matter, 5, 1031-1038 (1993).

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7. Example problems

The LAMMPS distribution includes an examples sub-directory with several sample problems. Each problem is in a sub-directory of its own. Most are 2d models so that they run quickly, requiring at most a couple of minutes to run on a desktop machine. Each problem has an input script (in.*) and produces a log file (log.*) and dump file (dump.*) when it runs. Some use a data file (data.*) of initial coordinates as additional input. A few sample log file outputs on different machines and different numbers of processors are included in the directories to compare your answers to. E.g. a log file like log.crack.foo.P means it ran on P processors of machine "foo".

For examples that use input data files, many of them were produced by Pizza.py or setup tools described in the Additional Tools section of the LAMMPS documentation and provided with the LAMMPS distribution.

If you uncomment the dump command in the input script, a text dump file will be produced, which can be animated by various visualization programs. It can also be animated using the xmovie tool described in the Additional Tools section of the LAMMPS documentation.

If you uncomment the dump image command in the input script, and assuming you have built LAMMPS with a JPG library, JPG snapshot images will be produced when the simulation runs. They can be quickly post-processed into a movie using commands described on the dump image doc page.

Animations of many of these examples can be viewed on the Movies section of the LAMMPS WWW Site.

These are the sample problems in the examples sub-directories:

balance	dynamic load balancing, 2d system
body	body particles, 2d system
colloid	big colloid particles in a small particle solvent, 2d system
comb	models using the COMB potential
crack	crack propagation in a 2d solid
cuda	use of the USER-CUDA package for GPU acceleration
dipole	point dipolar particles, 2d system
dreiding	methanol via Dreiding FF
eim	NaCl using the EIM potential
ellipse	ellipsoidal particles in spherical solvent, 2d system
flow	Couette and Poiseuille flow in a 2d channel
friction	frictional contact of spherical asperities between 2d surfaces
gpu	use of the GPU package for GPU acceleration
hugoniostat	Hugoniostat shock dynamics
indent	spherical indenter into a 2d solid
intel	use of the USER-INTEL package for CPU or Intel(R) Xeon Phi(TM) coprocessor
kim	use of potentials in Knowledge Base for Interatomic Models (KIM)
line	line segment particles in 2d rigid bodies
meam	MEAM test for SiC and shear (same as shear examples)
melt	rapid melt of 3d LJ system
micelle	self-assembly of small lipid-like molecules into 2d bilayers

min	energy minimization of 2d LJ melt
msst	MSST shock dynamics
nb3b	use of nonbonded 3-body harmonic pair style
neb	nudged elastic band (NEB) calculation for barrier finding
nemd	non-equilibrium MD of 2d sheared system
obstacle	flow around two voids in a 2d channel
peptide	dynamics of a small solvated peptide chain (5-mer)
peri	Peridynamic model of cylinder impacted by indenter
pour	pouring of granular particles into a 3d box, then chute flow
prd	parallel replica dynamics of vacancy diffusion in bulk Si
qeq	use of the QEQ pacakge for charge equilibration
reax	RDX and TATB models using the ReaxFF
rigid	rigid bodies modeled as independent or coupled
shear	sideways shear applied to 2d solid, with and without a void
snap	NVE dynamics for BCC tantalum crystal using SNAP potential
srd	stochastic rotation dynamics (SRD) particles as solvent
tad	temperature-accelerated dynamics of vacancy diffusion in bulk Si
tri	triangular particles in rigid bodies

vashishta: models using the Vashishta potential

Here is how you might run and visualize one of the sample problems:

```
cd indent
cp ../../src/lmp_linux .           # copy LAMMPS executable to this dir
lmp_linux -in in.indent            # run the problem
```

Running the simulation produces the files *dump.indent* and *log.lammps*. You can visualize the dump file as follows:

```
../../tools/xmovie/xmovie -scale dump.indent
```

If you uncomment the dump image line(s) in the input script a series of JPG images will be produced by the run. These can be viewed individually or turned into a movie or animated by tools like ImageMagick or QuickTime or various Windows-based tools. See the dump image doc page for more details. E.g. this Imagemagick command would create a GIF file suitable for viewing in a browser.

```
% convert -loop 1 *.jpg foo.gif
```

There is also a COUPLE directory with examples of how to use LAMMPS as a library, either by itself or in tandem with another code or library. See the COUPLE/README file to get started.

There is also an ELASTIC directory with an example script for computing elastic constants at zero temperature, using an Si example. See the ELASTIC/in.elastic file for more info.

There is also an ELASTIC_T directory with an example script for computing elastic constants at finite temperature, using an Si example. See the ELASTIC_T/in.elastic file for more info.

There is also a USER directory which contains subdirectories of user-provided examples for user packages. See the README files in those directories for more info. See the Section_start.html file for more info about user

packages.

8. Performance & scalability

LAMMPS performance on several prototypical benchmarks and machines is discussed on the Benchmarks page of the LAMMPS WWW Site where CPU timings and parallel efficiencies are listed. Here, the benchmarks are described briefly and some useful rules of thumb about their performance are highlighted.

These are the 5 benchmark problems:

1. LJ = atomic fluid, Lennard-Jones potential with 2.5 sigma cutoff (55 neighbors per atom), NVE integration
2. Chain = bead-spring polymer melt of 100-mer chains, FENE bonds and LJ pairwise interactions with a 2^(1/6) sigma cutoff (5 neighbors per atom), NVE integration
3. EAM = metallic solid, Cu EAM potential with 4.95 Angstrom cutoff (45 neighbors per atom), NVE integration
4. Chute = granular chute flow, frictional history potential with 1.1 sigma cutoff (7 neighbors per atom), NVE integration
5. Rhodo = rhodopsin protein in solvated lipid bilayer, CHARMM force field with a 10 Angstrom LJ cutoff (440 neighbors per atom), particle-particle particle-mesh (PPPM) for long-range Coulombics, NPT integration

The input files for running the benchmarks are included in the LAMMPS distribution, as are sample output files. Each of the 5 problems has 32,000 atoms and runs for 100 timesteps. Each can be run as a serial benchmarks (on one processor) or in parallel. In parallel, each benchmark can be run as a fixed-size or scaled-size problem. For fixed-size benchmarking, the same 32K atom problem is run on various numbers of processors. For scaled-size benchmarking, the model size is increased with the number of processors. E.g. on 8 processors, a 256K-atom problem is run; on 1024 processors, a 32-million atom problem is run, etc.

A useful metric from the benchmarks is the CPU cost per atom per timestep. Since LAMMPS performance scales roughly linearly with problem size and timesteps, the run time of any problem using the same model (atom style, force field, cutoff, etc) can then be estimated. For example, on a 1.7 GHz Pentium desktop machine (Intel icc compiler under Red Hat Linux), the CPU run-time in seconds/atom/timestep for the 5 problems is

Problem:	LJ	Chain	EAM	Chute	Rhodopsin
CPU/atom/step:	4.55E-6	2.18E-6	9.38E-6	2.18E-6	1.11E-4
Ratio to LJ:	1.0	0.48	2.06	0.48	24.5

The ratios mean that if the atomic LJ system has a normalized cost of 1.0, the bead-spring chains and granular systems run 2x faster, while the EAM metal and solvated protein models run 2x and 25x slower respectively. The bulk of these cost differences is due to the expense of computing a particular pairwise force field for a given number of neighbors per atom.

Performance on a parallel machine can also be predicted from the one-processor timings if the parallel efficiency can be estimated. The communication bandwidth and latency of a particular parallel machine affects the efficiency. On most machines LAMMPS will give fixed-size parallel efficiencies on these benchmarks above 50% so long as the atoms/processor count is a few 100 or greater - i.e. on 64 to 128 processors. Likewise, scaled-size parallel efficiencies will typically be 80% or greater up to very large processor counts. The benchmark data on the LAMMPS WWW Site gives specific examples on some different machines, including a run of 3/4 of a billion LJ atoms on 1500 processors that ran at 85% parallel efficiency.

9. Additional tools

LAMMPS is designed to be a computational kernel for performing molecular dynamics computations. Additional pre- and post-processing steps are often necessary to setup and analyze a simulation. A few additional tools are provided with the LAMMPS distribution and are described in this section.

Our group has also written and released a separate toolkit called Pizza.py which provides tools for doing setup, analysis, plotting, and visualization for LAMMPS simulations. Pizza.py is written in Python and is available for download from the Pizza.py WWW site.

Note that many users write their own setup or analysis tools or use other existing codes and convert their output to a LAMMPS input format or vice versa. The tools listed here are included in the LAMMPS distribution as examples of auxiliary tools. Some of them are not actively supported by Sandia, as they were contributed by LAMMPS users. If you have problems using them, we can direct you to the authors.

The source code for each of these codes is in the tools sub-directory of the LAMMPS distribution. There is a Makefile (which you may need to edit for your platform) which will build several of the tools which reside in that directory. Some of them are larger packages in their own sub-directories with their own Makefiles.

- amber2lmp
- binary2txt
- ch2lmp
- chain
- colvars
- createatoms
- data2xmovie
- eam database
- eam generate
- eff
- emacs
- fep
- i-pi
- ipp
- kate
- lmp2arc
- lmp2cfg
- lmp2vmd
- matlab
- micelle2d
- moltemplate
- msi2lmp
- phonon
- polymer bonding
- pymol_asphere
- python
- reax
- restart2data
- vim
- xmgrace
- xmovie

amber2lmp tool

The amber2lmp sub-directory contains two Python scripts for converting files back-and-forth between the AMBER MD code and LAMMPS. See the README file in amber2lmp for more information.

These tools were written by Keir Novik while he was at Queen Mary University of London. Keir is no longer there and cannot support these tools which are out-of-date with respect to the current LAMMPS version (and maybe with respect to AMBER as well). Since we don't use these tools at Sandia, you'll need to experiment with them and make necessary modifications yourself.

binary2txt tool

The file binary2txt.cpp converts one or more binary LAMMPS dump file into ASCII text files. The syntax for running the tool is

```
binary2txt file1 file2 ...
```

which creates file1.txt, file2.txt, etc. This tool must be compiled on a platform that can read the binary file created by a LAMMPS run, since binary files are not compatible across all platforms.

ch2lmp tool

The ch2lmp sub-directory contains tools for converting files back-and-forth between the CHARMM MD code and LAMMPS.

They are intended to make it easy to use CHARMM as a builder and as a post-processor for LAMMPS. Using charmm2lammps.pl, you can convert an ensemble built in CHARMM into its LAMMPS equivalent. Using lammps2pdb.pl you can convert LAMMPS atom dumps into pdb files.

See the README file in the ch2lmp sub-directory for more information.

These tools were created by Pieter in't Veld (pjintve at sandia.gov) and Paul Crozier (pscrozi at sandia.gov) at Sandia.

chain tool

The file chain.f creates a LAMMPS data file containing bead-spring polymer chains and/or monomer solvent atoms. It uses a text file containing chain definition parameters as an input. The created chains and solvent atoms can strongly overlap, so LAMMPS needs to run the system initially with a "soft" pair potential to un-overlap it. The syntax for running the tool is

```
chain <def.chain > data.file
```

See the def.chain or def.chain.ab files in the tools directory for examples of definition files. This tool was used to create the system for the chain benchmark.

colvars tools

The colvars directory contains a collection of tools for postprocessing data produced by the colvars collective variable library. To compile the tools, edit the makefile for your system and run "make".

Please report problems and issues the colvars library and its tools at: https://github.com/colvars/colvars/issues

abf_integrate:

MC-based integration of multidimensional free energy gradient Version 20110511

```
Syntax: ./abf_integrate <filename > [-n  <nsteps >] [-t  <temp >] [-m [0|1] (metadynamics)] [-h  <hi
```

The LAMMPS interface to the colvars collective variable library, as well as these tools, were created by Axel Kohlmeyer (akohlmey at gmail.com) at ICTP, Italy.

---

createatoms tool

The tools/createatoms directory contains a Fortran program called createAtoms.f which can generate a variety of interesting crystal structures and geometries and output the resulting list of atom coordinates in LAMMPS or other formats.

See the included Manual.pdf for details.

The tool is authored by Xiaowang Zhou (Sandia), xzhou at sandia.gov.

---

data2xmovie tool

The file data2xmovie.c converts a LAMMPS data file into a snapshot suitable for visualizing with the xmovie tool, as if it had been output with a dump command from LAMMPS itself. The syntax for running the tool is

```
data2xmovie [options] <infile > outfile
```

See the top of the data2xmovie.c file for a discussion of the options.

---

eam database tool

The tools/eam_database directory contains a Fortran program that will generate EAM alloy setfl potential files for any combination of 16 elements: Cu, Ag, Au, Ni, Pd, Pt, Al, Pb, Fe, Mo, Ta, W, Mg, Co, Ti, Zr. The files can then be used with the pair_style eam/alloy command.

The tool is authored by Xiaowang Zhou (Sandia), xzhou at sandia.gov, and is based on his paper:

X. W. Zhou, R. A. Johnson, and H. N. G. Wadley, Phys. Rev. B, 69, 144113 (2004).

---

eam generate tool

The tools/eam_generate directory contains several one-file C programs that convert an analytic formula into a tabulated embedded atom method (EAM) setfl potential file. The potentials they produce are in the potentials directory, and can be used with the pair_style eam/alloy command.

The source files and potentials were provided by Gerolf Ziegenhain (gerolf at ziegenhain.com).

---

eff tool

The tools/eff directory contains various scripts for generating structures and post-processing output for simulations using the electron force field (eFF).

These tools were provided by Andres Jaramillo-Botero at CalTech (ajaramil at wag.caltech.edu).

---

emacs tool

The tools/emacs directory contains a Lips add-on file for Emacs that enables a lammps-mode for editing of input scripts when using Emacs, with various highlighting options setup.

These tools were provided by Aidan Thompson at Sandia (athomps at sandia.gov).

---

fep tool

The tools/fep directory contains Python scripts useful for post-processing results from performing free-energy perturbation simulations using the USER-FEP package.

The scripts were contributed by Agilio Padua (Universite Blaise Pascal Clermont-Ferrand), agilio.padua at univ-bpclermont.fr.

See README file in the tools/fep directory.

---

i-pi tool

The tools/i-pi directory contains a version of the i-PI package, with all the LAMMPS-unrelated files removed. It is provided so that it can be used with the fix ipi command to perform path-integral molecular dynamics (PIMD).

The i-PI package was created and is maintained by Michele Ceriotti, michele.ceriotti at gmail.com, to interface to a variety of molecular dynamics codes.

See the tools/i-pi/manual.pdf file for an overview of i-PI, and the fix ipi doc page for further details on running PIMD calculations with LAMMPS.

---

ipp tool

The tools/ipp directory contains a Perl script ipp which can be used to facilitate the creation of a complicated file (say, a lammps input script or tools/createatoms input file) using a template file.

ipp was created and is maintained by Reese Jones (Sandia), rjones at sandia.gov.

See two examples in the tools/ipp directory. One of them is for the tools/createatoms tool's input file.

---

kate tool

The file in the tools/kate directory is an add-on to the Kate editor in the KDE suite that allow syntax highlighting of LAMMPS input scripts. See the README.txt file for details.

The file was provided by Alessandro Luigi Sellerio (alessandro.sellerio at ieni.cnr.it).

---

lmp2arc tool

The lmp2arc sub-directory contains a tool for converting LAMMPS output files to the format for Accelrys' Insight MD code (formerly MSI/Biosym and its Discover MD code). See the README file for more information.

This tool was written by John Carpenter (Cray), Michael Peachey (Cray), and Steve Lustig (Dupont). John is now at the Mayo Clinic (jec at mayo.edu), but still fields questions about the tool.

This tool was updated for the current LAMMPS C++ version by Jeff Greathouse at Sandia (jagreat at sandia.gov).

---

lmp2cfg tool

The lmp2cfg sub-directory contains a tool for converting LAMMPS output files into a series of *.cfg files which can be read into the AtomEye visualizer. See the README file for more information.

This tool was written by Ara Kooser at Sandia (askoose at sandia.gov).

---

lmp2vmd tool

The lmp2vmd sub-directory contains a README.txt file that describes details of scripts and plugin support within the VMD package for visualizing LAMMPS dump files.

The VMD plugins and other supporting scripts were written by Axel Kohlmeyer (akohlmey at cmm.chem.upenn.edu) at U Penn.

---

matlab tool

The matlab sub-directory contains several MATLAB scripts for post-processing LAMMPS output. The scripts include readers for log and dump files, a reader for EAM potential files, and a converter that reads LAMMPS dump files and produces CFG files that can be visualized with the AtomEye visualizer.

See the README.pdf file for more information.

These scripts were written by Arun Subramaniyan at Purdue Univ (asubrama at purdue.edu).

---

micelle2d tool

The file micelle2d.f creates a LAMMPS data file containing short lipid chains in a monomer solution. It uses a text file containing lipid definition parameters as an input. The created molecules and solvent atoms can strongly overlap, so LAMMPS needs to run the system initially with a "soft" pair potential to un-overlap it. The syntax for running the tool is

```
micelle2d <def.micelle2d > data.file
```

See the def.micelle2d file in the tools directory for an example of a definition file. This tool was used to create the system for the micelle example.

---

moltemplate tool

The moltemplate sub-directory contains a Python-based tool for building molecular systems based on a text-file description, and creating LAMMPS data files that encode their molecular topology as lists of bonds, angles, dihedrals, etc. See the README.TXT file for more information.

This tool was written by Andrew Jewett (jewett.aij at gmail.com), who supports it. It has its own WWW page at http://moltemplate.org.

---

msi2lmp tool

The msi2lmp sub-directory contains a tool for creating LAMMPS input data files from Accelrys' Insight MD code (formerly MSI/Biosym and its Discover MD code). See the README file for more information.

This tool was written by John Carpenter (Cray), Michael Peachey (Cray), and Steve Lustig (Dupont). John is now at the Mayo Clinic (jec at mayo.edu), but still fields questions about the tool.

This tool may be out-of-date with respect to the current LAMMPS and Insight versions. Since we don't use it at Sandia, you'll need to experiment with it yourself.

---

phonon tool

The phonon sub-directory contains a post-processing tool useful for analyzing the output of the fix phonon command in the USER-PHONON package.

See the README file for instruction on building the tool and what library it needs. And see the examples/USER/phonon directory for example problems that can be post-processed with this tool.

This tool was written by Ling-Ti Kong at Shanghai Jiao Tong University.

---

polymer bonding tool

The polybond sub-directory contains a Python-based tool useful for performing "programmable polymer bonding". The Python file lmpsdata.py provides a "Lmpsdata" class with various methods which can be invoked by a user-written Python script to create data files with complex bonding topologies.

See the Manual.pdf for details and example scripts.

This tool was written by Zachary Kraus at Georgia Tech.

---

pymol_asphere tool

The pymol_asphere sub-directory contains a tool for converting a LAMMPS dump file that contains orientation info for ellipsoidal particles into an input file for the PyMol visualization package.

Specifically, the tool triangulates the ellipsoids so they can be viewed as true ellipsoidal particles within PyMol. See the README and examples directory within pymol_asphere for more information.

This tool was written by Mike Brown at Sandia.

---

python tool

The python sub-directory contains several Python scripts that perform common LAMMPS post-processing tasks, such as:

- extract thermodynamic info from a log file as columns of numbers
- plot two columns of thermodynamic info from a log file using GnuPlot
- sort the snapshots in a dump file by atom ID

- convert multiple NEB dump files into one dump file for viz
- convert dump files into XYZ, CFG, or PDB format for viz by other packages

These are simple scripts built on Pizza.py modules. See the README for more info on Pizza.py and how to use these scripts.

---

reax tool

The reax sub-directory contains stand-alond codes that can post-process the output of the fix reax/bonds command from a LAMMPS simulation using ReaxFF. See the README.txt file for more info.

These tools were written by Aidan Thompson at Sandia.

---

restart2data tool

NOTE: This tool is now obsolete and is not included in the current LAMMPS distribution. This is becaues there is now a write_data command, which can create a data file from within an input script. Running LAMMPS with the "-r" command-line switch as follows:

lmp_g++ -r restartfile datafile

is the same as running a 2-line input script:

read_restart restartfile write_data datafile

which will produce the same data file that the restart2data tool used to create. The following information is included in case you have an older version of LAMMPS which still includes the restart2data tool.

The file restart2data.cpp converts a binary LAMMPS restart file into an ASCII data file. The syntax for running the tool is

```
restart2data restart-file data-file (input-file)
```

Input-file is optional and if specified will contain LAMMPS input commands for the masses and force field parameters, instead of putting those in the data-file. Only a few force field styles currently support this option.

This tool must be compiled on a platform that can read the binary file created by a LAMMPS run, since binary files are not compatible across all platforms.

Note that a text data file has less precision than a binary restart file. Hence, continuing a run from a converted data file will typically not conform as closely to a previous run as will restarting from a binary restart file.

If a "%" appears in the specified restart-file, the tool expects a set of multiple files to exist. See the restart and write_restart commands for info on how such sets of files are written by LAMMPS, and how the files are named.

---

vim tool

The files in the tools/vim directory are add-ons to the VIM editor that allow easier editing of LAMMPS input scripts. See the README.txt file for details.

These files were provided by Gerolf Ziegenhain (gerolf at ziegenhain.com)

---

xmgrace tool

The files in the tools/xmgrace directory can be used to plot the thermodynamic data in LAMMPS log files via the xmgrace plotting package. There are several tools in the directory that can be used in post-processing mode. The lammpsplot.cpp file can be compiled and used to create plots from the current state of a running LAMMPS simulation.

See the README file for details.

These files were provided by Vikas Varshney (vv0210 at gmail.com)

---

xmovie tool

The xmovie tool is an X-based visualization package that can read LAMMPS dump files and animate them. It is in its own sub-directory with the tools directory. You may need to modify its Makefile so that it can find the appropriate X libraries to link against.

The syntax for running xmovie is

```
xmovie [options] dump.file1 dump.file2 ...
```

If you just type "xmovie" you will see a list of options. Note that by default, LAMMPS dump files are in scaled coordinates, so you typically need to use the -scale option with xmovie. When xmovie runs it opens a visualization window and a control window. The control options are straightforward to use.

Xmovie was mostly written by Mike Uttormark (U Wisconsin) while he spent a summer at Sandia. It displays 2d projections of a 3d domain. While simple in design, it is an amazingly fast program that can render large numbers of atoms very quickly. It's a useful tool for debugging LAMMPS input and output and making sure your simulation is doing what you think it should. The animations on the Examples page of the LAMMPS WWW site were created with xmovie.

I've lost contact with Mike, so I hope he's comfortable with us distributing his great tool!

10. Modifying & extending LAMMPS

This section describes how to customize LAMMPS by modifying and extending its source code.

LAMMPS is designed in a modular fashion so as to be easy to modify and extend with new functionality. In fact, about 75% of its source code is files added in this fashion.

In this section, changes and additions users can make are listed along with minimal instructions. If you add a new feature to LAMMPS and think it will be of interest to general users, we encourage you to submit it to the developers for inclusion in the released version of LAMMPS. Information about how to do this is provided below.

The best way to add a new feature is to find a similar feature in LAMMPS and look at the corresponding source and header files to figure out what it does. You will need some knowledge of C++ to be able to understand the hi-level structure of LAMMPS and its class organization, but functions (class methods) that do actual computations are written in vanilla C-style code and operate on simple C-style data structures (vectors and arrays).

Most of the new features described in this section require you to write a new C++ derived class (except for exceptions described below, where you can make small edits to existing files). Creating a new class requires 2 files, a source code file (*.cpp) and a header file (*.h). The derived class must provide certain methods to work as a new option. Depending on how different your new feature is compared to existing features, you can either derive from the base class itself, or from a derived class that already exists. Enabling LAMMPS to invoke the new class is as simple as putting the two source files in the src dir and re-building LAMMPS.

The advantage of C++ and its object-orientation is that all the code and variables needed to define the new feature are in the 2 files you write, and thus shouldn't make the rest of LAMMPS more complex or cause side-effect bugs.

Here is a concrete example. Suppose you write 2 files pair_foo.cpp and pair_foo.h that define a new class PairFoo that computes pairwise potentials described in the classic 1997 paper by Foo, et al. If you wish to invoke those potentials in a LAMMPS input script with a command like

```
pair_style foo 0.1 3.5
```

then your pair_foo.h file should be structured as follows:

```
#ifdef PAIR_CLASS
PairStyle(foo,PairFoo)
#else
...
(class definition for PairFoo)
...
#endif
```

where "foo" is the style keyword in the pair_style command, and PairFoo is the class name defined in your pair_foo.cpp and pair_foo.h files.

When you re-build LAMMPS, your new pairwise potential becomes part of the executable and can be invoked with a pair_style command like the example above. Arguments like 0.1 and 3.5 can be defined and processed by your new class.

As illustrated by this pairwise example, many kinds of options are referred to in the LAMMPS documentation as the "style" of a particular command.

The instructions below give the header file for the base class that these styles are derived from. Public variables in that file are ones used and set by the derived classes which are also used by the base class. Sometimes they are also used by the rest of LAMMPS. Virtual functions in the base class header file which are set = 0 are ones you must define in your new derived class to give it the functionality LAMMPS expects. Virtual functions that are not set to 0 are functions you can optionally define.

Additionally, new output options can be added directly to the thermo.cpp, dump_custom.cpp, and variable.cpp files as explained below.

Here are additional guidelines for modifying LAMMPS and adding new functionality:

- Think about whether what you want to do would be better as a pre- or post-processing step. Many computations are more easily and more quickly done that way.
- Don't do anything within the timestepping of a run that isn't parallel. E.g. don't accumulate a bunch of data on a single processor and analyze it. You run the risk of seriously degrading the parallel efficiency.
- If your new feature reads arguments or writes output, make sure you follow the unit conventions discussed by the units command.
- If you add something you think is truly useful and doesn't impact LAMMPS performance when it isn't used, send an email to the developers. We might be interested in adding it to the LAMMPS distribution. See further details on this at the bottom of this page.

10.1 Atom styles

Classes that define an atom style are derived from the AtomVec class and managed by the Atom class. The atom style determines what attributes are associated with an atom. A new atom style can be created if one of the existing atom styles does not define all the attributes you need to store and communicate with atoms.

Atom_vec_atomic.cpp is a simple example of an atom style.

Here is a brief description of methods you define in your new derived class. See atom_vec.h for details.

init	one time setup (optional)
grow	re-allocate atom arrays to longer lengths (required)
grow_reset	make array pointers in Atom and AtomVec classes consistent (required)
copy	copy info for one atom to another atom's array locations (required)
pack_comm	store an atom's info in a buffer communicated every timestep (required)
pack_comm_vel	add velocity info to communication buffer (required)
pack_comm_hybrid	store extra info unique to this atom style (optional)
unpack_comm	retrieve an atom's info from the buffer (required)
unpack_comm_vel	also retrieve velocity info (required)
unpack_comm_hybrid	retreive extra info unique to this atom style (optional)
pack_reverse	store an atom's info in a buffer communicating partial forces (required)
pack_reverse_hybrid	store extra info unique to this atom style (optional)
unpack_reverse	retrieve an atom's info from the buffer (required)
unpack_reverse_hybrid	retreive extra info unique to this atom style (optional)
pack_border	store an atom's info in a buffer communicated on neighbor re-builds (required)
pack_border_vel	add velocity info to buffer (required)
pack_border_hybrid	store extra info unique to this atom style (optional)
unpack_border	retrieve an atom's info from the buffer (required)
unpack_border_vel	also retrieve velocity info (required)
unpack_border_hybrid	retreive extra info unique to this atom style (optional)
pack_exchange	store all an atom's info to migrate to another processor (required)
unpack_exchange	retrieve an atom's info from the buffer (required)
size_restart	number of restart quantities associated with proc's atoms (required)
pack_restart	pack atom quantities into a buffer (required)
unpack_restart	unpack atom quantities from a buffer (required)
create_atom	create an individual atom of this style (required)
data_atom	parse an atom line from the data file (required)
data_atom_hybrid	parse additional atom info unique to this atom style (optional)
data_vel	parse one line of velocity information from data file (optional)
data_vel_hybrid	parse additional velocity data unique to this atom style (optional)
memory_usage	tally memory allocated by atom arrays (required)

The constructor of the derived class sets values for several variables that you must set when defining a new atom style, which are documented in atom_vec.h. New atom arrays are defined in atom.cpp. Search for the word "customize" and you will find locations you will need to modify.

NOTE: It is possible to add some attributes, such as a molecule ID, to atom styles that do not have them via the fix property/atom command. This command also allows new custom attributes consisting of extra integer or floating-point values to be added to atoms. See the fix property/atom doc page for examples of cases where this is useful and details on how to initialize, access, and output the custom values.

New pair styles, fixes, or computes can be added to LAMMPS, as discussed below. The code for these classes can use the per-atom properties defined by fix property/atom. The Atom class has a find_custom() method that is useful in this context:

```
int index = atom->find_custom(char *name, int &flag);
```

The "name" of a custom attribute, as specified in the fix property/atom command, is checked to verify that it exists and its index is returned. The method also sets flag = 0/1 depending on whether it is an integer or floating-point attribute. The vector of values associated with the attribute can then be accessed using the returned index as

```
int *ivector = atom->ivector[index];
double *dvector = atom->dvector[index];
```

Ivector or dvector are vectors of length Nlocal = # of owned atoms, which store the attributes of individual atoms.

10.2 Bond, angle, dihedral, improper potentials

Classes that compute molecular interactions are derived from the Bond, Angle, Dihedral, and Improper classes. New styles can be created to add new potentials to LAMMPS.

Bond_harmonic.cpp is the simplest example of a bond style. Ditto for the harmonic forms of the angle, dihedral, and improper style commands.

Here is a brief description of common methods you define in your new derived class. See bond.h, angle.h, dihedral.h, and improper.h for details and specific additional methods.

init	check if all coefficients are set, calls *init_style* (optional)
init_style	check if style specific conditions are met (optional)
compute	compute the molecular interactions (required)
settings	apply global settings for all types (optional)
coeff	set coefficients for one type (required)
equilibrium_distance	length of bond, used by SHAKE (required, bond only)
equilibrium_angle	opening of angle, used by SHAKE (required, angle only)
write & read_restart	writes/reads coeffs to restart files (required)
single	force and energy of a single bond or angle (required, bond or angle only)
memory_usage	tally memory allocated by the style (optional)

10.3 Compute styles

Classes that compute scalar and vector quantities like temperature and the pressure tensor, as well as classes that compute per-atom quantities like kinetic energy and the centro-symmetry parameter are derived from the Compute class. New styles can be created to add new calculations to LAMMPS.

Compute_temp.cpp is a simple example of computing a scalar temperature. Compute_ke_atom.cpp is a simple example of computing per-atom kinetic energy.

Here is a brief description of methods you define in your new derived class. See compute.h for details.

init	perform one time setup (required)
init_list	neighbor list setup, if needed (optional)
compute_scalar	compute a scalar quantity (optional)
compute_vector	compute a vector of quantities (optional)

compute_peratom	compute one or more quantities per atom (optional)
compute_local	compute one or more quantities per processor (optional)
pack_comm	pack a buffer with items to communicate (optional)
unpack_comm	unpack the buffer (optional)
pack_reverse	pack a buffer with items to reverse communicate (optional)
unpack_reverse	unpack the buffer (optional)
remove_bias	remove velocity bias from one atom (optional)
remove_bias_all	remove velocity bias from all atoms in group (optional)
restore_bias	restore velocity bias for one atom after remove_bias (optional)
restore_bias_all	same as before, but for all atoms in group (optional)
pair_tally_callback	callback function for *tally*-style computes (optional).
memory_usage	tally memory usage (optional)

Tally-style computes are a special case, as their computation is done in two stages: the callback function is registered with the pair style and then called from the Pair::ev_tally() function, which is called for each pair after force and energy has been computed for this pair. Then the tallied values are retrieved with the standard compute_scalar or compute_vector or compute_peratom methods. The USER-TALLY package provides *examples*_compute_tally.html for utilizing this mechanism.

10.4 Dump styles

10.5 Dump custom output options

Classes that dump per-atom info to files are derived from the Dump class. To dump new quantities or in a new format, a new derived dump class can be added, but it is typically simpler to modify the DumpCustom class contained in the dump_custom.cpp file.

Dump_atom.cpp is a simple example of a derived dump class.

Here is a brief description of methods you define in your new derived class. See dump.h for details.

write_header	write the header section of a snapshot of atoms
count	count the number of lines a processor will output
pack	pack a proc's output data into a buffer
write_data	write a proc's data to a file

See the dump command and its *custom* style for a list of keywords for atom information that can already be dumped by DumpCustom. It includes options to dump per-atom info from Compute classes, so adding a new derived Compute class is one way to calculate new quantities to dump.

Alternatively, you can add new keywords to the dump custom command. Search for the word "customize" in dump_custom.cpp to see the half-dozen or so locations where code will need to be added.

10.6 Fix styles

In LAMMPS, a "fix" is any operation that is computed during timestepping that alters some property of the system. Essentially everything that happens during a simulation besides force computation, neighbor list

construction, and output, is a "fix". This includes time integration (update of coordinates and velocities), force constraints or boundary conditions (SHAKE or walls), and diagnostics (compute a diffusion coefficient). New styles can be created to add new options to LAMMPS.

Fix_setforce.cpp is a simple example of setting forces on atoms to prescribed values. There are dozens of fix options already in LAMMPS; choose one as a template that is similar to what you want to implement.

Here is a brief description of methods you can define in your new derived class. See fix.h for details.

setmask	determines when the fix is called during the timestep (required)
init	initialization before a run (optional)
setup_pre_exchange	called before atom exchange in setup (optional)
setup_pre_force	called before force computation in setup (optional)
setup	called immediately before the 1st timestep and after forces are computed (optional)
min_setup_pre_force	like setup_pre_force, but for minimizations instead of MD runs (optional)
min_setup	like setup, but for minimizations instead of MD runs (optional)
initial_integrate	called at very beginning of each timestep (optional)
pre_exchange	called before atom exchange on re-neighboring steps (optional)
pre_neighbor	called before neighbor list build (optional)
pre_force	called before pair & molecular forces are computed (optional)
post_force	called after pair & molecular forces are computed and communicated (optional)
final_integrate	called at end of each timestep (optional)
end_of_step	called at very end of timestep (optional)
write_restart	dumps fix info to restart file (optional)
restart	uses info from restart file to re-initialize the fix (optional)
grow_arrays	allocate memory for atom-based arrays used by fix (optional)
copy_arrays	copy atom info when an atom migrates to a new processor (optional)
pack_exchange	store atom's data in a buffer (optional)
unpack_exchange	retrieve atom's data from a buffer (optional)
pack_restart	store atom's data for writing to restart file (optional)
unpack_restart	retrieve atom's data from a restart file buffer (optional)
size_restart	size of atom's data (optional)
maxsize_restart	max size of atom's data (optional)
setup_pre_force_respa	same as setup_pre_force, but for rRESPA (optional)
initial_integrate_respa	same as initial_integrate, but for rRESPA (optional)
post_integrate_respa	called after the first half integration step is done in rRESPA (optional)
pre_force_respa	same as pre_force, but for rRESPA (optional)
post_force_respa	same as post_force, but for rRESPA (optional)
final_integrate_respa	same as final_integrate, but for rRESPA (optional)
min_pre_force	called after pair & molecular forces are computed in minimizer (optional)
min_post_force	called after pair & molecular forces are computed and communicated in minmizer (optional)
min_store	store extra data for linesearch based minimization on a LIFO stack (optional)
min_pushstore	push the minimization LIFO stack one element down (optional)
min_popstore	pop the minimization LIFO stack one element up (optional)

min_clearstore	clear minimization LIFO stack (optional)
min_step	reset or move forward on line search minimization (optional)
min_dof	report number of degrees of freedom *added* by this fix in minimization (optional)
max_alpha	report maximum allowed step size during linesearch minimization (optional)
pack_comm	pack a buffer to communicate a per-atom quantity (optional)
unpack_comm	unpack a buffer to communicate a per-atom quantity (optional)
pack_reverse_comm	pack a buffer to reverse communicate a per-atom quantity (optional)
unpack_reverse_comm	unpack a buffer to reverse communicate a per-atom quantity (optional)
dof	report number of degrees of freedom *removed* by this fix during MD (optional)
compute_scalar	return a global scalar property that the fix computes (optional)
compute_vector	return a component of a vector property that the fix computes (optional)
compute_array	return a component of an array property that the fix computes (optional)
deform	called when the box size is changed (optional)
reset_target	called when a change of the target temperature is requested during a run (optional)
reset_dt	is called when a change of the time step is requested during a run (optional)
modify_param	called when a fix_modify request is executed (optional)
memory_usage	report memory used by fix (optional)
thermo	compute quantities for thermodynamic output (optional)

Typically, only a small fraction of these methods are defined for a particular fix. Setmask is mandatory, as it determines when the fix will be invoked during the timestep. Fixes that perform time integration (*nve*, *nvt*, *npt*) implement initial_integrate() and final_integrate() to perform velocity Verlet updates. Fixes that constrain forces implement post_force().

Fixes that perform diagnostics typically implement end_of_step(). For an end_of_step fix, one of your fix arguments must be the variable "nevery" which is used to determine when to call the fix and you must set this variable in the constructor of your fix. By convention, this is the first argument the fix defines (after the ID, group-ID, style).

If the fix needs to store information for each atom that persists from timestep to timestep, it can manage that memory and migrate the info with the atoms as they move from processors to processor by implementing the grow_arrays, copy_arrays, pack_exchange, and unpack_exchange methods. Similarly, the pack_restart and unpack_restart methods can be implemented to store information about the fix in restart files. If you wish an integrator or force constraint fix to work with rRESPA (see the run_style command), the initial_integrate, post_force_integrate, and final_integrate_respa methods can be implemented. The thermo method enables a fix to contribute values to thermodynamic output, as printed quantities and/or to be summed to the potential energy of the system.

10.7 Input script commands

New commands can be added to LAMMPS input scripts by adding new classes that have a "command" method. For example, the create_atoms, read_data, velocity, and run commands are all implemented in this fashion. When such a command is encountered in the LAMMPS input script, LAMMPS simply creates a class with the corresponding name, invokes the "command" method of the class, and passes it the arguments from the input script. The command method can perform whatever operations it wishes on LAMMPS data structures.

The single method your new class must define is as follows:

command	operations performed by the new command

Of course, the new class can define other methods and variables as needed.

10.8 Kspace computations

Classes that compute long-range Coulombic interactions via K-space representations (Ewald, PPPM) are derived from the KSpace class. New styles can be created to add new K-space options to LAMMPS.

Ewald.cpp is an example of computing K-space interactions.

Here is a brief description of methods you define in your new derived class. See kspace.h for details.

init	initialize the calculation before a run
setup	computation before the 1st timestep of a run
compute	every-timestep computation
memory_usage	tally of memory usage

10.9 Minimization styles

Classes that perform energy minimization derived from the Min class. New styles can be created to add new minimization algorithms to LAMMPS.

Min_cg.cpp is an example of conjugate gradient minimization.

Here is a brief description of methods you define in your new derived class. See min.h for details.

init	initialize the minimization before a run
run	perform the minimization
memory_usage	tally of memory usage

10.10 Pairwise potentials

Classes that compute pairwise interactions are derived from the Pair class. In LAMMPS, pairwise calculation include manybody potentials such as EAM or Tersoff where particles interact without a static bond topology. New styles can be created to add new pair potentials to LAMMPS.

Pair_lj_cut.cpp is a simple example of a Pair class, though it includes some optional methods to enable its use with rRESPA.

Here is a brief description of the class methods in pair.h:

compute	workhorse routine that computes pairwise interactions
settings	reads the input script line with arguments you define
coeff	set coefficients for one i,j type pair
init_one	perform initialization for one i,j type pair
init_style	initialization specific to this pair style

write & read_restart	write/read i,j pair coeffs to restart files
write & read_restart_settings	write/read global settings to restart files
single	force and energy of a single pairwise interaction between 2 atoms
compute_inner/middle/outer	versions of compute used by rRESPA

The inner/middle/outer routines are optional.

10.11 Region styles

Classes that define geometric regions are derived from the Region class. Regions are used elsewhere in LAMMPS to group atoms, delete atoms to create a void, insert atoms in a specified region, etc. New styles can be created to add new region shapes to LAMMPS.

Region_sphere.cpp is an example of a spherical region.

Here is a brief description of methods you define in your new derived class. See region.h for details.

match	determine whether a point is in the region

10.11 Body styles

Classes that define body particles are derived from the Body class. Body particles can represent complex entities, such as surface meshes of discrete points, collections of sub-particles, deformable objects, etc.

See Section_howto 14 of the manual for an overview of using body particles and the body doc page for details on the various body styles LAMMPS supports. New styles can be created to add new kinds of body particles to LAMMPS.

Body_nparticle.cpp is an example of a body particle that is treated as a rigid body containing N sub-particles.

Here is a brief description of methods you define in your new derived class. See body.h for details.

data_body	process a line from the Bodies section of a data file
noutrow	number of sub-particles output is generated for
noutcol	number of values per-sub-particle output is generated for
output	output values for the Mth sub-particle
pack_comm_body	body attributes to communicate every timestep
unpack_comm_body	unpacking of those attributes
pack_border_body	body attributes to communicate when reneighboring is done
unpack_border_body	unpacking of those attributes

10.13 Thermodynamic output options

There is one class that computes and prints thermodynamic information to the screen and log file; see the file thermo.cpp.

There are two styles defined in thermo.cpp: "one" and "multi". There is also a flexible "custom" style which allows the user to explicitly list keywords for quantities to print when thermodynamic info is output. See the thermo_style command for a list of defined quantities.

The thermo styles (one, multi, etc) are simply lists of keywords. Adding a new style thus only requires defining a new list of keywords. Search for the word "customize" with references to "thermo style" in thermo.cpp to see the two locations where code will need to be added.

New keywords can also be added to thermo.cpp to compute new quantities for output. Search for the word "customize" with references to "keyword" in thermo.cpp to see the several locations where code will need to be added.

Note that the thermo_style custom command already allows for thermo output of quantities calculated by fixes, computes, and variables. Thus, it may be simpler to compute what you wish via one of those constructs, than by adding a new keyword to the thermo command.

10.14 Variable options

There is one class that computes and stores variable information in LAMMPS; see the file variable.cpp. The value associated with a variable can be periodically printed to the screen via the print, fix print, or thermo_style custom commands. Variables of style "equal" can compute complex equations that involve the following types of arguments:

```
thermo keywords = ke, vol, atoms, ...
other variables = v_a, v_myvar, ...
math functions = div(x,y), mult(x,y), add(x,y), ...
group functions = mass(group), xcm(group,x), ...
atom values = x[123], y[3], vx[34], ...
compute values = c_mytemp[0], c_thermo_press[3], ...
```

Adding keywords for the thermo_style custom command (which can then be accessed by variables) was discussed here on this page.

Adding a new math function of one or two arguments can be done by editing one section of the Variable::evaulate() method. Search for the word "customize" to find the appropriate location.

Adding a new group function can be done by editing one section of the Variable::evaulate() method. Search for the word "customize" to find the appropriate location. You may need to add a new method to the Group class as well (see the group.cpp file).

Accessing a new atom-based vector can be done by editing one section of the Variable::evaulate() method. Search for the word "customize" to find the appropriate location.

Adding new compute styles (whose calculated values can then be accessed by variables) was discussed here on this page.

10.15 Submitting new features for inclusion in LAMMPS

We encourage users to submit new features to the developers that they add to LAMMPS, especially if you think they will be of interest to other users. If they are broadly useful we may add them as core files to LAMMPS or as

part of a standard package. Else we will add them as a user-contributed file or package. Examples of user packages are in src sub-directories that start with USER. The USER-MISC package is simply a collection of (mostly) unrelated single files, which is the simplest way to have your contribution quickly added to the LAMMPS distribution. You can see a list of the both standard and user packages by typing "make package" in the LAMMPS src directory.

Note that by providing us the files to release, you are agreeing to make them open-source, i.e. we can release them under the terms of the GPL, used as a license for the rest of LAMMPS. See Section 1.4 for details.

With user packages and files, all we are really providing (aside from the fame and fortune that accompanies having your name in the source code and on the Authors page of the LAMMPS WWW site), is a means for you to distribute your work to the LAMMPS user community, and a mechanism for others to easily try out your new feature. This may help you find bugs or make contact with new collaborators. Note that you're also implicitly agreeing to support your code which means answer questions, fix bugs, and maintain it if LAMMPS changes in some way that breaks it (an unusual event).

NOTE: If you prefer to actively develop and support your add-on feature yourself, then you may wish to make it available for download from your own website, as a user package that LAMMPS users can add to their copy of LAMMPS. See the Offsite LAMMPS packages and tools page of the LAMMPS web site for examples of groups that do this. We are happy to advertise your package and web site from that page. Simply email the developers with info about your package and we will post it there.

The previous sections of this doc page describe how to add new "style" files of various kinds to LAMMPS. Packages are simply collections of one or more new class files which are invoked as a new style within a LAMMPS input script. If designed correctly, these additions typically do not require changes to the main core of LAMMPS; they are simply add-on files. If you think your new feature requires non-trivial changes in core LAMMPS files, you'll need to communicate with the developers, since we may or may not want to make those changes. An example of a trivial change is making a parent-class method "virtual" when you derive a new child class from it.

Here are the steps you need to follow to submit a single file or user package for our consideration. Following these steps will save both you and us time. See existing files in packages in the src dir for examples.

- All source files you provide must compile with the most current version of LAMMPS.
- If you want your file(s) to be added to main LAMMPS or one of its standard packages, then it needs to be written in a style compatible with other LAMMPS source files. This is so the developers can understand it and hopefully maintain it. This basically means that the code accesses data structures, performs its operations, and is formatted similar to other LAMMPS source files, including the use of the error class for error and warning messages.
- If you want your contribution to be added as a user-contributed feature, and it's a single file (actually a *.cpp and *.h file) it can rapidly be added to the USER-MISC directory. Send us the one-line entry to add to the USER-MISC/README file in that dir, along with the 2 source files. You can do this multiple times if you wish to contribute several individual features.
- If you want your contribution to be added as a user-contribution and it is several related featues, it is probably best to make it a user package directory with a name like USER-FOO. In addition to your new files, the directory should contain a README text file. The README should contain your name and contact information and a brief description of what your new package does. If your files depend on other LAMMPS style files also being installed (e.g. because your file is a derived class from the other LAMMPS class), then an Install.sh file is also needed to check for those dependencies. See other README and Install.sh files in other USER directories as examples. Send us a tarball of this USER-FOO directory.
- Your new source files need to have the LAMMPS copyright, GPL notice, and your name and email

address at the top, like other user-contributed LAMMPS source files. They need to create a class that is inside the LAMMPS namespace. If the file is for one of the USER packages, including USER-MISC, then we are not as picky about the coding style (see above). I.e. the files do not need to be in the same stylistic format and syntax as other LAMMPS files, though that would be nice for developers as well as users who try to read your code.

- You must also create a documentation file for each new command or style you are adding to LAMMPS. This will be one file for a single-file feature. For a package, it might be several files. These are simple text files which we auto-convert to HTML. Thus they must be in the same format as other *.txt files in the lammps/doc directory for similar commands and styles; use one or more of them as a starting point. As appropriate, the text files can include links to equations (see doc/Eqs/*.tex for examples, we auto-create the associated JPG files), or figures (see doc/JPG for examples), or even additional PDF files with further details (see doc/PDF for examples). The doc page should also include literature citations as appropriate; see the bottom of doc/fix_nh.txt for examples and the earlier part of the same file for how to format the cite itself. The "Restrictions" section of the doc page should indicate that your command is only available if LAMMPS is built with the appropriate USER-MISC or USER-FOO package. See other user package doc files for examples of how to do this. The txt2html tool we use to convert to HTML can be downloaded from this site, so you can perform the HTML conversion yourself to proofread your doc page.
- For a new package (or even a single command) you can include one or more example scripts. These should run in no more than 1 minute, even on a single processor, and not require large data files as input. See directories under examples/USER for examples of input scripts other users provided for their packages.
- If there is a paper of yours describing your feature (either the algorithm/science behind the feature itself, or its initial usage, or its implementation in LAMMPS), you can add the citation to the *.cpp source file. See src/USER-EFF/atom_vec_electron.cpp for an example. A LaTeX citation is stored in a variable at the top of the file and a single line of code that references the variable is added to the constructor of the class. Whenever a user invokes your feature from their input script, this will cause LAMMPS to output the citation to a log.cite file and prompt the user to examine the file. Note that you should only use this for a paper you or your group authored. E.g. adding a cite in the code for a paper by Nose and Hoover if you write a fix that implements their integrator is not the intended usage. That kind of citation should just be in the doc page you provide.

Finally, as a general rule-of-thumb, the more clear and self-explanatory you make your doc and README files, and the easier you make it for people to get started, e.g. by providing example scripts, the more likely it is that users will try out your new feature.

(Foo) Foo, Morefoo, and Maxfoo, J of Classic Potentials, 75, 345 (1997).

11. Python interface to LAMMPS

LAMMPS can work together with Python in two ways. First, Python can wrap LAMMPS through the LAMMPS library interface, so that a Python script can create one or more instances of LAMMPS and launch one or more simulations. In Python lingo, this is "extending" Python with LAMMPS.

Second, LAMMPS can use the Python interpreter, so that a LAMMPS input script can invoke Python code, and pass information back-and-forth between the input script and Python functions you write. The Python code can also callback to LAMMPS to query or change its attributes. In Python lingo, this is "embedding" Python in LAMMPS.

This section describes how to do both.

If you are not familiar with it, Python is a powerful scripting and programming language which can essentially do anything that faster, lower-level languages like C or C++ can do, but typically with much fewer lines of code. When used in embedded mode, Python can perform operations that the simplistic LAMMPS input script syntax cannot. Python can be also be used as a "glue" language to drive a program through its library interface, or to hook multiple pieces of software together, such as a simulation package plus a visualization package, or to run a coupled multiscale or multiphysics model.

See Section_howto 10 of the manual and the couple directory of the distribution for more ideas about coupling LAMMPS to other codes. See Section_howto 19 for a description of the LAMMPS library interface provided in src/library.cpp and src/library.h, and how to extend it for your needs. As described below, that interface is what is exposed to Python either when calling LAMMPS from Python or when calling Python from a LAMMPS input script and then calling back to LAMMPS from Python code. The library interface is designed to be easy to add functions to. Thus the Python interface to LAMMPS is also easy to extend as well.

If you create interesting Python scripts that run LAMMPS or interesting Python functions that can be called from a LAMMPS input script, that you think would be useful to other users, please email them to the developers. We can include them in the LAMMPS distribution.

11.1 Overview of running LAMMPS from Python

The LAMMPS distribution includes a python directory with all you need to run LAMMPS from Python. The python/lammps.py file wraps the LAMMPS library interface, with one wrapper function per LAMMPS library function. This file makes it is possible to do the following either from a Python script, or interactively from a Python prompt: create one or more instances of LAMMPS, invoke LAMMPS commands or give it an input script, run LAMMPS incrementally, extract LAMMPS results, an modify internal LAMMPS variables. From a Python script you can do this in serial or parallel. Running Python interactively in parallel does not generally work, unless

you have a version of Python that extends standard Python to enable multiple instances of Python to read what you type.

To do all of this, you must first build LAMMPS as a shared library, then insure that your Python can find the python/lammps.py file and the shared library. These steps are explained in subsequent sections 11.3 and 11.4. Sections 11.5 and 11.6 discuss using MPI from a parallel Python program and how to test that you are ready to use LAMMPS from Python. Section 11.7 lists all the functions in the current LAMMPS library interface and how to call them from Python.

Section 11.8 gives some examples of coupling LAMMPS to other tools via Python. For example, LAMMPS can easily be coupled to a GUI or other visualization tools that display graphs or animations in real time as LAMMPS runs. Examples of such scripts are inlcluded in the python directory.

Two advantages of using Python to run LAMMPS are how concise the language is, and that it can be run interactively, enabling rapid development and debugging of programs. If you use it to mostly invoke costly operations within LAMMPS, such as running a simulation for a reasonable number of timesteps, then the overhead cost of invoking LAMMPS thru Python will be negligible.

The Python wrapper for LAMMPS uses the amazing and magical (to me) "ctypes" package in Python, which auto-generates the interface code needed between Python and a set of C interface routines for a library. Ctypes is part of standard Python for versions 2.5 and later. You can check which version of Python you have installed, by simply typing "python" at a shell prompt.

11.2 Overview of using Python from a LAMMPS script

NOTE: It is not currently possible to use the python command described in this section with Python 3, only with Python 2. The C API changed from Python 2 to 3 and the LAMMPS code is not compatible with both.

LAMMPS has a python command which can be used in an input script to define and execute a Python function that you write the code for. The Python function can also be assigned to a LAMMPS python-style variable via the variable command. Each time the variable is evaluated, either in the LAMMPS input script itself, or by another LAMMPS command that uses the variable, this will trigger the Python function to be invoked.

The Python code for the function can be included directly in the input script or in an auxiliary file. The function can have arguments which are mapped to LAMMPS variables (also defined in the input script) and it can return a value to a LAMMPS variable. This is thus a mechanism for your input script to pass information to a piece of Python code, ask Python to execute the code, and return information to your input script.

Note that a Python function can be arbitrarily complex. It can import other Python modules, instantiate Python classes, call other Python functions, etc. The Python code that you provide can contain more code than the single function. It can contain other functions or Python classes, as well as global variables or other mechanisms for storing state between calls from LAMMPS to the function.

The Python function you provide can consist of "pure" Python code that only performs operations provided by standard Python. However, the Python function can also "call back" to LAMMPS through its Python-wrapped library interface, in the manner described in the previous section 11.1. This means it can issue LAMMPS input script commands or query and set internal LAMMPS state. As an example, this can be useful in an input script to create a more complex loop with branching logic, than can be created using the simple looping and brancing logic enabled by the next and if commands.

See the python doc page and the variable doc page for its python-style variables for more info, including examples of Python code you can write for both pure Python operations and callbacks to LAMMPS.

To run pure Python code from LAMMPS, you only need to build LAMMPS with the PYTHON package installed:

```
make yes-python
make machine
```

Note that this will link LAMMPS with the Python library on your system, which typically requires several auxiliary system libraries to also be linked. The list of these libraries and the paths to find them are specified in the lib/python/Makefile.lammps file. You need to insure that file contains the correct information for your version of Python and your machine to successfully build LAMMPS. See the lib/python/README file for more info.

If you want to write Python code with callbacks to LAMMPS, then you must also follow the steps overviewed in the preceeding section (11.1) for running LAMMPS from Python. I.e. you must build LAMMPS as a shared library and insure that Python can find the python/lammps.py file and the shared library.

11.3 Building LAMMPS as a shared library

Instructions on how to build LAMMPS as a shared library are given in Section_start 5. A shared library is one that is dynamically loadable, which is what Python requires to wrap LAMMPS. On Linux this is a library file that ends in ".so", not ".a".

From the src directory, type

```
make foo mode=shlib
```

where foo is the machine target name, such as linux or g++ or serial. This should create the file liblammps_foo.so in the src directory, as well as a soft link liblammps.so, which is what the Python wrapper will load by default. Note that if you are building multiple machine versions of the shared library, the soft link is always set to the most recently built version.

NOTE: If you are building LAMMPS with an MPI or FFT library or other auxiliary libraries (used by various packages), then all of these extra libraries must also be shared libraries. If the LAMMPS shared-library build fails with an error complaining about this, see Section_start 5 for more details.

11.4 Installing the Python wrapper into Python

For Python to invoke LAMMPS, there are 2 files it needs to know about:

- python/lammps.py
- src/liblammps.so

Lammps.py is the Python wrapper on the LAMMPS library interface. Liblammps.so is the shared LAMMPS library that Python loads, as described above.

You can insure Python can find these files in one of two ways:

- set two environment variables
- run the python/install.py script

If you set the paths to these files as environment variables, you only have to do it once. For the csh or tcsh shells, add something like this to your ~/.cshrc file, one line for each of the two files:

```
setenv PYTHONPATH ${PYTHONPATH}:/home/sjplimp/lammps/python
setenv LD_LIBRARY_PATH ${LD_LIBRARY_PATH}:/home/sjplimp/lammps/src
```

If you use the python/install.py script, you need to invoke it every time you rebuild LAMMPS (as a shared library) or make changes to the python/lammps.py file.

You can invoke install.py from the python directory as

```
% python install.py [libdir] [pydir]
```

The optional libdir is where to copy the LAMMPS shared library to; the default is /usr/local/lib. The optional pydir is where to copy the lammps.py file to; the default is the site-packages directory of the version of Python that is running the install script.

Note that libdir must be a location that is in your default LD_LIBRARY_PATH, like /usr/local/lib or /usr/lib. And pydir must be a location that Python looks in by default for imported modules, like its site-packages dir. If you want to copy these files to non-standard locations, such as within your own user space, you will need to set your PYTHONPATH and LD_LIBRARY_PATH environment variables accordingly, as above.

If the install.py script does not allow you to copy files into system directories, prefix the python command with "sudo". If you do this, make sure that the Python that root runs is the same as the Python you run. E.g. you may need to do something like

```
% sudo /usr/local/bin/python install.py [libdir] [pydir]
```

You can also invoke install.py from the make command in the src directory as

```
% make install-python
```

In this mode you cannot append optional arguments. Again, you may need to prefix this with "sudo". In this mode you cannot control which Python is invoked by root.

Note that if you want Python to be able to load different versions of the LAMMPS shared library (see this section below), you will need to manually copy files like liblammps_g++.so into the appropriate system directory. This is not needed if you set the LD_LIBRARY_PATH environment variable as described above.

11.5 Extending Python with MPI to run in parallel

If you wish to run LAMMPS in parallel from Python, you need to extend your Python with an interface to MPI. This also allows you to make MPI calls directly from Python in your script, if you desire.

There are several Python packages available that purport to wrap MPI as a library and allow MPI functions to be called from Python.

These include

- pyMPI
- maroonmpi
- mpi4py

- myMPI
- Pypar

All of these except pyMPI work by wrapping the MPI library and exposing (some portion of) its interface to your Python script. This means Python cannot be used interactively in parallel, since they do not address the issue of interactive input to multiple instances of Python running on different processors. The one exception is pyMPI, which alters the Python interpreter to address this issue, and (I believe) creates a new alternate executable (in place of "python" itself) as a result.

In principle any of these Python/MPI packages should work to invoke LAMMPS in parallel and to make MPI calls themselves from a Python script which is itself running in parallel. However, when I downloaded and looked at a few of them, their documentation was incomplete and I had trouble with their installation. It's not clear if some of the packages are still being actively developed and supported.

The packages Pypar and mpi4py have both been successfully tested with LAMMPS. Pypar is simpler and easy to set up and use, but supports only a subset of MPI. Mpi4py is more MPI-feature complete, but also a bit more complex to use. As of version 2.0.0, mpi4py is the only python MPI wrapper that allows passing a custom MPI communicator to the LAMMPS constructor, which means one can easily run one or more LAMMPS instances on subsets of the total MPI ranks.

Pypar requires the ubiquitous Numpy package be installed in your Python. After launching Python, type

```
import numpy
```

to see if it is installed. If not, here is how to install it (version 1.3.0b1 as of April 2009). Unpack the numpy tarball and from its top-level directory, type

```
python setup.py build
sudo python setup.py install
```

The "sudo" is only needed if required to copy Numpy files into your Python distribution's site-packages directory.

To install Pypar (version pypar-2.1.4_94 as of Aug 2012), unpack it and from its "source" directory, type

```
python setup.py build
sudo python setup.py install
```

Again, the "sudo" is only needed if required to copy Pypar files into your Python distribution's site-packages directory.

If you have successully installed Pypar, you should be able to run Python and type

```
import pypar
```

without error. You should also be able to run python in parallel on a simple test script

```
% mpirun -np 4 python test.py
```

where test.py contains the lines

```
import pypar
print "Proc %d out of %d procs" % (pypar.rank(),pypar.size())
```

and see one line of output for each processor you run on.

NOTE: To use Pypar and LAMMPS in parallel from Python, you must insure both are using the same version of MPI. If you only have one MPI installed on your system, this is not an issue, but it can be if you have multiple MPIs. Your LAMMPS build is explicit about which MPI it is using, since you specify the details in your lo-level src/MAKE/Makefile.foo file. Pypar uses the "mpicc" command to find information about the MPI it uses to build against. And it tries to load "libmpi.so" from the LD_LIBRARY_PATH. This may or may not find the MPI library that LAMMPS is using. If you have problems running both Pypar and LAMMPS together, this is an issue you may need to address, e.g. by moving other MPI installations so that Pypar finds the right one.

To install mpi4py (version mpi4py-2.0.0 as of Oct 2015), unpack it and from its main directory, type

```
python setup.py build
sudo python setup.py install
```

Again, the "sudo" is only needed if required to copy mpi4py files into your Python distribution's site-packages directory. To install with user privilege into the user local directory type

```
python setup.py install --user
```

If you have successully installed mpi4py, you should be able to run Python and type

```
from mpi4py import MPI
```

without error. You should also be able to run python in parallel on a simple test script

```
% mpirun -np 4 python test.py
```

where test.py contains the lines

```
from mpi4py import MPI
comm = MPI.COMM_WORLD
print "Proc %d out of %d procs" % (comm.Get_rank(),comm.Get_size())
```

and see one line of output for each processor you run on.

NOTE: To use mpi4py and LAMMPS in parallel from Python, you must insure both are using the same version of MPI. If you only have one MPI installed on your system, this is not an issue, but it can be if you have multiple MPIs. Your LAMMPS build is explicit about which MPI it is using, since you specify the details in your lo-level src/MAKE/Makefile.foo file. Mpi4py uses the "mpicc" command to find information about the MPI it uses to build against. And it tries to load "libmpi.so" from the LD_LIBRARY_PATH. This may or may not find the MPI library that LAMMPS is using. If you have problems running both mpi4py and LAMMPS together, this is an issue you may need to address, e.g. by moving other MPI installations so that mpi4py finds the right one.

11.6 Testing the Python-LAMMPS interface

To test if LAMMPS is callable from Python, launch Python interactively and type:

```
>>> from lammps import lammps
>>> lmp = lammps()
```

If you get no errors, you're ready to use LAMMPS from Python. If the 2nd command fails, the most common error to see is

```
OSError: Could not load LAMMPS dynamic library
```

which means Python was unable to load the LAMMPS shared library. This typically occurs if the system can't find the LAMMPS shared library or one of the auxiliary shared libraries it depends on, or if something about the library is incompatible with your Python. The error message should give you an indication of what went wrong.

You can also test the load directly in Python as follows, without first importing from the lammps.py file:

```
>>> from ctypes import CDLL
>>> CDLL("liblammps.so")
```

If an error occurs, carefully go thru the steps in Section_start 5 and above about building a shared library and about insuring Python can find the necessary two files it needs.

Test LAMMPS and Python in serial:

To run a LAMMPS test in serial, type these lines into Python interactively from the bench directory:

```
>>> from lammps import lammps
>>> lmp = lammps()
>>> lmp.file("in.lj")
```

Or put the same lines in the file test.py and run it as

```
% python test.py
```

Either way, you should see the results of running the in.lj benchmark on a single processor appear on the screen, the same as if you had typed something like:

```
lmp_g++ -in in.lj
```

Test LAMMPS and Python in parallel:

To run LAMMPS in parallel, assuming you have installed the Pypar package as discussed above, create a test.py file containing these lines:

```
import pypar
from lammps import lammps
lmp = lammps()
lmp.file("in.lj")
print "Proc %d out of %d procs has" % (pypar.rank(),pypar.size()),lmp
pypar.finalize()
```

To run LAMMPS in parallel, assuming you have installed the mpi4py package as discussed above, create a test.py file containing these lines:

```
from mpi4py import MPI
from lammps import lammps
lmp = lammps()
lmp.file("in.lj")
me = MPI.COMM_WORLD.Get_rank()
nprocs = MPI.COMM_WORLD.Get_size()
print "Proc %d out of %d procs has" % (me,nprocs),lmp
MPI.Finalize()
```

You can either script in parallel as:

```
% mpirun -np 4 python test.py
```

and you should see the same output as if you had typed

```
% mpirun -np 4 lmp_g++ -in in.lj
```

Note that if you leave out the 3 lines from test.py that specify Pypar commands you will instantiate and run LAMMPS independently on each of the P processors specified in the mpirun command. In this case you should get 4 sets of output, each showing that a LAMMPS run was made on a single processor, instead of one set of output showing that LAMMPS ran on 4 processors. If the 1-processor outputs occur, it means that Pypar is not working correctly.

Also note that once you import the PyPar module, Pypar initializes MPI for you, and you can use MPI calls directly in your Python script, as described in the Pypar documentation. The last line of your Python script should be pypar.finalize(), to insure MPI is shut down correctly.

Running Python scripts:

Note that any Python script (not just for LAMMPS) can be invoked in one of several ways:

```
% python foo.script
% python -i foo.script
% foo.script
```

The last command requires that the first line of the script be something like this:

```
#!/usr/local/bin/python
#!/usr/local/bin/python -i
```

where the path points to where you have Python installed, and that you have made the script file executable:

```
% chmod +x foo.script
```

Without the "-i" flag, Python will exit when the script finishes. With the "-i" flag, you will be left in the Python interpreter when the script finishes, so you can type subsequent commands. As mentioned above, you can only run Python interactively when running Python on a single processor, not in parallel.

11.7 Using LAMMPS from Python

As described above, the Python interface to LAMMPS consists of a Python "lammps" module, the source code for which is in python/lammps.py, which creates a "lammps" object, with a set of methods that can be invoked on that object. The sample Python code below assumes you have first imported the "lammps" module in your Python script, as follows:

```
from lammps import lammps
```

These are the methods defined by the lammps module. If you look at the files src/library.cpp and src/library.h you will see that they correspond one-to-one with calls you can make to the LAMMPS library from a C++ or C or Fortran program.

```
lmp = lammps()           # create a LAMMPS object using the default liblammps.so library
                         4 optional args are allowed: name, cmdargs, ptr, comm
lmp = lammps(ptr=lmpptr) # use lmpptr as previously created LAMMPS object
lmp = lammps(comm=split) # create a LAMMPS object with a custom communicator, requires mpi4py 2.0.0
lmp = lammps(name="g++")   # create a LAMMPS object using the liblammps_g++.so library
```

```
lmp = lammps(name="g++",cmdargs=list)    # add LAMMPS command-line args, e.g. list = ["-echo","scree

lmp.close()              # destroy a LAMMPS object
```

version = lmp.version() # return the numerical version id, e.g. LAMMPS 2 Sep 2015 -> 20150902

```
lmp.file(file)           # run an entire input script, file = "in.lj"
lmp.command(cmd)         # invoke a single LAMMPS command, cmd = "run 100"

xlo = lmp.extract_global(name,type)  # extract a global quantity
                                     # name = "boxxlo", "nlocal", etc
                                     # type = 0 = int
                                     #        1 = double

coords = lmp.extract_atom(name,type)       # extract a per-atom quantity
                                           # name = "x", "type", etc
                                           # type = 0 = vector of ints
                                           #        1 = array of ints
                                           #        2 = vector of doubles
                                           #        3 = array of doubles

eng = lmp.extract_compute(id,style,type)  # extract value(s) from a compute
v3 = lmp.extract_fix(id,style,type,i,j)   # extract value(s) from a fix
                                          # id = ID of compute or fix
                                          # style = 0 = global data
                                          #         1 = per-atom data
                                          #         2 = local data
                                          # type = 0 = scalar
                                          #        1 = vector
                                          #        2 = array
                                          # i,j = indices of value in global vector or array

var = lmp.extract_variable(name,group,flag)  # extract value(s) from a variable
                                             # name = name of variable
                                             # group = group ID (ignored for equal-style variables)
                                             # flag = 0 = equal-style variable
                                             #        1 = atom-style variable

flag = lmp.set_variable(name,value)       # set existing named string-style variable to value, flag
natoms = lmp.get_natoms()                 # total # of atoms as int
data = lmp.gather_atoms(name,type,count)  # return atom attribute of all atoms gathered into data, o
                                          # name = "x", "charge", "type", etc
                                          # count = # of per-atom values, 1 or 3, etc
lmp.scatter_atoms(name,type,count,data)   # scatter atom attribute of all atoms from data, ordered b
                                          # name = "x", "charge", "type", etc
                                          # count = # of per-atom values, 1 or 3, etc
```

The lines

```
from lammps import lammps
lmp = lammps()
```

create an instance of LAMMPS, wrapped in a Python class by the lammps Python module, and return an instance of the Python class as lmp. It is used to make all subequent calls to the LAMMPS library.

Additional arguments can be used to tell Python the name of the shared library to load or to pass arguments to the LAMMPS instance, the same as if LAMMPS were launched from a command-line prompt.

If the ptr argument is set like this:

```
lmp = lammps(ptr=lmpptr)
```

then lmpptr must be an argument passed to Python via the LAMMPS python command, when it is used to define a Python function that is invoked by the LAMMPS input script. This mode of using Python with LAMMPS is described above in 11.2. The variable lmpptr refers to the instance of LAMMPS that called the embedded Python interpreter. Using it as an argument to lammps() allows the returned Python class instance "lmp" to make calls to that instance of LAMMPS. See the python command doc page for examples using this syntax.

Note that you can create multiple LAMMPS objects in your Python script, and coordinate and run multiple simulations, e.g.

```
from lammps import lammps
lmp1 = lammps()
lmp2 = lammps()
lmp1.file("in.file1")
lmp2.file("in.file2")
```

The file() and command() methods allow an input script or single commands to be invoked.

The extract_global(), extract_atom(), extract_compute(), extract_fix(), and extract_variable() methods return values or pointers to data structures internal to LAMMPS.

For extract_global() see the src/library.cpp file for the list of valid names. New names could easily be added. A double or integer is returned. You need to specify the appropriate data type via the type argument.

For extract_atom(), a pointer to internal LAMMPS atom-based data is returned, which you can use via normal Python subscripting. See the extract() method in the src/atom.cpp file for a list of valid names. Again, new names could easily be added. A pointer to a vector of doubles or integers, or a pointer to an array of doubles (double **) or integers (int **) is returned. You need to specify the appropriate data type via the type argument.

For extract_compute() and extract_fix(), the global, per-atom, or local data calulated by the compute or fix can be accessed. What is returned depends on whether the compute or fix calculates a scalar or vector or array. For a scalar, a single double value is returned. If the compute or fix calculates a vector or array, a pointer to the internal LAMMPS data is returned, which you can use via normal Python subscripting. The one exception is that for a fix that calculates a global vector or array, a single double value from the vector or array is returned, indexed by I (vector) or I and J (array). I,J are zero-based indices. The I,J arguments can be left out if not needed. See Section_howto 15 of the manual for a discussion of global, per-atom, and local data, and of scalar, vector, and array data types. See the doc pages for individual computes and fixes for a description of what they calculate and store.

For extract_variable(), an equal-style or atom-style variable is evaluated and its result returned.

For equal-style variables a single double value is returned and the group argument is ignored. For atom-style variables, a vector of doubles is returned, one value per atom, which you can use via normal Python subscripting. The values will be zero for atoms not in the specified group.

The get_natoms() method returns the total number of atoms in the simulation, as an int.

The gather_atoms() method returns a ctypes vector of ints or doubles as specified by type, of length count*natoms, for the property of all the atoms in the simulation specified by name, ordered by count and then by atom ID. The vector can be used via normal Python subscripting. If atom IDs are not consecutively ordered within LAMMPS, a None is returned as indication of an error.

Note that the data structure gather_atoms("x") returns is different from the data structure returned by extract_atom("x") in four ways. (1) Gather_atoms() returns a vector which you index as x[i]; extract_atom() returns an array which you index as x[i][j]. (2) Gather_atoms() orders the atoms by atom ID while extract_atom() does not. (3) Gathert_atoms() returns a list of all atoms in the simulation; extract_atoms() returns just the atoms local to each processor. (4) Finally, the gather_atoms() data structure is a copy of the atom coords stored internally in LAMMPS, whereas extract_atom() returns an array that effectively points directly to the internal data. This means you can change values inside LAMMPS from Python by assigning a new values to the extract_atom() array. To do this with the gather_atoms() vector, you need to change values in the vector, then invoke the scatter_atoms() method.

The scatter_atoms() method takes a vector of ints or doubles as specified by type, of length count*natoms, for the property of all the atoms in the simulation specified by name, ordered by bount and then by atom ID. It uses the vector of data to overwrite the corresponding properties for each atom inside LAMMPS. This requires LAMMPS to have its "map" option enabled; see the atom_modify command for details. If it is not, or if atom IDs are not consecutively ordered, no coordinates are reset.

The array of coordinates passed to scatter_atoms() must be a ctypes vector of ints or doubles, allocated and initialized something like this:

```
from ctypes import *
natoms = lmp.get_natoms()
n3 = 3*natoms
x = (n3*c_double)()
x[0] = x coord of atom with ID 1
x[1] = y coord of atom with ID 1
x[2] = z coord of atom with ID 1
x[3] = x coord of atom with ID 2
...
x[n3-1] = z coord of atom with ID natoms
lmp.scatter_coords("x",1,3,x)
```

Alternatively, you can just change values in the vector returned by gather_atoms("x",1,3), since it is a ctypes vector of doubles.

As noted above, these Python class methods correspond one-to-one with the functions in the LAMMPS library interface in src/library.cpp and library.h. This means you can extend the Python wrapper via the following steps:

- Add a new interface function to src/library.cpp and src/library.h.
- Rebuild LAMMPS as a shared library.
- Add a wrapper method to python/lammps.py for this interface function.
- You should now be able to invoke the new interface function from a Python script. Isn't ctypes amazing?

11.8 Example Python scripts that use LAMMPS

These are the Python scripts included as demos in the python/examples directory of the LAMMPS distribution, to illustrate the kinds of things that are possible when Python wraps LAMMPS. If you create your own scripts, send them to us and we can include them in the LAMMPS distribution.

trivial.py	read/run a LAMMPS input script thru Python
demo.py	invoke various LAMMPS library interface routines

simple.py	run in parallel
similar to examples/COUPLE/simple/simple.cpp	split.py
same as simple.py but running in parallel on a subset of procs	gui.py
GUI go/stop/temperature-slider to control LAMMPS	plot.py
real-time temeperature plot with GnuPlot via Pizza.py	viz_tool.py
real-time viz via some viz package	vizplotgui_tool.py
combination of viz_tool.py and plot.py and gui.py	

For the viz_tool.py and vizplotgui_tool.py commands, replace "tool" with "gl" or "atomeye" or "pymol" or "vmd", depending on what visualization package you have installed.

Note that for GL, you need to be able to run the Pizza.py GL tool, which is included in the pizza sub-directory. See the Pizza.py doc pages for more info:

Note that for AtomEye, you need version 3, and there is a line in the scripts that specifies the path and name of the executable. See the AtomEye WWW pages here or here for more details:

```
http://mt.seas.upenn.edu/Archive/Graphics/A
http://mt.seas.upenn.edu/Archive/Graphics/A3/A3.html
```

The latter link is to AtomEye 3 which has the scriping capability needed by these Python scripts.

Note that for PyMol, you need to have built and installed the open-source version of PyMol in your Python, so that you can import it from a Python script. See the PyMol WWW pages here or here for more details:

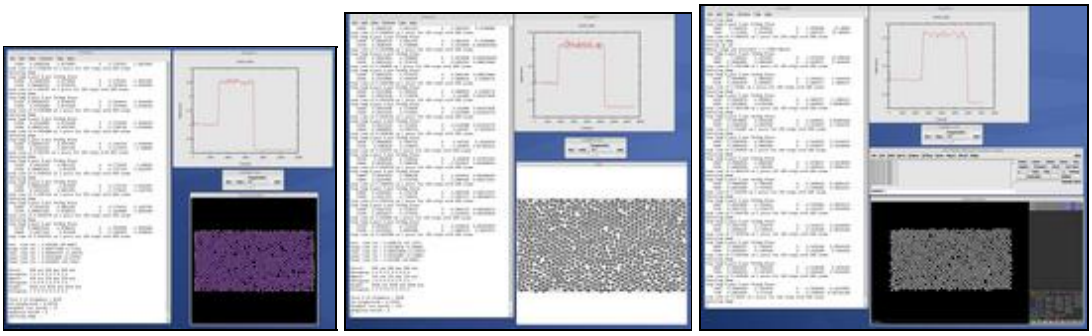
```
http://www.pymol.org
http://sourceforge.net/scm/?type=svn&group_id=4546
```

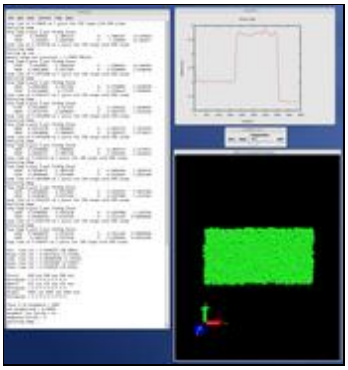
The latter link is to the open-source version.

Note that for VMD, you need a fairly current version (1.8.7 works for me) and there are some lines in the pizza/vmd.py script for 4 PIZZA variables that have to match the VMD installation on your system.

See the python/README file for instructions on how to run them and the source code for individual scripts for comments about what they do.

Here are screenshots of the vizplotgui_tool.py script in action for different visualization package options. Click to see larger images:





12. Errors

This section describes the errors you can encounter when using LAMMPS, either conceptually, or as printed out by the program.

12.1 Common problems

If two LAMMPS runs do not produce the same answer on different machines or different numbers of processors, this is typically not a bug. In theory you should get identical answers on any number of processors and on any machine. In practice, numerical round-off can cause slight differences and eventual divergence of molecular dynamics phase space trajectories within a few 100s or few 1000s of timesteps. However, the statistical properties of the two runs (e.g. average energy or temperature) should still be the same.

If the velocity command is used to set initial atom velocities, a particular atom can be assigned a different velocity when the problem is run on a different number of processors or on different machines. If this happens, the phase space trajectories of the two simulations will rapidly diverge. See the discussion of the *loop* option in the velocity command for details and options that avoid this issue.

Similarly, the create_atoms command generates a lattice of atoms. For the same physical system, the ordering and numbering of atoms by atom ID may be different depending on the number of processors.

Some commands use random number generators which may be setup to produce different random number streams on each processor and hence will produce different effects when run on different numbers of processors. A commonly-used example is the fix langevin command for thermostatting.

A LAMMPS simulation typically has two stages, setup and run. Most LAMMPS errors are detected at setup time; others like a bond stretching too far may not occur until the middle of a run.

LAMMPS tries to flag errors and print informative error messages so you can fix the problem. Of course, LAMMPS cannot figure out your physics or numerical mistakes, like choosing too big a timestep, specifying erroneous force field coefficients, or putting 2 atoms on top of each other! If you run into errors that LAMMPS doesn't catch that you think it should flag, please send an email to the developers.

If you get an error message about an invalid command in your input script, you can determine what command is causing the problem by looking in the log.lammps file or using the echo command to see it on the screen. If you get an error like "Invalid ... style", with ... being fix, compute, pair, etc, it means that you mistyped the style name or that the command is part of an optional package which was not compiled into your executable. The list of available styles in your executable can be listed by using the -h command-line argument. The installation and compilation of optional packages is explained in the installation instructions.

For a given command, LAMMPS expects certain arguments in a specified order. If you mess this up, LAMMPS will often flag the error, but it may also simply read a bogus argument and assign a value that is valid, but not what you wanted. E.g. trying to read the string "abc" as an integer value of 0. Careful reading of the associated doc page for the command should allow you to fix these problems. Note that some commands allow for variables

to be specified in place of numeric constants so that the value can be evaluated and change over the course of a run. This is typically done with the syntax *v_name* for a parameter, where name is the name of the variable. This is only allowed if the command documentation says it is.

Generally, LAMMPS will print a message to the screen and logfile and exit gracefully when it encounters a fatal error. Sometimes it will print a WARNING to the screen and logfile and continue on; you can decide if the WARNING is important or not. A WARNING message that is generated in the middle of a run is only printed to the screen, not to the logfile, to avoid cluttering up thermodynamic output. If LAMMPS crashes or hangs without spitting out an error message first then it could be a bug (see this section) or one of the following cases:

LAMMPS runs in the available memory a processor allows to be allocated. Most reasonable MD runs are compute limited, not memory limited, so this shouldn't be a bottleneck on most platforms. Almost all large memory allocations in the code are done via C-style malloc's which will generate an error message if you run out of memory. Smaller chunks of memory are allocated via C++ "new" statements. If you are unlucky you could run out of memory just when one of these small requests is made, in which case the code will crash or hang (in parallel), since LAMMPS doesn't trap on those errors.

Illegal arithmetic can cause LAMMPS to run slow or crash. This is typically due to invalid physics and numerics that your simulation is computing. If you see wild thermodynamic values or NaN values in your LAMMPS output, something is wrong with your simulation. If you suspect this is happening, it is a good idea to print out thermodynamic info frequently (e.g. every timestep) via the thermo so you can monitor what is happening. Visualizing the atom movement is also a good idea to insure your model is behaving as you expect.

In parallel, one way LAMMPS can hang is due to how different MPI implementations handle buffering of messages. If the code hangs without an error message, it may be that you need to specify an MPI setting or two (usually via an environment variable) to enable buffering or boost the sizes of messages that can be buffered.

12.2 Reporting bugs

If you are confident that you have found a bug in LAMMPS, follow these steps.

Check the New features and bug fixes section of the LAMMPS WWW site to see if the bug has already been reported or fixed or the Unfixed bug to see if a fix is pending.

Check the mailing list to see if it has been discussed before.

If not, send an email to the mailing list describing the problem with any ideas you have as to what is causing it or where in the code the problem might be. The developers will ask for more info if needed, such as an input script or data files.

The most useful thing you can do to help us fix the bug is to isolate the problem. Run it on the smallest number of atoms and fewest number of processors and with the simplest input script that reproduces the bug and try to identify what command or combination of commands is causing the problem.

As a last resort, you can send an email directly to the developers.

12.3 Error & warning messages

These are two alphabetic lists of the ERROR and WARNING messages LAMMPS prints out and the reason why. If the explanation here is not sufficient, the documentation for the offending command may help. Error and warning messages also list the source file and line number where the error was generated. For example, this

message

ERROR: Illegal velocity command (velocity.cpp:78)

means that line #78 in the file src/velocity.cpp generated the error. Looking in the source code may help you figure out what went wrong.

Note that error messages from user-contributed packages are not listed here. If such an error occurs and is not self-explanatory, you'll need to look in the source code or contact the author of the package.

Errors:

1-3 bond count is inconsistent
: An inconsistency was detected when computing the number of 1-3 neighbors for each atom. This likely means something is wrong with the bond topologies you have defined.

1-4 bond count is inconsistent
: An inconsistency was detected when computing the number of 1-4 neighbors for each atom. This likely means something is wrong with the bond topologies you have defined.

Accelerator sharing is not currently supported on system
: Multiple MPI processes cannot share the accelerator on your system. For NVIDIA GPUs, see the nvidia-smi command to change this setting.

All angle coeffs are not set
: All angle coefficients must be set in the data file or by the angle_coeff command before running a simulation.

All atom IDs = 0 but atom_modify id = yes
: Self-explanatory.

All atoms of a swapped type must have same charge.
: Self-explanatory.

All atoms of a swapped type must have the same charge.
: Self-explanatory.

All bond coeffs are not set
: All bond coefficients must be set in the data file or by the bond_coeff command before running a simulation.

All dihedral coeffs are not set
: All dihedral coefficients must be set in the data file or by the dihedral_coeff command before running a simulation.

All improper coeffs are not set
: All improper coefficients must be set in the data file or by the improper_coeff command before running a simulation.

All masses are not set
: For atom styles that define masses for each atom type, all masses must be set in the data file or by the mass command before running a simulation. They must also be set before using the velocity command.

All mol IDs should be set for fix gcmc group atoms
: The molecule flag is on, yet not all molecule ids in the fix group have been set to non-zero positive values by the user. This is an error since all atoms in the fix gcmc group are eligible for deletion, rotation, and translation and therefore must have valid molecule ids.

All pair coeffs are not set
: All pair coefficients must be set in the data file or by the pair_coeff command before running a simulation.

All read_dump x,y,z fields must be specified for scaled, triclinic coords
: For triclinic boxes and scaled coordinates you must specify all 3 of the x,y,z fields, else LAMMPS cannot reconstruct the unscaled coordinates.

All universe/uloop variables must have same # of values
: Self-explanatory.

All variables in next command must be same style
: Self-explanatory.

Angle atom missing in delete_bonds
: The delete_bonds command cannot find one or more atoms in a particular angle on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid angle.

Angle atom missing in set command
: The set command cannot find one or more atoms in a particular angle on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid angle.

Angle atoms %d %d %d missing on proc %d at step %ld
: One or more of 3 atoms needed to compute a particular angle are missing on this processor. Typically this is because the pairwise cutoff is set too short or the angle has blown apart and an atom is too far away.

Angle atoms missing on proc %d at step %ld
: One or more of 3 atoms needed to compute a particular angle are missing on this processor. Typically this is because the pairwise cutoff is set too short or the angle has blown apart and an atom is too far away.

Angle coeff for hybrid has invalid style
: Angle style hybrid uses another angle style as one of its coefficients. The angle style used in the angle_coeff command or read from a restart file is not recognized.

Angle coeffs are not set
: No angle coefficients have been assigned in the data file or via the angle_coeff command.

Angle extent > half of periodic box length
: This error was detected by the neigh_modify check yes setting. It is an error because the angle atoms are so far apart it is ambiguous how it should be defined.

Angle potential must be defined for SHAKE
: When shaking angles, an angle_style potential must be used.

Angle style hybrid cannot have hybrid as an argument
: Self-explanatory.

Angle style hybrid cannot have none as an argument
: Self-explanatory.

Angle style hybrid cannot use same angle style twice
: Self-explanatory.

Angle table must range from 0 to 180 degrees
: Self-explanatory.

Angle table parameters did not set N
: List of angle table parameters must include N setting.

Angle_coeff command before angle_style is defined
: Coefficients cannot be set in the data file or via the angle_coeff command until an angle_style has been assigned.

Angle_coeff command before simulation box is defined
: The angle_coeff command cannot be used before a read_data, read_restart, or create_box command.

Angle_coeff command when no angles allowed
: The chosen atom style does not allow for angles to be defined.

Angle_style command when no angles allowed
: The chosen atom style does not allow for angles to be defined.

Angles assigned incorrectly
: Angles read in from the data file were not assigned correctly to atoms. This means there is something invalid about the topology definitions.

Angles defined but no angle types
: The data file header lists angles but no angle types.

Append boundary must be shrink/minimum
: The boundary style of the face where atoms are added must be of type m (shrink/minimum).

Arccos of invalid value in variable formula
: Argument of arccos() must be between -1 and 1.

Arcsin of invalid value in variable formula
: Argument of arcsin() must be between -1 and 1.

Assigning body parameters to non-body atom
: Self-explanatory.

Assigning ellipsoid parameters to non-ellipsoid atom
: Self-explanatory.

Assigning line parameters to non-line atom
: Self-explanatory.

Assigning quat to non-body atom
: Self-explanatory.

Assigning tri parameters to non-tri atom
: Self-explanatory.

At least one atom of each swapped type must be present to define charges.
: Self-explanatory.

Atom IDs must be consecutive for velocity create loop all
: Self-explanatory.

Atom IDs must be used for molecular systems
: Atom IDs are used to identify and find partner atoms in bonds.

Atom count changed in fix neb
: This is not allowed in a NEB calculation.

Atom count is inconsistent, cannot write data file
: The sum of atoms across processors does not equal the global number of atoms. Probably some atoms have been lost.

Atom count is inconsistent, cannot write restart file
: Sum of atoms across processors does not equal initial total count. This is probably because you have lost some atoms.

Atom in too many rigid bodies - boost MAXBODY
: Fix poems has a parameter MAXBODY (in fix_poems.cpp) which determines the maximum number of rigid bodies a single atom can belong to (i.e. a multibody joint). The bodies you have defined exceed this limit.

Atom sort did not operate correctly
: This is an internal LAMMPS error. Please report it to the developers.

Atom sorting has bin size = 0.0
: The neighbor cutoff is being used as the bin size, but it is zero. Thus you must explicitly list a bin size in the atom_modify sort command or turn off sorting.

Atom style hybrid cannot have hybrid as an argument
: Self-explanatory.

Atom style hybrid cannot use same atom style twice
: Self-explanatory.

Atom style template molecule must have atom types
: The defined molecule(s) does not specify atom types.

Atom style was redefined after using fix property/atom
: This is not allowed.

Atom type must be zero in fix gcmc mol command
: Self-explanatory.

Atom vector in equal-style variable formula
: Atom vectors generate one value per atom which is not allowed in an equal-style variable.

Atom-style variable in equal-style variable formula
: Atom-style variables generate one value per atom which is not allowed in an equal-style variable.

Atom_modify id command after simulation box is defined

The atom_modify id command cannot be used after a read_data, read_restart, or create_box command.

Atom_modify map command after simulation box is defined

The atom_modify map command cannot be used after a read_data, read_restart, or create_box command.

Atom_modify sort and first options cannot be used together

Self-explanatory.

Atom_style command after simulation box is defined

The atom_style command cannot be used after a read_data, read_restart, or create_box command.

Atom_style line can only be used in 2d simulations

Self-explanatory.

Atom_style tri can only be used in 3d simulations

Self-explanatory.

Atomfile variable could not read values

Check the file assigned to the variable.

Atomfile variable in equal-style variable formula

Self-explanatory.

Atomfile-style variable in equal-style variable formula

Self-explanatory.

Attempt to pop empty stack in fix box/relax

Internal LAMMPS error. Please report it to the developers.

Attempt to push beyond stack limit in fix box/relax

Internal LAMMPS error. Please report it to the developers.

Attempting to rescale a 0.0 temperature

Cannot rescale a temperature that is already 0.0.

Bad FENE bond

Two atoms in a FENE bond have become so far apart that the bond cannot be computed.

Bad TIP4P angle type for PPPM/TIP4P

Specified angle type is not valid.

Bad TIP4P angle type for PPPMDisp/TIP4P

Specified angle type is not valid.

Bad TIP4P bond type for PPPM/TIP4P

Specified bond type is not valid.

Bad TIP4P bond type for PPPMDisp/TIP4P

Specified bond type is not valid.

Bad fix ID in fix append/atoms command

The value of the fix_id for keyword spatial must start with the suffix f_.

Bad grid of processors

The 3d grid of processors defined by the processors command does not match the number of processors LAMMPS is being run on.

Bad kspace_modify kmax/ewald parameter

Kspace_modify values for the kmax/ewald keyword must be integers > 0

Bad kspace_modify slab parameter

Kspace_modify value for the slab/volume keyword must be >= 2.0.

Bad matrix inversion in mldivide3

This error should not occur unless the matrix is badly formed.

Bad principal moments

Fix rigid did not compute the principal moments of inertia of a rigid group of atoms correctly.

Bad quadratic solve for particle/line collision

This is an internal error. It should nornally not occur.

Bad quadratic solve for particle/tri collision

This is an internal error. It should nornally not occur.

Bad real space Coulomb cutoff in fix tune/kspace

Fix tune/kspace tried to find the optimal real space Coulomb cutoff using the Newton-Rhaphson method,

but found a non-positive or NaN cutoff

Balance command before simulation box is defined

The balance command cannot be used before a read_data, read_restart, or create_box command.

Balance produced bad splits

This should not occur. It means two or more cutting plane locations are on top of each other or out of order. Report the problem to the developers.

Balance rcb cannot be used with comm_style brick

Comm_style tiled must be used instead.

Balance shift string is invalid

The string can only contain the characters "x", "y", or "z".

Bias compute does not calculate a velocity bias

The specified compute must compute a bias for temperature.

Bias compute does not calculate temperature

The specified compute must compute temperature.

Bias compute group does not match compute group

The specified compute must operate on the same group as the parent compute.

Big particle in fix srd cannot be point particle

Big particles must be extended spheriods or ellipsoids.

Bigint setting in lmptype.h is invalid

Size of bigint is less than size of tagint.

Bigint setting in lmptype.h is not compatible

Format of bigint stored in restart file is not consistent with LAMMPS version you are running. See the settings in src/lmptype.h

Bitmapped lookup tables require int/float be same size

Cannot use pair tables on this machine, because of word sizes. Use the pair_modify command with table 0 instead.

Bitmapped table in file does not match requested table

Setting for bitmapped table in pair_coeff command must match table in file exactly.

Bitmapped table is incorrect length in table file

Number of table entries is not a correct power of 2.

Bond and angle potentials must be defined for TIP4P

Cannot use TIP4P pair potential unless bond and angle potentials are defined.

Bond atom missing in box size check

The 2nd atoms needed to compute a particular bond is missing on this processor. Typically this is because the pairwise cutoff is set too short or the bond has blown apart and an atom is too far away.

Bond atom missing in delete_bonds

The delete_bonds command cannot find one or more atoms in a particular bond on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid bond.

Bond atom missing in image check

The 2nd atom in a particular bond is missing on this processor. Typically this is because the pairwise cutoff is set too short or the bond has blown apart and an atom is too far away.

Bond atom missing in set command

The set command cannot find one or more atoms in a particular bond on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid bond.

Bond atoms %d %d missing on proc %d at step %ld

The 2nd atom needed to compute a particular bond is missing on this processor. Typically this is because the pairwise cutoff is set too short or the bond has blown apart and an atom is too far away.

Bond atoms missing on proc %d at step %ld

The 2nd atom needed to compute a particular bond is missing on this processor. Typically this is because the pairwise cutoff is set too short or the bond has blown apart and an atom is too far away.

Bond coeff for hybrid has invalid style

Bond style hybrid uses another bond style as one of its coefficients. The bond style used in the

bond_coeff command or read from a restart file is not recognized.

Bond coeffs are not set
No bond coefficients have been assigned in the data file or via the bond_coeff command.

Bond extent > half of periodic box length
This error was detected by the neigh_modify check yes setting. It is an error because the bond atoms are so far apart it is ambiguous how it should be defined.

Bond potential must be defined for SHAKE
Cannot use fix shake unless bond potential is defined.

Bond style hybrid cannot have hybrid as an argument
Self-explanatory.

Bond style hybrid cannot have none as an argument
Self-explanatory.

Bond style hybrid cannot use same bond style twice
Self-explanatory.

Bond style quartic cannot be used with 3,4-body interactions
No angle, dihedral, or improper styles can be defined when using bond style quartic.

Bond style quartic cannot be used with atom style template
This bond style can change the bond topology which is not allowed with this atom style.

Bond style quartic requires special_bonds = 1,1,1
This is a restriction of the current bond quartic implementation.

Bond table parameters did not set N
List of bond table parameters must include N setting.

Bond table values are not increasing
The values in the tabulated file must be monotonically increasing.

BondAngle coeff for hybrid angle has invalid format
No "ba" field should appear in data file entry.

BondBond coeff for hybrid angle has invalid format
No "bb" field should appear in data file entry.

Bond_coeff command before bond_style is defined
Coefficients cannot be set in the data file or via the bond_coeff command until an bond_style has been assigned.

Bond_coeff command before simulation box is defined
The bond_coeff command cannot be used before a read_data, read_restart, or create_box command.

Bond_coeff command when no bonds allowed
The chosen atom style does not allow for bonds to be defined.

Bond_style command when no bonds allowed
The chosen atom style does not allow for bonds to be defined.

Bonds assigned incorrectly
Bonds read in from the data file were not assigned correctly to atoms. This means there is something invalid about the topology definitions.

Bonds defined but no bond types
The data file header lists bonds but no bond types.

Both restart files must use % or neither
Self-explanatory.

Both restart files must use MPI-IO or neither
Self-explanatory.

Both sides of boundary must be periodic
Cannot specify a boundary as periodic only on the lo or hi side. Must be periodic on both sides.

Boundary command after simulation box is defined
The boundary command cannot be used after a read_data, read_restart, or create_box command.

Box bounds are invalid
The box boundaries specified in the read_data file are invalid. The lo value must be less than the hi value

for all 3 dimensions.

Box command after simulation box is defined
The box command cannot be used after a read_data, read_restart, or create_box command.

CPU neighbor lists must be used for ellipsoid/sphere mix.
When using Gay-Berne or RE-squared pair styles with both ellipsoidal and spherical particles, the neighbor list must be built on the CPU

Can not specify Pxy/Pxz/Pyz in fix box/relax with non-triclinic box
Only triclinic boxes can be used with off-diagonal pressure components. See the region prism command for details.

Can not specify Pxy/Pxz/Pyz in fix nvt/npt/nph with non-triclinic box
Only triclinic boxes can be used with off-diagonal pressure components. See the region prism command for details.

Can only use -plog with multiple partitions
Self-explanatory. See doc page discussion of command-line switches.

Can only use -pscreen with multiple partitions
Self-explanatory. See doc page discussion of command-line switches.

Can only use Kokkos supported regions with Kokkos package
Self-explanatory.

Can only use NEB with 1-processor replicas
This is current restriction for NEB as implemented in LAMMPS.

Can only use TAD with 1-processor replicas for NEB
This is current restriction for NEB as implemented in LAMMPS.

Cannot (yet) do analytic differentiation with pppm/gpu
This is a current restriction of this command.

Cannot (yet) request ghost atoms with Kokkos half neighbor list
This feature is not yet supported.

Cannot (yet) use 'electron' units with dipoles
This feature is not yet supported.

Cannot (yet) use Ewald with triclinic box and slab correction
This feature is not yet supported.

Cannot (yet) use K-space slab correction with compute group/group for triclinic systems
This option is not yet supported.

Cannot (yet) use MSM with 2d simulation
This feature is not yet supported.

Cannot (yet) use PPPM with triclinic box and TIP4P
This feature is not yet supported.

Cannot (yet) use PPPM with triclinic box and kspace_modify diff ad
This feature is not yet supported.

Cannot (yet) use PPPM with triclinic box and slab correction
This feature is not yet supported.

Cannot (yet) use kspace slab correction with long-range dipoles and non-neutral systems or per-atom energy
This feature is not yet supported.

Cannot (yet) use kspace_modify diff ad with compute group/group
This option is not yet supported.

Cannot (yet) use kspace_style pppm/stagger with triclinic systems
This feature is not yet supported.

Cannot (yet) use molecular templates with Kokkos
Self-explanatory.

Cannot (yet) use respa with Kokkos
Self-explanatory.

Cannot (yet) use rigid bodies with fix deform and Kokkos
Self-explanatory.

Cannot (yet) use rigid bodies with fix nh and Kokkos
: Self-explanatory.

Cannot (yet) use single precision with MSM (remove -DFFT_SINGLE from Makefile and recompile)
: Single precision cannot be used with MSM.

Cannot add atoms to fix move variable
: Atoms can not be added afterwards to this fix option.

Cannot append atoms to a triclinic box
: The simulation box must be defined with edges alligned with the Cartesian axes.

Cannot balance in z dimension for 2d simulation
: Self-explanatory.

Cannot change box ortho/triclinic with certain fixes defined
: This is because those fixes store the shape of the box. You need to use unfix to discard the fix, change the box, then redefine a new fix.

Cannot change box ortho/triclinic with dumps defined
: This is because some dumps store the shape of the box. You need to use undump to discard the dump, change the box, then redefine a new dump.

Cannot change box tilt factors for orthogonal box
: Cannot use tilt factors unless the simulation box is non-orthogonal.

Cannot change box to orthogonal when tilt is non-zero
: Self-explanatory.

Cannot change box z boundary to nonperiodic for a 2d simulation
: Self-explanatory.

Cannot change dump_modify every for dump dcd
: The frequency of writing dump dcd snapshots cannot be changed.

Cannot change dump_modify every for dump xtc
: The frequency of writing dump xtc snapshots cannot be changed.

Cannot change timestep once fix srd is setup
: This is because various SRD properties depend on the timestep size.

Cannot change timestep with fix pour
: This is because fix pour pre-computes the time delay for particles to fall out of the insertion volume due to gravity.

Cannot change to comm_style brick from tiled layout
: Self-explanatory.

Cannot change_box after reading restart file with per-atom info
: This is because the restart file info cannot be migrated with the atoms. You can get around this by performing a 0-timestep run which will assign the restart file info to actual atoms.

Cannot change_box in xz or yz for 2d simulation
: Self-explanatory.

Cannot change_box in z dimension for 2d simulation
: Self-explanatory.

Cannot clear group all
: This operation is not allowed.

Cannot close restart file - MPI error: %s
: This error was generated by MPI when reading/writing an MPI-IO restart file.

Cannot compute initial g_ewald_disp
: LAMMPS failed to compute an initial guess for the PPPM_disp g_ewald_6 factor that partitions the computation between real space and k-space for Disptersion interactions.

Cannot create an atom map unless atoms have IDs
: The simulation requires a mapping from global atom IDs to local atoms, but the atoms that have been defined have no IDs.

Cannot create atoms with undefined lattice
: Must use the lattice command before using the create_atoms command.

Cannot create/grow a vector/array of pointers for %s
: LAMMPS code is making an illegal call to the templated memory allocaters, to create a vector or array of pointers.

Cannot create_atoms after reading restart file with per-atom info
: The per-atom info was stored to be used when by a fix that you may re-define. If you add atoms before re-defining the fix, then there will not be a correct amount of per-atom info.

Cannot create_box after simulation box is defined
: A simulation box can only be defined once.

Cannot currently use pair reax with pair hybrid
: This is not yet supported.

Cannot currently use pppm/gpu with fix balance.
: Self-explanatory.

Cannot delete group all
: Self-explanatory.

Cannot delete group currently used by a compute
: Self-explanatory.

Cannot delete group currently used by a dump
: Self-explanatory.

Cannot delete group currently used by a fix
: Self-explanatory.

Cannot delete group currently used by atom_modify first
: Self-explanatory.

Cannot delete_atoms bond yes for non-molecular systems
: Self-explanatory.

Cannot displace_atoms after reading restart file with per-atom info
: This is because the restart file info cannot be migrated with the atoms. You can get around this by performing a 0-timestep run which will assign the restart file info to actual atoms.

Cannot do GCMC on atoms in atom_modify first group
: This is a restriction due to the way atoms are organized in a list to enable the atom_modify first command.

Cannot do atom/swap on atoms in atom_modify first group
: This is a restriction due to the way atoms are organized in a list to enable the atom_modify first command.

Cannot dump sort on atom IDs with no atom IDs defined
: Self-explanatory.

Cannot dump sort when multiple dump files are written
: In this mode, each processor dumps its atoms to a file, so no sorting is allowed.

Cannot embed Python when also extending Python with LAMMPS
: When running LAMMPS via Python through the LAMMPS library interface you cannot also user the input script python command.

Cannot evaporate atoms in atom_modify first group
: This is a restriction due to the way atoms are organized in a list to enable the atom_modify first command.

Cannot find create_bonds group ID
: Self-explanatory.

Cannot find delete_bonds group ID
: Group ID used in the delete_bonds command does not exist.

Cannot find specified group ID for core particles
: Self-explanatory.

Cannot find specified group ID for shell particles
: Self-explanatory.

Cannot have both pair_modify shift and tail set to yes

These 2 options are contradictory.

Cannot intersect groups using a dynamic group

This operation is not allowed.

Cannot mix molecular and molecule template atom styles

Self-explanatory.

Cannot open -reorder file

Self-explanatory.

Cannot open ADP potential file %s

The specified ADP potential file cannot be opened. Check that the path and name are correct.

Cannot open AIREBO potential file %s

The specified AIREBO potential file cannot be opened. Check that the path and name are correct.

Cannot open BOP potential file %s

The specified BOP potential file cannot be opened. Check that the path and name are correct.

Cannot open COMB potential file %s

The specified COMB potential file cannot be opened. Check that the path and name are correct.

Cannot open COMB3 lib.comb3 file

The COMB3 library file cannot be opened. Check that the path and name are correct.

Cannot open COMB3 potential file %s

The specified COMB3 potential file cannot be opened. Check that the path and name are correct.

Cannot open EAM potential file %s

The specified EAM potential file cannot be opened. Check that the path and name are correct.

Cannot open EIM potential file %s

The specified EIM potential file cannot be opened. Check that the path and name are correct.

Cannot open LCBOP potential file %s

The specified LCBOP potential file cannot be opened. Check that the path and name are correct.

Cannot open MEAM potential file %s

The specified MEAM potential file cannot be opened. Check that the path and name are correct.

Cannot open SNAP coefficient file %s

The specified SNAP coefficient file cannot be opened. Check that the path and name are correct.

Cannot open SNAP parameter file %s

The specified SNAP parameter file cannot be opened. Check that the path and name are correct.

Cannot open Stillinger-Weber potential file %s

The specified SW potential file cannot be opened. Check that the path and name are correct.

Cannot open Tersoff potential file %s

The specified potential file cannot be opened. Check that the path and name are correct.

Cannot open Vashishta potential file %s

The specified Vashishta potential file cannot be opened. Check that the path and name are correct.

Cannot open balance output file

Self-explanatory.

Cannot open coul/streitz potential file %s

The specified coul/streitz potential file cannot be opened. Check that the path and name are correct.

Cannot open custom file

Self-explanatory.

Cannot open data file %s

The specified file cannot be opened. Check that the path and name are correct.

Cannot open dir to search for restart file

Using a "*" in the name of the restart file will open the current directory to search for matching file names.

Cannot open dump file

Self-explanatory.

Cannot open dump file %s

The output file for the dump command cannot be opened. Check that the path and name are correct.

Cannot open file %s
: The specified file cannot be opened. Check that the path and name are correct. If the file is a compressed file, also check that the gzip executable can be found and run.

Cannot open file variable file %s
: The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix ave/chunk file %s
: The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix ave/correlate file %s
: The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix ave/histo file %s
: The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix ave/spatial file %s
: The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix ave/time file %s
: The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix balance output file
: Self-explanatory.

Cannot open fix poems file %s
: The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix print file %s
: The output file generated by the fix print command cannot be opened

Cannot open fix qeq parameter file %s
: The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix qeq/comb file %s
: The output file for the fix qeq/combs command cannot be opened. Check that the path and name are correct.

Cannot open fix reax/bonds file %s
: The output file for the fix reax/bonds command cannot be opened. Check that the path and name are correct.

Cannot open fix rigid infile %s
: The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix rigid restart file %s
: The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix rigid/small infile %s
: The specified file cannot be opened. Check that the path and name are correct.

Cannot open fix tmd file %s
: The output file for the fix tmd command cannot be opened. Check that the path and name are correct.

Cannot open fix ttm file %s
: The output file for the fix ttm command cannot be opened. Check that the path and name are correct.

Cannot open gzipped file
: LAMMPS was compiled without support for reading and writing gzipped files through a pipeline to the gzip program with -DLAMMPS_GZIP.

Cannot open input script %s
: Self-explanatory.

Cannot open log.cite file
: This file is created when you use some LAMMPS features, to indicate what paper you should cite on behalf of those who implemented the feature. Check that you have write priveleges into the directory you are running in.

Cannot open log.lammps for writing
: The default LAMMPS log file cannot be opened. Check that the directory you are running in allows for files to be created.

Cannot open logfile

The LAMMPS log file named in a command-line argument cannot be opened. Check that the path and name are correct.

Cannot open logfile %s
The LAMMPS log file specified in the input script cannot be opened. Check that the path and name are correct.

Cannot open molecule file %s
The specified file cannot be opened. Check that the path and name are correct.

Cannot open nb3b/harmonic potential file %s
The specified potential file cannot be opened. Check that the path and name are correct.

Cannot open pair_write file
The specified output file for pair energies and forces cannot be opened. Check that the path and name are correct.

Cannot open polymorphic potential file %s
The specified polymorphic potential file cannot be opened. Check that the path and name are correct.

Cannot open print file %s
Self-explanatory.

Cannot open processors output file
Self-explanatory.

Cannot open restart file %s
Self-explanatory.

Cannot open restart file for reading - MPI error: %s
This error was generated by MPI when reading/writing an MPI-IO restart file.

Cannot open restart file for writing - MPI error: %s
This error was generated by MPI when reading/writing an MPI-IO restart file.

Cannot open screen file
The screen file specified as a command-line argument cannot be opened. Check that the directory you are running in allows for files to be created.

Cannot open temporary file for world counter.
Self-explanatory.

Cannot open universe log file
For a multi-partition run, the master log file cannot be opened. Check that the directory you are running in allows for files to be created.

Cannot open universe screen file
For a multi-partition run, the master screen file cannot be opened. Check that the directory you are running in allows for files to be created.

Cannot read from restart file - MPI error: %s
This error was generated by MPI when reading/writing an MPI-IO restart file.

Cannot read_data without add keyword after simulation box is defined
Self-explanatory.

Cannot read_restart after simulation box is defined
The read_restart command cannot be used after a read_data, read_restart, or create_box command.

Cannot redefine variable as a different style
An equal-style variable can be re-defined but only if it was originally an equal-style variable.

Cannot replicate 2d simulation in z dimension
The replicate command cannot replicate a 2d simulation in the z dimension.

Cannot replicate with fixes that store atom quantities
Either fixes are defined that create and store atom-based vectors or a restart file was read which included atom-based vectors for fixes. The replicate command cannot duplicate that information for new atoms. You should use the replicate command before fixes are applied to the system.

Cannot reset timestep with a dynamic region defined
Dynamic regions (see the region command) have a time dependence. Thus you cannot change the timestep when one or more of these are defined.

Cannot reset timestep with a time-dependent fix defined
: You cannot reset the timestep when a fix that keeps track of elapsed time is in place.

Cannot run 2d simulation with nonperiodic Z dimension
: Use the boundary command to make the z dimension periodic in order to run a 2d simulation.

Cannot set bond topology types for atom style template
: The bond, angle, etc types cannot be changed for this atom style since they are static settings in the molecule template files.

Cannot set both respa pair and inner/middle/outer
: In the rRESPA integrator, you must compute pairwise potentials either all together (pair), or in pieces (inner/middle/outer). You can't do both.

Cannot set cutoff/multi before simulation box is defined
: Self-explanatory.

Cannot set dpd/theta for this atom style
: Self-explanatory.

Cannot set dump_modify flush for dump xtc
: Self-explanatory.

Cannot set mass for this atom style
: This atom style does not support mass settings for each atom type. Instead they are defined on a per-atom basis in the data file.

Cannot set meso/cv for this atom style
: Self-explanatory.

Cannot set meso/e for this atom style
: Self-explanatory.

Cannot set meso/rho for this atom style
: Self-explanatory.

Cannot set non-zero image flag for non-periodic dimension
: Self-explanatory.

Cannot set non-zero z velocity for 2d simulation
: Self-explanatory.

Cannot set quaternion for atom that has none
: Self-explanatory.

Cannot set quaternion with xy components for 2d system
: Self-explanatory.

Cannot set respa hybrid and any of pair/inner/middle/outer
: In the rRESPA integrator, you must compute pairwise potentials either all together (pair), with different cutoff regions (inner/middle/outer), or per hybrid sub-style (hybrid). You cannot mix those.

Cannot set respa middle without inner/outer
: In the rRESPA integrator, you must define both a inner and outer setting in order to use a middle setting.

Cannot set restart file size - MPI error: %s
: This error was generated by MPI when reading/writing an MPI-IO restart file.

Cannot set smd/contact/radius for this atom style
: Self-explanatory.

Cannot set smd/mass/density for this atom style
: Self-explanatory.

Cannot set temperature for fix rigid/nph
: The temp keyword cannot be specified.

Cannot set theta for atom that is not a line
: Self-explanatory.

Cannot set this attribute for this atom style
: The attribute being set does not exist for the defined atom style.

Cannot set variable z velocity for 2d simulation
: Self-explanatory.

Cannot skew triclinic box in z for 2d simulation
: Self-explanatory.

Cannot subtract groups using a dynamic group
: This operation is not allowed.

Cannot union groups using a dynamic group
: This operation is not allowed.

Cannot use -cuda on and -kokkos on together
: This is not allowed since both packages can use GPUs.

Cannot use -cuda on without USER-CUDA installed
: The USER-CUDA package must be installed via "make yes-user-cuda" before LAMMPS is built.

Cannot use -kokkos on without KOKKOS installed
: Self-explanatory.

Cannot use -reorder after -partition
: Self-explanatory. See doc page discussion of command-line switches.

Cannot use Ewald with 2d simulation
: The kspace style ewald cannot be used in 2d simulations. You can use 2d Ewald in a 3d simulation; see the kspace_modify command.

Cannot use Ewald/disp solver on system with no charge, dipole, or LJ particles
: No atoms in system have a non-zero charge or dipole, or are LJ particles. Change charges/dipoles or change options of the kspace solver/pair style.

Cannot use EwaldDisp with 2d simulation
: This is a current restriction of this command.

Cannot use GPU package with USER-CUDA package enabled
: You cannot use both the GPU and USER-CUDA packages together. Use one or the other.

Cannot use Kokkos pair style with rRESPA inner/middle
: Self-explanatory.

Cannot use NEB unless atom map exists
: Use the atom_modify command to create an atom map.

Cannot use NEB with a single replica
: Self-explanatory.

Cannot use NEB with atom_modify sort enabled
: This is current restriction for NEB implemented in LAMMPS.

Cannot use PPPM with 2d simulation
: The kspace style pppm cannot be used in 2d simulations. You can use 2d PPPM in a 3d simulation; see the kspace_modify command.

Cannot use PPPMDisp with 2d simulation
: The kspace style pppm/disp cannot be used in 2d simulations. You can use 2d pppm/disp in a 3d simulation; see the kspace_modify command.

Cannot use PRD with a changing box
: The current box dimensions are not copied between replicas

Cannot use PRD with a time-dependent fix defined
: PRD alters the timestep in ways that will mess up these fixes.

Cannot use PRD with a time-dependent region defined
: PRD alters the timestep in ways that will mess up these regions.

Cannot use PRD with atom_modify sort enabled
: This is a current restriction of PRD. You must turn off sorting, which is enabled by default, via the atom_modify command.

Cannot use PRD with multi-processor replicas unless atom map exists
: Use the atom_modify command to create an atom map.

Cannot use TAD unless atom map exists for NEB
: See atom_modify map command to set this.

Cannot use TAD with a single replica for NEB

NEB requires multiple replicas.

Cannot use TAD with atom_modify sort enabled for NEB

This is a current restriction of NEB.

Cannot use a damped dynamics min style with fix box/relax

This is a current restriction in LAMMPS. Use another minimizer style.

Cannot use a damped dynamics min style with per-atom DOF

This is a current restriction in LAMMPS. Use another minimizer style.

Cannot use append/atoms in periodic dimension

The boundary style of the face where atoms are added can not be of type p (periodic).

Cannot use atomfile-style variable unless atom map exists

Self-explanatory. See the atom_modify command to create a map.

Cannot use both com and bias with compute temp/chunk

Self-explanatory.

Cannot use chosen neighbor list style with buck/coul/cut/kk

Self-explanatory.

Cannot use chosen neighbor list style with buck/coul/long/kk

Self-explanatory.

Cannot use chosen neighbor list style with buck/kk

That style is not supported by Kokkos.

Cannot use chosen neighbor list style with coul/cut/kk

That style is not supported by Kokkos.

Cannot use chosen neighbor list style with coul/debye/kk

Self-explanatory.

Cannot use chosen neighbor list style with coul/dsf/kk

That style is not supported by Kokkos.

Cannot use chosen neighbor list style with coul/wolf/kk

That style is not supported by Kokkos.

Cannot use chosen neighbor list style with lj/charmm/coul/charmm/implicit/kk

Self-explanatory.

Cannot use chosen neighbor list style with lj/charmm/coul/charmm/kk

Self-explanatory.

Cannot use chosen neighbor list style with lj/charmm/coul/long/kk

Self-explanatory.

Cannot use chosen neighbor list style with lj/class2/coul/cut/kk

Self-explanatory.

Cannot use chosen neighbor list style with lj/class2/coul/long/kk

Self-explanatory.

Cannot use chosen neighbor list style with lj/class2/kk

Self-explanatory.

Cannot use chosen neighbor list style with lj/cut/coul/cut/kk

That style is not supported by Kokkos.

Cannot use chosen neighbor list style with lj/cut/coul/debye/kk

Self-explanatory.

Cannot use chosen neighbor list style with lj/cut/coul/long/kk

That style is not supported by Kokkos.

Cannot use chosen neighbor list style with lj/cut/kk

That style is not supported by Kokkos.

Cannot use chosen neighbor list style with lj/expand/kk

Self-explanatory.

Cannot use chosen neighbor list style with lj/gromacs/coul/gromacs/kk

Self-explanatory.

Cannot use chosen neighbor list style with lj/gromacs/kk

Self-explanatory.

Cannot use chosen neighbor list style with lj/sdk/kk

That style is not supported by Kokkos.

Cannot use chosen neighbor list style with pair eam/kk

That style is not supported by Kokkos.

Cannot use chosen neighbor list style with pair eam/kk/alloy

Self-explanatory.

Cannot use chosen neighbor list style with pair eam/kk/fs

Self-explanatory.

Cannot use chosen neighbor list style with pair sw/kk

Self-explanatory.

Cannot use chosen neighbor list style with tersoff/kk

Self-explanatory.

Cannot use chosen neighbor list style with tersoff/zbl/kk

Self-explanatory.

Cannot use compute chunk/atom bin z for 2d model

Self-explanatory.

Cannot use compute cluster/atom unless atoms have IDs

Atom IDs are used to identify clusters.

Cannot use create_atoms rotate unless single style

Self-explanatory.

Cannot use create_bonds unless atoms have IDs

This command requires a mapping from global atom IDs to local atoms, but the atoms that have been defined have no IDs.

Cannot use create_bonds with non-molecular system

Self-explanatory.

Cannot use cwiggle in variable formula between runs

This is a function of elapsed time.

Cannot use delete_atoms bond yes with atom_style template

This is because the bonds for that atom style are hardwired in the molecule template.

Cannot use delete_atoms unless atoms have IDs

Your atoms do not have IDs, so the delete_atoms command cannot be used.

Cannot use delete_bonds with non-molecular system

Your choice of atom style does not have bonds.

Cannot use dump_modify fileper without % in dump file name

Self-explanatory.

Cannot use dump_modify nfile without % in dump file name

Self-explanatory.

Cannot use dynamic group with fix adapt atom

This is not yet supported.

Cannot use fix TMD unless atom map exists

Using this fix requires the ability to lookup an atom index, which is provided by an atom map. An atom map does not exist (by default) for non-molecular problems. Using the atom_modify map command will force an atom map to be created.

Cannot use fix ave/spatial z for 2 dimensional model

Self-explanatory.

Cannot use fix bond/break with non-molecular systems

Only systems with bonds that can be changed can be used. Atom_style template does not qualify.

Cannot use fix bond/create with non-molecular systems

Only systems with bonds that can be changed can be used. Atom_style template does not qualify.

Cannot use fix bond/swap with non-molecular systems

Only systems with bonds that can be changed can be used. Atom_style template does not qualify.

Cannot use fix box/relax on a 2nd non-periodic dimension
: When specifying an off-diagonal pressure component, the 2nd of the two dimensions must be periodic. E.g. if the xy component is specified, then the y dimension must be periodic.

Cannot use fix box/relax on a non-periodic dimension
: When specifying a diagonal pressure component, the dimension must be periodic.

Cannot use fix box/relax with both relaxation and scaling on a tilt factor
: When specifying scaling on a tilt factor component, that component can not also be controlled by the barostat. E.g. if scalexy yes is specified and also keyword tri or xy, this is wrong.

Cannot use fix box/relax with tilt factor scaling on a 2nd non-periodic dimension
: When specifying scaling on a tilt factor component, the 2nd of the two dimensions must be periodic. E.g. if the xy component is specified, then the y dimension must be periodic.

Cannot use fix deform on a shrink-wrapped boundary
: The x, y, z options cannot be applied to shrink-wrapped dimensions.

Cannot use fix deform tilt on a shrink-wrapped 2nd dim
: This is because the shrink-wrapping will change the value of the strain implied by the tilt factor.

Cannot use fix deform trate on a box with zero tilt
: The trate style alters the current strain.

Cannot use fix deposit rigid and not molecule
: Self-explanatory.

Cannot use fix deposit rigid and shake
: These two attributes are conflicting.

Cannot use fix deposit shake and not molecule
: Self-explanatory.

Cannot use fix enforce2d with 3d simulation
: Self-explanatory.

Cannot use fix gcmc in a 2d simulation
: Fix gcmc is set up to run in 3d only. No 2d simulations with fix gcmc are allowed.

Cannot use fix gcmc shake and not molecule
: Self-explanatory.

Cannot use fix msst without per-type mass defined
: Self-explanatory.

Cannot use fix npt and fix deform on same component of stress tensor
: This would be changing the same box dimension twice.

Cannot use fix nvt/npt/nph on a 2nd non-periodic dimension
: When specifying an off-diagonal pressure component, the 2nd of the two dimensions must be periodic. E.g. if the xy component is specified, then the y dimension must be periodic.

Cannot use fix nvt/npt/nph on a non-periodic dimension
: When specifying a diagonal pressure component, the dimension must be periodic.

Cannot use fix nvt/npt/nph with both xy dynamics and xy scaling
: Self-explanatory.

Cannot use fix nvt/npt/nph with both xz dynamics and xz scaling
: Self-explanatory.

Cannot use fix nvt/npt/nph with both yz dynamics and yz scaling
: Self-explanatory.

Cannot use fix nvt/npt/nph with xy scaling when y is non-periodic dimension
: The 2nd dimension in the barostatted tilt factor must be periodic.

Cannot use fix nvt/npt/nph with xz scaling when z is non-periodic dimension
: The 2nd dimension in the barostatted tilt factor must be periodic.

Cannot use fix nvt/npt/nph with yz scaling when z is non-periodic dimension
: The 2nd dimension in the barostatted tilt factor must be periodic.

Cannot use fix pour rigid and not molecule
: Self-explanatory.

Cannot use fix pour rigid and shake
: These two attributes are conflicting.

Cannot use fix pour shake and not molecule
: Self-explanatory.

Cannot use fix pour with triclinic box
: This option is not yet supported.

Cannot use fix press/berendsen and fix deform on same component of stress tensor
: These commands both change the box size/shape, so you cannot use both together.

Cannot use fix press/berendsen on a non-periodic dimension
: Self-explanatory.

Cannot use fix press/berendsen with triclinic box
: Self-explanatory.

Cannot use fix reax/bonds without pair_style reax
: Self-explantory.

Cannot use fix rigid npt/nph and fix deform on same component of stress tensor
: This would be changing the same box dimension twice.

Cannot use fix rigid npt/nph on a non-periodic dimension
: When specifying a diagonal pressure component, the dimension must be periodic.

Cannot use fix rigid/small npt/nph on a non-periodic dimension
: When specifying a diagonal pressure component, the dimension must be periodic.

Cannot use fix shake with non-molecular system
: Your choice of atom style does not have bonds.

Cannot use fix ttm with 2d simulation
: This is a current restriction of this fix due to the grid it creates.

Cannot use fix ttm with triclinic box
: This is a current restriction of this fix due to the grid it creates.

Cannot use fix tune/kspace without a kspace style
: Self-explanatory.

Cannot use fix tune/kspace without a pair style
: This fix (tune/kspace) can only be used when a pair style has been specified.

Cannot use fix wall in periodic dimension
: Self-explanatory.

Cannot use fix wall zlo/zhi for a 2d simulation
: Self-explanatory.

Cannot use fix wall/reflect in periodic dimension
: Self-explanatory.

Cannot use fix wall/reflect zlo/zhi for a 2d simulation
: Self-explanatory.

Cannot use fix wall/srd in periodic dimension
: Self-explanatory.

Cannot use fix wall/srd more than once
: Nor is their a need to since multiple walls can be specified in one command.

Cannot use fix wall/srd without fix srd
: Self-explanatory.

Cannot use fix wall/srd zlo/zhi for a 2d simulation
: Self-explanatory.

Cannot use fix_deposit unless atoms have IDs
: Self-explanatory.

Cannot use fix_pour unless atoms have IDs
: Self-explanatory.

Cannot use include command within an if command
: Self-explanatory.

Cannot use lines with fix srd unless overlap is set
: This is because line segements are connected to each other.

Cannot use multiple fix wall commands with pair brownian
: Self-explanatory.

Cannot use multiple fix wall commands with pair lubricate
: Self-explanatory.

Cannot use multiple fix wall commands with pair lubricate/poly
: Self-explanatory.

Cannot use multiple fix wall commands with pair lubricateU
: Self-explanatory.

Cannot use neigh_modify exclude with GPU neighbor builds
: This is a current limitation of the GPU implementation in LAMMPS.

Cannot use neighbor bins - box size << cutoff
: Too many neighbor bins will be created. This typically happens when the simulation box is very small in some dimension, compared to the neighbor cutoff. Use the "nsq" style instead of "bin" style.

Cannot use newton pair with beck/gpu pair style
: Self-explanatory.

Cannot use newton pair with born/coul/long/gpu pair style
: Self-explanatory.

Cannot use newton pair with born/coul/wolf/gpu pair style
: Self-explanatory.

Cannot use newton pair with born/gpu pair style
: Self-explantory.

Cannot use newton pair with buck/coul/cut/gpu pair style
: Self-explanatory.

Cannot use newton pair with buck/coul/long/gpu pair style
: Self-explanatory.

Cannot use newton pair with buck/gpu pair style
: Self-explanatory.

Cannot use newton pair with colloid/gpu pair style
: Self-explanatory.

Cannot use newton pair with coul/cut/gpu pair style
: Self-explanatory.

Cannot use newton pair with coul/debye/gpu pair style
: Self-explanatory.

Cannot use newton pair with coul/dsf/gpu pair style
: Self-explanatory.

Cannot use newton pair with coul/long/gpu pair style
: Self-explanatory.

Cannot use newton pair with dipole/cut/gpu pair style
: Self-explanatory.

Cannot use newton pair with dipole/sf/gpu pair style
: Self-explanatory.

Cannot use newton pair with dpd/gpu pair style
: Self-explanatory.

Cannot use newton pair with dpd/tstat/gpu pair style
: Self-explanatory.

Cannot use newton pair with eam/alloy/gpu pair style
: Self-explanatory.

Cannot use newton pair with eam/fs/gpu pair style
: Self-explanatory.

Cannot use newton pair with eam/gpu pair style

Self-explanatory.

Cannot use newton pair with gauss/gpu pair style

Self-explanatory.

Cannot use newton pair with gayberne/gpu pair style

Self-explanatory.

Cannot use newton pair with lj/charmm/coul/long/gpu pair style

Self-explanatory.

Cannot use newton pair with lj/class2/coul/long/gpu pair style

Self-explanatory.

Cannot use newton pair with lj/class2/gpu pair style

Self-explanatory.

Cannot use newton pair with lj/cubic/gpu pair style

Self-explanatory.

Cannot use newton pair with lj/cut/coul/cut/gpu pair style

Self-explanatory.

Cannot use newton pair with lj/cut/coul/debye/gpu pair style

Self-explanatory.

Cannot use newton pair with lj/cut/coul/dsf/gpu pair style

Self-explanatory.

Cannot use newton pair with lj/cut/coul/long/gpu pair style

Self-explanatory.

Cannot use newton pair with lj/cut/coul/msm/gpu pair style

Self-explanatory.

Cannot use newton pair with lj/cut/gpu pair style

Self-explanatory.

Cannot use newton pair with lj/expand/gpu pair style

Self-explanatory.

Cannot use newton pair with lj/gromacs/gpu pair style

Self-explanatory.

Cannot use newton pair with lj/sdk/coul/long/gpu pair style

Self-explanatory.

Cannot use newton pair with lj/sdk/gpu pair style

Self-explanatory.

Cannot use newton pair with lj96/cut/gpu pair style

Self-explanatory.

Cannot use newton pair with mie/cut/gpu pair style

Self-explanatory.

Cannot use newton pair with morse/gpu pair style

Self-explanatory.

Cannot use newton pair with resquared/gpu pair style

Self-explanatory.

Cannot use newton pair with soft/gpu pair style

Self-explanatory.

Cannot use newton pair with table/gpu pair style

Self-explanatory.

Cannot use newton pair with yukawa/colloid/gpu pair style

Self-explanatory.

Cannot use newton pair with yukawa/gpu pair style

Self-explanatory.

Cannot use newton pair with zbl/gpu pair style

Self-explantory.

Cannot use non-zero forces in an energy minimization

Fix setforce cannot be used in this manner. Use fix addforce instead.

Cannot use nonperiodic boundares with fix ttm

This fix requires a fully periodic simulation box.

Cannot use nonperiodic boundaries with Ewald

For kspace style ewald, all 3 dimensions must have periodic boundaries unless you use the kspace_modify command to define a 2d slab with a non-periodic z dimension.

Cannot use nonperiodic boundaries with EwaldDisp

For kspace style ewald/disp, all 3 dimensions must have periodic boundaries unless you use the kspace_modify command to define a 2d slab with a non-periodic z dimension.

Cannot use nonperiodic boundaries with PPPM

For kspace style pppm, all 3 dimensions must have periodic boundaries unless you use the kspace_modify command to define a 2d slab with a non-periodic z dimension.

Cannot use nonperiodic boundaries with PPPMDisp

For kspace style pppm/disp, all 3 dimensions must have periodic boundaries unless you use the kspace_modify command to define a 2d slab with a non-periodic z dimension.

Cannot use order greater than 8 with pppm/gpu.

Self-explanatory.

Cannot use package gpu neigh yes with triclinic box

This is a current restriction in LAMMPS.

Cannot use pair hybrid with GPU neighbor list builds

Neighbor list builds must be done on the CPU for this pair style.

Cannot use pair tail corrections with 2d simulations

The correction factors are only currently defined for 3d systems.

Cannot use processors part command without using partitions

See the command-line -partition switch.

Cannot use ramp in variable formula between runs

This is because the ramp() function is time dependent.

Cannot use read_data add before simulation box is defined

Self-explanatory.

Cannot use read_data extra with add flag

Self-explanatory.

Cannot use read_data offset without add flag

Self-explanatory.

Cannot use read_data shift without add flag

Self-explanatory.

Cannot use region INF or EDGE when box does not exist

Regions that extend to the box boundaries can only be used after the create_box command has been used.

Cannot use set atom with no atom IDs defined

Atom IDs are not defined, so they cannot be used to identify an atom.

Cannot use set mol with no molecule IDs defined

Self-explanatory.

Cannot use swiggle in variable formula between runs

This is a function of elapsed time.

Cannot use tris with fix srd unless overlap is set

This is because triangles are connected to each other.

Cannot use variable energy with constant efield in fix efield

LAMMPS computes the energy itself when the E-field is constant.

Cannot use variable energy with constant force in fix addforce

This is because for constant force, LAMMPS can compute the change in energy directly.

Cannot use variable every setting for dump dcd

The format of DCD dump files requires snapshots be output at a constant frequency.

Cannot use variable every setting for dump xtc

The format of this file requires snapshots at regular intervals.

Cannot use vdisplace in variable formula between runs

This is a function of elapsed time.

Cannot use velocity bias command without temp keyword

Self-explanatory.

Cannot use velocity create loop all unless atoms have IDs

Atoms in the simulation to do not have IDs, so this style of velocity creation cannot be performed.

Cannot use wall in periodic dimension

Self-explanatory.

Cannot use write_restart fileper without % in restart file name

Self-explanatory.

Cannot use write_restart nfile without % in restart file name

Self-explanatory.

Cannot wiggle and shear fix wall/gran

Cannot specify both options at the same time.

Cannot write to restart file - MPI error: %s

This error was generated by MPI when reading/writing an MPI-IO restart file.

Cannot yet use KSpace solver with grid with comm style tiled

This is current restriction in LAMMPS.

Cannot yet use comm_style tiled with multi-mode comm

Self-explanatory.

Cannot yet use comm_style tiled with triclinic box

Self-explanatory.

Cannot yet use compute tally with Kokkos

This feature is not yet supported.

Cannot yet use fix bond/break with this improper style

This is a current restriction in LAMMPS.

Cannot yet use fix bond/create with this improper style

This is a current restriction in LAMMPS.

Cannot yet use minimize with Kokkos

This feature is not yet supported.

Cannot yet use pair hybrid with Kokkos

This feature is not yet supported.

Cannot zero Langevin force of 0 atoms

The group has zero atoms, so you cannot request its force be zeroed.

Cannot zero gld force for zero atoms

There are no atoms currently in the group.

Cannot zero momentum of no atoms

Self-explanatory.

Change_box command before simulation box is defined

Self-explanatory.

Change_box volume used incorrectly

The "dim volume" option must be used immediately following one or two settings for "dim1 ..." (and optionally "dim2 ...") and must be for a different dimension, i.e. dim != dim1 and dim != dim2.

Chunk/atom compute does not exist for compute angmom/chunk

Self-explanatory.

Chunk/atom compute does not exist for compute com/chunk

Self-explanatory.

Chunk/atom compute does not exist for compute gyration/chunk

Self-explanatory.

Chunk/atom compute does not exist for compute inertia/chunk

Self-explanatory.

Chunk/atom compute does not exist for compute msd/chunk
Self-explanatory.
Chunk/atom compute does not exist for compute omega/chunk
Self-explanatory.
Chunk/atom compute does not exist for compute property/chunk
Self-explanatory.
Chunk/atom compute does not exist for compute temp/chunk
Self-explanatory.
Chunk/atom compute does not exist for compute torque/chunk
Self-explanatory.
Chunk/atom compute does not exist for compute vcm/chunk
Self-explanatory.
Chunk/atom compute does not exist for fix ave/chunk
Self-explanatory.
Comm tiled invalid index in box drop brick
Internal error check in comm_style tiled which should not occur. Contact the developers.
Comm tiled mis-match in box drop brick
Internal error check in comm_style tiled which should not occur. Contact the developers.
Comm_modify group != atom_modify first group
Self-explanatory.
Communication cutoff for comm_style tiled cannot exceed periodic box length
Self-explanatory.
Communication cutoff too small for SNAP micro load balancing
This can happen if you change the neighbor skin after your pair_style command or if your box dimensions grow during a run. You can set the cutoff explicitly via the comm_modify cutoff command.
Compute %s does not allow use of dynamic group
Dynamic groups have not yet been enabled for this compute.
Compute ID for compute chunk /atom does not exist
Self-explanatory.
Compute ID for compute chunk/atom does not exist
Self-explanatory.
Compute ID for compute reduce does not exist
Self-explanatory.
Compute ID for compute slice does not exist
Self-explanatory.
Compute ID for fix ave/atom does not exist
Self-explanatory.
Compute ID for fix ave/chunk does not exist
Self-explanatory.
Compute ID for fix ave/correlate does not exist
Self-explanatory.
Compute ID for fix ave/histo does not exist
Self-explanatory.
Compute ID for fix ave/spatial does not exist
Self-explanatory.
Compute ID for fix ave/time does not exist
Self-explanatory.
Compute ID for fix store/state does not exist
Self-explanatory.
Compute ID for fix vector does not exist
Self-explanatory.
Compute ID must be alphanumeric or underscore characters

Self-explanatory.

Compute angle/local used when angles are not allowed

The atom style does not support angles.

Compute angmom/chunk does not use chunk/atom compute

The style of the specified compute is not chunk/atom.

Compute body/local requires atom style body

Self-explanatory.

Compute bond/local used when bonds are not allowed

The atom style does not support bonds.

Compute centro/atom requires a pair style be defined

This is because the computation of the centro-symmetry values uses a pairwise neighbor list.

Compute chunk/atom bin/cylinder radius is too large for periodic box

Radius cannot be bigger than 1/2 of a non-axis periodic dimention.

Compute chunk/atom bin/sphere radius is too large for periodic box

Radius cannot be bigger than 1/2 of any periodic dimention.

Compute chunk/atom compute array is accessed out-of-range

The index for the array is out of bounds.

Compute chunk/atom compute does not calculate a per-atom array

Self-explanatory.

Compute chunk/atom compute does not calculate a per-atom vector

Self-explanatory.

Compute chunk/atom compute does not calculate per-atom values

Self-explanatory.

Compute chunk/atom cylinder axis must be z for 2d

Self-explanatory.

Compute chunk/atom fix array is accessed out-of-range

the index for the array is out of bounds.

Compute chunk/atom fix does not calculate a per-atom array

Self-explanatory.

Compute chunk/atom fix does not calculate a per-atom vector

Self-explanatory.

Compute chunk/atom fix does not calculate per-atom values

Self-explanatory.

Compute chunk/atom for triclinic boxes requires units reduced

Self-explanatory.

Compute chunk/atom ids once but nchunk is not once

You cannot assign chunks IDs to atom permanently if the number of chunks may change.

Compute chunk/atom molecule for non-molecular system

Self-explanatory.

Compute chunk/atom sphere z origin must be 0.0 for 2d

Self-explanatory.

Compute chunk/atom stores no IDs for compute property/chunk

It will only store IDs if its compress option is enabled.

Compute chunk/atom stores no coord1 for compute property/chunk

Only certain binning options for comptue chunk/atom store coordinates.

Compute chunk/atom stores no coord2 for compute property/chunk

Only certain binning options for comptue chunk/atom store coordinates.

Compute chunk/atom stores no coord3 for compute property/chunk

Only certain binning options for comptue chunk/atom store coordinates.

Compute chunk/atom variable is not atom-style variable

Self-explanatory.

Compute chunk/atom without bins cannot use discard mixed

That discard option only applies to the binning styles.

Compute cluster/atom cutoff is longer than pairwise cutoff

Cannot identify clusters beyond cutoff.

Compute cluster/atom requires a pair style be defined

This is so that the pair style defines a cutoff distance which is used to find clusters.

Compute cna/atom cutoff is longer than pairwise cutoff

Self-explantory.

Compute cna/atom requires a pair style be defined

Self-explantory.

Compute com/chunk does not use chunk/atom compute

The style of the specified compute is not chunk/atom.

Compute contact/atom requires a pair style be defined

Self-explantory.

Compute contact/atom requires atom style sphere

Self-explanatory.

Compute coord/atom cutoff is longer than pairwise cutoff

Cannot compute coordination at distances longer than the pair cutoff, since those atoms are not in the neighbor list.

Compute coord/atom requires a pair style be defined

Self-explantory.

Compute damage/atom requires peridynamic potential

Damage is a Peridynamic-specific metric. It requires you to be running a Peridynamics simulation.

Compute dihedral/local used when dihedrals are not allowed

The atom style does not support dihedrals.

Compute dilatation/atom cannot be used with this pair style

Self-explanatory.

Compute dilatation/atom requires Peridynamic pair style

Self-explanatory.

Compute does not allow an extra compute or fix to be reset

This is an internal LAMMPS error. Please report it to the developers.

Compute erotate/asphere requires atom style ellipsoid or line or tri

Self-explanatory.

Compute erotate/asphere requires extended particles

This compute cannot be used with point paritlces.

Compute erotate/rigid with non-rigid fix-ID

Self-explanatory.

Compute erotate/sphere requires atom style sphere

Self-explanatory.

Compute erotate/sphere/atom requires atom style sphere

Self-explanatory.

Compute event/displace has invalid fix event assigned

This is an internal LAMMPS error. Please report it to the developers.

Compute group/group group ID does not exist

Self-explanatory.

Compute gyration/chunk does not use chunk/atom compute

The style of the specified compute is not chunk/atom.

Compute heat/flux compute ID does not compute ke/atom

Self-explanatory.

Compute heat/flux compute ID does not compute pe/atom

Self-explanatory.

Compute heat/flux compute ID does not compute stress/atom

Self-explanatory.

Compute hexorder/atom cutoff is longer than pairwise cutoff
: Cannot compute order parameter beyond cutoff.

Compute hexorder/atom requires a pair style be defined
: Self-explantory.

Compute improper/local used when impropers are not allowed
: The atom style does not support impropers.

Compute inertia/chunk does not use chunk/atom compute
: The style of the specified compute is not chunk/atom.

Compute ke/rigid with non-rigid fix-ID
: Self-explanatory.

Compute msd/chunk does not use chunk/atom compute
: The style of the specified compute is not chunk/atom.

Compute msd/chunk nchunk is not static
: This is required because the MSD cannot be computed consistently if the number of chunks is changing. Compute chunk/atom allows setting nchunk to be static.

Compute nve/asphere requires atom style ellipsoid
: Self-explanatory.

Compute nvt/nph/npt asphere requires atom style ellipsoid
: Self-explanatory.

Compute nvt/nph/npt body requires atom style body
: Self-explanatory.

Compute omega/chunk does not use chunk/atom compute
: The style of the specified compute is not chunk/atom.

Compute orientorder/atom cutoff is longer than pairwise cutoff
: Cannot compute order parameter beyond cutoff.

Compute orientorder/atom requires a pair style be defined
: Self-explantory.

Compute pair must use group all
: Pair styles accumlate energy on all atoms.

Compute pe must use group all
: Energies computed by potentials (pair, bond, etc) are computed on all atoms.

Compute plasticity/atom cannot be used with this pair style
: Self-explanatory.

Compute plasticity/atom requires Peridynamic pair style
: Self-explanatory.

Compute pressure must use group all
: Virial contributions computed by potentials (pair, bond, etc) are computed on all atoms.

Compute pressure requires temperature ID to include kinetic energy
: The keflag cannot be used unless a temperature compute is provided.

Compute pressure temperature ID does not compute temperature
: The compute ID assigned to a pressure computation must compute temperature.

Compute property/atom floating point vector does not exist
: The command is accessing a vector added by the fix property/atom command, that does not exist.

Compute property/atom for atom property that isn't allocated
: Self-explanatory.

Compute property/atom integer vector does not exist
: The command is accessing a vector added by the fix property/atom command, that does not exist.

Compute property/chunk does not use chunk/atom compute
: The style of the specified compute is not chunk/atom.

Compute property/local cannot use these inputs together
: Only inputs that generate the same number of datums can be used togther. E.g. bond and angle quantities cannot be mixed.

Compute property/local does not (yet) work with atom_style template
: Self-explanatory.

Compute property/local for property that isn't allocated
: Self-explanatory.

Compute rdf requires a pair style be defined
: Self-explanatory.

Compute reduce compute array is accessed out-of-range
: An index for the array is out of bounds.

Compute reduce compute calculates global values
: A compute that calculates peratom or local values is required.

Compute reduce compute does not calculate a local array
: Self-explanatory.

Compute reduce compute does not calculate a local vector
: Self-explanatory.

Compute reduce compute does not calculate a per-atom array
: Self-explanatory.

Compute reduce compute does not calculate a per-atom vector
: Self-explanatory.

Compute reduce fix array is accessed out-of-range
: An index for the array is out of bounds.

Compute reduce fix calculates global values
: A fix that calculates peratom or local values is required.

Compute reduce fix does not calculate a local array
: Self-explanatory.

Compute reduce fix does not calculate a local vector
: Self-explanatory.

Compute reduce fix does not calculate a per-atom array
: Self-explanatory.

Compute reduce fix does not calculate a per-atom vector
: Self-explanatory.

Compute reduce replace requires min or max mode
: Self-explanatory.

Compute reduce variable is not atom-style variable
: Self-explanatory.

Compute slice compute array is accessed out-of-range
: An index for the array is out of bounds.

Compute slice compute does not calculate a global array
: Self-explanatory.

Compute slice compute does not calculate a global vector
: Self-explanatory.

Compute slice compute does not calculate global vector or array
: Self-explanatory.

Compute slice compute vector is accessed out-of-range
: The index for the vector is out of bounds.

Compute slice fix array is accessed out-of-range
: An index for the array is out of bounds.

Compute slice fix does not calculate a global array
: Self-explanatory.

Compute slice fix does not calculate a global vector
: Self-explanatory.

Compute slice fix does not calculate global vector or array
: Self-explanatory.

Compute slice fix vector is accessed out-of-range
: The index for the vector is out of bounds.

Compute sna/atom cutoff is longer than pairwise cutoff
: Self-explanatory.

Compute sna/atom requires a pair style be defined
: Self-explanatory.

Compute snad/atom cutoff is longer than pairwise cutoff
: Self-explanatory.

Compute snad/atom requires a pair style be defined
: Self-explanatory.

Compute snav/atom cutoff is longer than pairwise cutoff
: Self-explanatory.

Compute snav/atom requires a pair style be defined
: Self-explanatory.

Compute stress/atom temperature ID does not compute temperature
: The specified compute must compute temperature.

Compute temp/asphere requires atom style ellipsoid
: Self-explanatory.

Compute temp/asphere requires extended particles
: This compute cannot be used with point paritlces.

Compute temp/body requires atom style body
: Self-explanatory.

Compute temp/body requires bodies
: This compute can only be applied to body particles.

Compute temp/chunk does not use chunk/atom compute
: The style of the specified compute is not chunk/atom.

Compute temp/cs requires ghost atoms store velocity
: Use the comm_modify vel yes command to enable this.

Compute temp/cs used when bonds are not allowed
: This compute only works on pairs of bonded particles.

Compute temp/partial cannot use vz for 2d systemx
: Self-explanatory.

Compute temp/profile cannot bin z for 2d systems
: Self-explanatory.

Compute temp/profile cannot use vz for 2d systemx
: Self-explanatory.

Compute temp/sphere requires atom style sphere
: Self-explanatory.

Compute ti kspace style does not exist
: Self-explanatory.

Compute ti pair style does not exist
: Self-explanatory.

Compute ti tail when pair style does not compute tail corrections
: Self-explanatory.

Compute torque/chunk does not use chunk/atom compute
: The style of the specified compute is not chunk/atom.

Compute used in dump between runs is not current
: The compute was not invoked on the current timestep, therefore it cannot be used in a dump between runs.

Compute used in variable between runs is not current
: Computes cannot be invoked by a variable in between runs. Thus they must have been evaluated on the last timestep of the previous run in order for their value(s) to be accessed. See the doc page for the

variable command for more info.

Compute used in variable thermo keyword between runs is not current

Some thermo keywords rely on a compute to calculate their value(s). Computes cannot be invoked by a variable in between runs. Thus they must have been evaluated on the last timestep of the previous run in order for their value(s) to be accessed. See the doc page for the variable command for more info.

Compute vcm/chunk does not use chunk/atom compute

The style of the specified compute is not chunk/atom.

Computed temperature for fix temp/berendsen cannot be 0.0

Self-explanatory.

Computed temperature for fix temp/rescale cannot be 0.0

Cannot rescale the temperature to a new value if the current temperature is 0.0.

Core/shell partner atom not found

Could not find one of the atoms in the bond pair.

Core/shell partners were not all found

Could not find or more atoms in the bond pairs.

Could not adjust g_ewald_6

The Newton-Raphson solver failed to converge to a good value for g_ewald. This error should not occur for typical problems. Please send an email to the developers.

Could not compute g_ewald

The Newton-Raphson solver failed to converge to a good value for g_ewald. This error should not occur for typical problems. Please send an email to the developers.

Could not compute grid size

The code is unable to compute a grid size consistent with the desired accuracy. This error should not occur for typical problems. Please send an email to the developers.

Could not compute grid size for Coulomb interaction

The code is unable to compute a grid size consistent with the desired accuracy. This error should not occur for typical problems. Please send an email to the developers.

Could not compute grid size for Dispersion

The code is unable to compute a grid size consistent with the desired accuracy. This error should not occur for typical problems. Please send an email to the developers.

Could not create 3d FFT plan

The FFT setup for the PPPM solver failed, typically due to lack of memory. This is an unusual error. Check the size of the FFT grid you are requesting.

Could not create 3d grid of processors

The specified constraints did not allow a Px by Py by Pz grid to be created where Px * Py * Pz = P = total number of processors.

Could not create 3d remap plan

The FFT setup in pppm failed.

Could not create Python function arguments

This is an internal Python error, possibly because the number of inputs to the function is too large.

Could not create numa grid of processors

The specified constraints did not allow this style of grid to be created. Usually this is because the total processor count is not a multiple of the cores/node or the user specified processor count is > 1 in one of the dimensions.

Could not create twolevel 3d grid of processors

The specified constraints did not allow this style of grid to be created.

Could not evaluate Python function input variable

Self-explanatory.

Could not find Python function

The provided Python code was run successfully, but it not define a callable function with the required name.

Could not find atom_modify first group ID

Self-explanatory.

Could not find change_box group ID

Group ID used in the change_box command does not exist.

Could not find compute ID for PRD

Self-explanatory.

Could not find compute ID for TAD

Self-explanatory.

Could not find compute ID for temperature bias

Self-explanatory.

Could not find compute ID to delete

Self-explanatory.

Could not find compute displace/atom fix ID

Self-explanatory.

Could not find compute event/displace fix ID

Self-explanatory.

Could not find compute group ID

Self-explanatory.

Could not find compute heat/flux compute ID

Self-explanatory.

Could not find compute msd fix ID

Self-explanatory.

Could not find compute msd/chunk fix ID

The compute creates an internal fix, which has been deleted.

Could not find compute pressure temperature ID

The compute ID for calculating temperature does not exist.

Could not find compute stress/atom temperature ID

Self-explanatory.

Could not find compute vacf fix ID

Self-explanatory.

Could not find compute/voronoi surface group ID

Self-explanatory.

Could not find compute_modify ID

Self-explanatory.

Could not find custom per-atom property ID

Self-explanatory.

Could not find delete_atoms group ID

Group ID used in the delete_atoms command does not exist.

Could not find delete_atoms region ID

Region ID used in the delete_atoms command does not exist.

Could not find displace_atoms group ID

Group ID used in the displace_atoms command does not exist.

Could not find dump custom compute ID

Self-explanatory.

Could not find dump custom fix ID

Self-explanatory.

Could not find dump custom variable name

Self-explanatory.

Could not find dump group ID

A group ID used in the dump command does not exist.

Could not find dump local compute ID

Self-explanatory.

Could not find dump local fix ID

Self-explanatory.

Could not find dump modify compute ID

Self-explanatory.

Could not find dump modify custom atom floating point property ID

Self-explanatory.

Could not find dump modify custom atom integer property ID

Self-explanatory.

Could not find dump modify fix ID

Self-explanatory.

Could not find dump modify variable name

Self-explanatory.

Could not find fix ID to delete

Self-explanatory.

Could not find fix adapt storage fix ID

This should not happen unless you explicitly deleted a secondary fix that fix adapt created internally.

Could not find fix gcmc exclusion group ID

Self-explanatory.

Could not find fix gcmc rotation group ID

Self-explanatory.

Could not find fix group ID

A group ID used in the fix command does not exist.

Could not find fix msst compute ID

Self-explanatory.

Could not find fix poems group ID

A group ID used in the fix poems command does not exist.

Could not find fix recenter group ID

A group ID used in the fix recenter command does not exist.

Could not find fix rigid group ID

A group ID used in the fix rigid command does not exist.

Could not find fix srd group ID

Self-explanatory.

Could not find fix_modify ID

A fix ID used in the fix_modify command does not exist.

Could not find fix_modify pressure ID

The compute ID for computing pressure does not exist.

Could not find fix_modify temperature ID

The compute ID for computing temperature does not exist.

Could not find group clear group ID

Self-explanatory.

Could not find group delete group ID

Self-explanatory.

Could not find pair fix ID

A fix is created internally by the pair style to store shear history information. You cannot delete it.

Could not find set group ID

Group ID specified in set command does not exist.

Could not find specified fix gcmc group ID

Self-explanatory.

Could not find thermo compute ID

Compute ID specified in thermo_style command does not exist.

Could not find thermo custom compute ID

The compute ID needed by thermo style custom to compute a requested quantity does not exist.

Could not find thermo custom fix ID

The fix ID needed by thermo style custom to compute a requested quantity does not exist.

Could not find thermo custom variable name

Self-explanatory.

Could not find thermo fix ID

Fix ID specified in thermo_style command does not exist.

Could not find thermo variable name

Self-explanatory.

Could not find thermo_modify pressure ID

The compute ID needed by thermo style custom to compute pressure does not exist.

Could not find thermo_modify temperature ID

The compute ID needed by thermo style custom to compute temperature does not exist.

Could not find undump ID

A dump ID used in the undump command does not exist.

Could not find velocity group ID

A group ID used in the velocity command does not exist.

Could not find velocity temperature ID

The compute ID needed by the velocity command to compute temperature does not exist.

Could not find/initialize a specified accelerator device

Could not initialize at least one of the devices specified for the gpu package

Could not grab element entry from EIM potential file

Self-explanatory

Could not grab global entry from EIM potential file

Self-explanatory.

Could not grab pair entry from EIM potential file

Self-explanatory.

Could not initialize embedded Python

The main module in Python was not accessible.

Could not open Python file

The specified file of Python code cannot be opened. Check that the path and name are correct.

Could not process Python file

The Python code in the specified file was not run sucessfully by Python, probably due to errors in the Python code.

Could not process Python string

The Python code in the here string was not run sucessfully by Python, probably due to errors in the Python code.

Coulomb PPPMDisp order has been reduced below minorder

The default minimum order is 2. This can be reset by the kspace_modify minorder command.

Coulomb cut not supported in pair_style buck/long/coul/coul

Must use long-range Coulombic interactions.

Coulomb cut not supported in pair_style lj/long/coul/long

Must use long-range Coulombic interactions.

Coulomb cut not supported in pair_style lj/long/tip4p/long

Must use long-range Coulombic interactions.

Coulomb cutoffs of pair hybrid sub-styles do not match

If using a Kspace solver, all Coulomb cutoffs of long pair styles must be the same.

Coulombic cut not supported in pair_style lj/long/dipole/long

Must use long-range Coulombic interactions.

Cound not find dump_modify ID

Self-explanatory.

Create_atoms command before simulation box is defined

The create_atoms command cannot be used before a read_data, read_restart, or create_box command.

Create_atoms molecule has atom IDs, but system does not

The atom_style id command can be used to force atom IDs to be stored.

Create_atoms molecule must have atom types

The defined molecule does not specify atom types.

Create_atoms molecule must have coordinates

The defined molecule does not specify coordinates.

Create_atoms region ID does not exist

A region ID used in the create_atoms command does not exist.

Create_bonds command before simulation box is defined

Self-explanatory.

Create_bonds command requires no kspace_style be defined

This is so that atom pairs that are already bonded to not appear in the neighbor list.

Create_bonds command requires special_bonds 1-2 weights be 0.0

This is so that atom pairs that are already bonded to not appear in the neighbor list.

Create_bonds max distance > neighbor cutoff

Can only create bonds for atom pairs that will be in neighbor list.

Create_bonds requires a pair style be defined

Self-explanatory.

Create_box region ID does not exist

Self-explanatory.

Create_box region does not support a bounding box

Not all regions represent bounded volumes. You cannot use such a region with the create_box command.

Custom floating point vector for fix store/state does not exist

The command is accessing a vector added by the fix property/atom command, that does not exist.

Custom integer vector for fix store/state does not exist

The command is accessing a vector added by the fix property/atom command, that does not exist.

Custom per-atom property ID is not floating point

Self-explanatory.

Custom per-atom property ID is not integer

Self-explanatory.

Cut-offs missing in pair_style lj/long/dipole/long

Self-explanatory.

Cutoffs missing in pair_style buck/long/coul/long

Self-exlanatory.

Cutoffs missing in pair_style lj/long/coul/long

Self-explanatory.

Cyclic loop in joint connections

Fix poems cannot (yet) work with coupled bodies whose joints connect the bodies in a ring (or cycle).

Degenerate lattice primitive vectors

Invalid set of 3 lattice vectors for lattice command.

Delete region ID does not exist

Self-explanatory.

Delete_atoms command before simulation box is defined

The delete_atoms command cannot be used before a read_data, read_restart, or create_box command.

Delete_atoms cutoff > max neighbor cutoff

Can only delete atoms in atom pairs that will be in neighbor list.

Delete_atoms mol yes requires atom attribute molecule

Cannot use this option with a non-molecular system.

Delete_atoms requires a pair style be defined

This is because atom deletion within a cutoff uses a pairwise neighbor list.

Delete_bonds command before simulation box is defined

The delete_bonds command cannot be used before a read_data, read_restart, or create_box command.

Delete_bonds command with no atoms existing

No atoms are yet defined so the delete_bonds command cannot be used.

Deposition region extends outside simulation box

Self-explanatory.

Did not assign all atoms correctly

Atoms read in from a data file were not assigned correctly to processors. This is likely due to some atom coordinates being outside a non-periodic simulation box.

Did not assign all restart atoms correctly

Atoms read in from the restart file were not assigned correctly to processors. This is likely due to some atom coordinates being outside a non-periodic simulation box. Normally this should not happen. You may wish to use the "remap" option on the read_restart command to see if this helps.

Did not find all elements in MEAM library file

The requested elements were not found in the MEAM file.

Did not find fix shake partner info

Could not find bond partners implied by fix shake command. This error can be triggered if the delete_bonds command was used before fix shake, and it removed bonds without resetting the 1-2, 1-3, 1-4 weighting list via the special keyword.

Did not find keyword in table file

Keyword used in pair_coeff command was not found in table file.

Did not set pressure for fix rigid/nph

The press keyword must be specified.

Did not set temp for fix rigid/nvt/small

Self-explanatory.

Did not set temp or press for fix rigid/npt/small

Self-explanatory.

Did not set temperature for fix rigid/nvt

The temp keyword must be specified.

Did not set temperature or pressure for fix rigid/npt

The temp and press keywords must be specified.

Dihedral atom missing in delete_bonds

The delete_bonds command cannot find one or more atoms in a particular dihedral on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid dihedral.

Dihedral atom missing in set command

The set command cannot find one or more atoms in a particular dihedral on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid dihedral.

Dihedral atoms %d %d %d %d missing on proc %d at step %ld

One or more of 4 atoms needed to compute a particular dihedral are missing on this processor. Typically this is because the pairwise cutoff is set too short or the dihedral has blown apart and an atom is too far away.

Dihedral atoms missing on proc %d at step %ld

One or more of 4 atoms needed to compute a particular dihedral are missing on this processor. Typically this is because the pairwise cutoff is set too short or the dihedral has blown apart and an atom is too far away.

Dihedral charmm is incompatible with Pair style

Dihedral style charmm must be used with a pair style charmm in order for the 1-4 epsilon/sigma parameters to be defined.

Dihedral coeff for hybrid has invalid style

Dihedral style hybrid uses another dihedral style as one of its coefficients. The dihedral style used in the dihedral_coeff command or read from a restart file is not recognized.

Dihedral coeffs are not set

No dihedral coefficients have been assigned in the data file or via the dihedral_coeff command.

Dihedral style hybrid cannot have hybrid as an argument

Self-explanatory.

Dihedral style hybrid cannot have none as an argument
: Self-explanatory.

Dihedral style hybrid cannot use same dihedral style twice
: Self-explanatory.

Dihedral/improper extent > half of periodic box length
: This error was detected by the neigh_modify check yes setting. It is an error because the dihedral atoms are so far apart it is ambiguous how it should be defined.

Dihedral_coeff command before dihedral_style is defined
: Coefficients cannot be set in the data file or via the dihedral_coeff command until an dihedral_style has been assigned.

Dihedral_coeff command before simulation box is defined
: The dihedral_coeff command cannot be used before a read_data, read_restart, or create_box command.

Dihedral_coeff command when no dihedrals allowed
: The chosen atom style does not allow for dihedrals to be defined.

Dihedral_style command when no dihedrals allowed
: The chosen atom style does not allow for dihedrals to be defined.

Dihedrals assigned incorrectly
: Dihedrals read in from the data file were not assigned correctly to atoms. This means there is something invalid about the topology definitions.

Dihedrals defined but no dihedral types
: The data file header lists dihedrals but no dihedral types.

Dimension command after simulation box is defined
: The dimension command cannot be used after a read_data, read_restart, or create_box command.

Dispersion PPPMDisp order has been reduced below minorder
: The default minimum order is 2. This can be reset by the kspace_modify minorder command.

Displace_atoms command before simulation box is defined
: The displace_atoms command cannot be used before a read_data, read_restart, or create_box command.

Distance must be > 0 for compute event/displace
: Self-explanatory.

Divide by 0 in influence function
: This should not normally occur. It is likely a problem with your model.

Divide by 0 in influence function of pair peri/lps
: This should not normally occur. It is likely a problem with your model.

Divide by 0 in variable formula
: Self-explanatory.

Domain too large for neighbor bins
: The domain has become extremely large so that neighbor bins cannot be used. Most likely, one or more atoms have been blown out of the simulation box to a great distance.

Double precision is not supported on this accelerator
: Self-explanatory

Dump atom/gz only writes compressed files
: The dump atom/gz output file name must have a .gz suffix.

Dump cfg arguments can not mix xs|ys|zs with xsu|ysu|zsu
: Self-explanatory.

Dump cfg arguments must start with 'mass type xs ys zs' or 'mass type xsu ysu zsu'
: This is a requirement of the CFG output format. See the dump cfg doc page for more details.

Dump cfg requires one snapshot per file
: Use the wildcard "*" character in the filename.

Dump cfg/gz only writes compressed files
: The dump cfg/gz output file name must have a .gz suffix.

Dump custom and fix not computed at compatible times
: The fix must produce per-atom quantities on timesteps that dump custom needs them.

Dump custom compute does not calculate per-atom array
: Self-explanatory.

Dump custom compute does not calculate per-atom vector
: Self-explanatory.

Dump custom compute does not compute per-atom info
: Self-explanatory.

Dump custom compute vector is accessed out-of-range
: Self-explanatory.

Dump custom fix does not compute per-atom array
: Self-explanatory.

Dump custom fix does not compute per-atom info
: Self-explanatory.

Dump custom fix does not compute per-atom vector
: Self-explanatory.

Dump custom fix vector is accessed out-of-range
: Self-explanatory.

Dump custom variable is not atom-style variable
: Only atom-style variables generate per-atom quantities, needed for dump output.

Dump custom/gz only writes compressed files
: The dump custom/gz output file name must have a .gz suffix.

Dump dcd of non-matching # of atoms
: Every snapshot written by dump dcd must contain the same # of atoms.

Dump dcd requires sorting by atom ID
: Use the dump_modify sort command to enable this.

Dump every variable returned a bad timestep
: The variable must return a timestep greater than the current timestep.

Dump file MPI-IO output not allowed with % in filename
: This is because a % signifies one file per processor and MPI-IO creates one large file for all processors.

Dump file does not contain requested snapshot
: Self-explanatory.

Dump file is incorrectly formatted
: Self-explanatory.

Dump image body yes requires atom style body
: Self-explanatory.

Dump image bond not allowed with no bond types
: Self-explanatory.

Dump image cannot perform sorting
: Self-explanatory.

Dump image line requires atom style line
: Self-explanatory.

Dump image persp option is not yet supported
: Self-explanatory.

Dump image requires one snapshot per file
: Use a "*" in the filename.

Dump image tri requires atom style tri
: Self-explanatory.

Dump local and fix not computed at compatible times
: The fix must produce per-atom quantities on timesteps that dump local needs them.

Dump local attributes contain no compute or fix
: Self-explanatory.

Dump local cannot sort by atom ID
: This is because dump local does not really dump per-atom info.

Dump local compute does not calculate local array
: Self-explanatory.

Dump local compute does not calculate local vector
: Self-explanatory.

Dump local compute does not compute local info
: Self-explanatory.

Dump local compute vector is accessed out-of-range
: Self-explanatory.

Dump local count is not consistent across input fields
: Every column of output must be the same length.

Dump local fix does not compute local array
: Self-explanatory.

Dump local fix does not compute local info
: Self-explanatory.

Dump local fix does not compute local vector
: Self-explanatory.

Dump local fix vector is accessed out-of-range
: Self-explanatory.

Dump modify bcolor not allowed with no bond types
: Self-explanatory.

Dump modify bdiam not allowed with no bond types
: Self-explanatory.

Dump modify compute ID does not compute per-atom array
: Self-explanatory.

Dump modify compute ID does not compute per-atom info
: Self-explanatory.

Dump modify compute ID does not compute per-atom vector
: Self-explanatory.

Dump modify compute ID vector is not large enough
: Self-explanatory.

Dump modify element names do not match atom types
: Number of element names must equal number of atom types.

Dump modify fix ID does not compute per-atom array
: Self-explanatory.

Dump modify fix ID does not compute per-atom info
: Self-explanatory.

Dump modify fix ID does not compute per-atom vector
: Self-explanatory.

Dump modify fix ID vector is not large enough
: Self-explanatory.

Dump modify variable is not atom-style variable
: Self-explanatory.

Dump sort column is invalid
: Self-explanatory.

Dump xtc requires sorting by atom ID
: Use the dump_modify sort command to enable this.

Dump xyz/gz only writes compressed files
: The dump xyz/gz output file name must have a .gz suffix.

Dump_modify buffer yes not allowed for this style
: Self-explanatory.

Dump_modify format string is too short
: There are more fields to be dumped in a line of output than your format string specifies.

Dump_modify region ID does not exist
: Self-explanatory.

Dumping an atom property that isn't allocated
: The chosen atom style does not define the per-atom quantity being dumped.

Duplicate atom IDs exist
: Self-explanatory.

Duplicate fields in read_dump command
: Self-explanatory.

Duplicate particle in PeriDynamic bond - simulation box is too small
: This is likely because your box length is shorter than 2 times the bond length.

Electronic temperature dropped below zero
: Something has gone wrong with the fix ttm electron temperature model.

Element not defined in potential file
: The specified element is not in the potential file.

Empty brackets in variable
: There is no variable syntax that uses empty brackets. Check the variable doc page.

Energy was not tallied on needed timestep
: You are using a thermo keyword that requires potentials to have tallied energy, but they didn't on this timestep. See the variable doc page for ideas on how to make this work.

Epsilon or sigma reference not set by pair style in PPPMDisp
: Self-explanatory.

Epsilon or sigma reference not set by pair style in ewald/n
: The pair style is not providing the needed epsilon or sigma values.

Error in vdw spline: inner radius > outer radius
: A pre-tabulated spline is invalid. Likely a problem with the potential parameters.

Error writing averaged chunk data
: Something in the output to the file triggered an error.

Error writing file header
: Something in the output to the file triggered an error.

Error writing out correlation data
: Something in the output to the file triggered an error.

Error writing out histogram data
: Something in the output to the file triggered an error.

Error writing out time averaged data
: Something in the output to the file triggered an error.

Failed to allocate %ld bytes for array %s
: Your LAMMPS simulation has run out of memory. You need to run a smaller simulation or on more processors.

Failed to open FFmpeg pipeline to file %s
: The specified file cannot be opened. Check that the path and name are correct and writable and that the FFmpeg executable can be found and run.

Failed to reallocate %ld bytes for array %s
: Your LAMMPS simulation has run out of memory. You need to run a smaller simulation or on more processors.

Fewer SRD bins than processors in some dimension
: This is not allowed. Make your SRD bin size smaller.

File variable could not read value
: Check the file assigned to the variable.

Final box dimension due to fix deform is < 0.0
: Self-explanatory.

Fix %s does not allow use of dynamic group
: Dynamic groups have not yet been enabled for this fix.

Fix ID for compute chunk/atom does not exist
: Self-explanatory.

Fix ID for compute erotate/rigid does not exist
: Self-explanatory.

Fix ID for compute ke/rigid does not exist
: Self-explanatory.

Fix ID for compute reduce does not exist
: Self-explanatory.

Fix ID for compute slice does not exist
: Self-explanatory.

Fix ID for fix ave/atom does not exist
: Self-explanatory.

Fix ID for fix ave/chunk does not exist
: Self-explanatory.

Fix ID for fix ave/correlate does not exist
: Self-explanatory.

Fix ID for fix ave/histo does not exist
: Self-explanatory.

Fix ID for fix ave/spatial does not exist
: Self-explanatory.

Fix ID for fix ave/time does not exist
: Self-explanatory.

Fix ID for fix store/state does not exist
: Self-explanatory

Fix ID for fix vector does not exist
: Self-explanatory.

Fix ID for read_data does not exist
: Self-explanatory.

Fix ID for velocity does not exist
: Self-explanatory.

Fix ID must be alphanumeric or underscore characters
: Self-explanatory.

Fix SRD: bad bin assignment for SRD advection
: Something has gone wrong in your SRD model; try using more conservative settings.

Fix SRD: bad search bin assignment
: Something has gone wrong in your SRD model; try using more conservative settings.

Fix SRD: bad stencil bin for big particle
: Something has gone wrong in your SRD model; try using more conservative settings.

Fix SRD: too many big particles in bin
: Reset the ATOMPERBIN parameter at the top of fix_srd.cpp to a larger value, and re-compile the code.

Fix SRD: too many walls in bin
: This should not happen unless your system has been setup incorrectly.

Fix adapt interface to this pair style not supported
: New coding for the pair style would need to be done.

Fix adapt kspace style does not exist
: Self-explanatory.

Fix adapt pair style does not exist
: Self-explanatory

Fix adapt pair style param not supported
: The pair style does not know about the parameter you specified.

Fix adapt requires atom attribute charge
: The atom style being used does not specify an atom charge.

Fix adapt requires atom attribute diameter
: The atom style being used does not specify an atom diameter.

Fix adapt type pair range is not valid for pair hybrid sub-style
: Self-explanatory.

Fix append/atoms requires a lattice be defined
: Use the lattice command for this purpose.

Fix ave/atom compute array is accessed out-of-range
: Self-explanatory.

Fix ave/atom compute does not calculate a per-atom array
: Self-explanatory.

Fix ave/atom compute does not calculate a per-atom vector
: A compute used by fix ave/atom must generate per-atom values.

Fix ave/atom compute does not calculate per-atom values
: A compute used by fix ave/atom must generate per-atom values.

Fix ave/atom fix array is accessed out-of-range
: Self-explanatory.

Fix ave/atom fix does not calculate a per-atom array
: Self-explanatory.

Fix ave/atom fix does not calculate a per-atom vector
: A fix used by fix ave/atom must generate per-atom values.

Fix ave/atom fix does not calculate per-atom values
: A fix used by fix ave/atom must generate per-atom values.

Fix ave/atom variable is not atom-style variable
: A variable used by fix ave/atom must generate per-atom values.

Fix ave/chunk compute does not calculate a per-atom array
: Self-explanatory.

Fix ave/chunk compute does not calculate a per-atom vector
: Self-explanatory.

Fix ave/chunk compute does not calculate per-atom values
: Self-explanatory.

Fix ave/chunk compute vector is accessed out-of-range
: Self-explanatory.

Fix ave/chunk does not use chunk/atom compute
: The specified conpute is not for a compute chunk/atom command.

Fix ave/chunk fix does not calculate a per-atom array
: Self-explanatory.

Fix ave/chunk fix does not calculate a per-atom vector
: Self-explanatory.

Fix ave/chunk fix does not calculate per-atom values
: Self-explanatory.

Fix ave/chunk fix vector is accessed out-of-range
: Self-explanatory.

Fix ave/chunk variable is not atom-style variable
: Self-explanatory.

Fix ave/correlate compute does not calculate a scalar
: Self-explanatory.

Fix ave/correlate compute does not calculate a vector
: Self-explanatory.

Fix ave/correlate compute vector is accessed out-of-range
: The index for the vector is out of bounds.

Fix ave/correlate fix does not calculate a scalar
: Self-explanatory.

Fix ave/correlate fix does not calculate a vector
Self-explanatory.
Fix ave/correlate fix vector is accessed out-of-range
The index for the vector is out of bounds.
Fix ave/correlate variable is not equal-style variable
Self-explanatory.
Fix ave/histo cannot input local values in scalar mode
Self-explanatory.
Fix ave/histo cannot input per-atom values in scalar mode
Self-explanatory.
Fix ave/histo compute array is accessed out-of-range
Self-explanatory.
Fix ave/histo compute does not calculate a global array
Self-explanatory.
Fix ave/histo compute does not calculate a global scalar
Self-explanatory.
Fix ave/histo compute does not calculate a global vector
Self-explanatory.
Fix ave/histo compute does not calculate a local array
Self-explanatory.
Fix ave/histo compute does not calculate a local vector
Self-explanatory.
Fix ave/histo compute does not calculate a per-atom array
Self-explanatory.
Fix ave/histo compute does not calculate a per-atom vector
Self-explanatory.
Fix ave/histo compute does not calculate local values
Self-explanatory.
Fix ave/histo compute does not calculate per-atom values
Self-explanatory.
Fix ave/histo compute vector is accessed out-of-range
Self-explanatory.
Fix ave/histo fix array is accessed out-of-range
Self-explanatory.
Fix ave/histo fix does not calculate a global array
Self-explanatory.
Fix ave/histo fix does not calculate a global scalar
Self-explanatory.
Fix ave/histo fix does not calculate a global vector
Self-explanatory.
Fix ave/histo fix does not calculate a local array
Self-explanatory.
Fix ave/histo fix does not calculate a local vector
Self-explanatory.
Fix ave/histo fix does not calculate a per-atom array
Self-explanatory.
Fix ave/histo fix does not calculate a per-atom vector
Self-explanatory.
Fix ave/histo fix does not calculate local values
Self-explanatory.
Fix ave/histo fix does not calculate per-atom values
Self-explanatory.

Fix ave/histo fix vector is accessed out-of-range
Self-explanatory.
Fix ave/histo input is invalid compute
Self-explanatory.
Fix ave/histo input is invalid fix
Self-explanatory.
Fix ave/histo input is invalid variable
Self-explanatory.
Fix ave/histo inputs are not all global, peratom, or local
All inputs in a single fix ave/histo command must be of the same style.
Fix ave/histo/weight value and weight vector lengths do not match
Self-explanatory.
Fix ave/spatial compute does not calculate a per-atom array
Self-explanatory.
Fix ave/spatial compute does not calculate a per-atom vector
A compute used by fix ave/spatial must generate per-atom values.
Fix ave/spatial compute does not calculate per-atom values
A compute used by fix ave/spatial must generate per-atom values.
Fix ave/spatial compute vector is accessed out-of-range
The index for the vector is out of bounds.
Fix ave/spatial fix does not calculate a per-atom array
Self-explanatory.
Fix ave/spatial fix does not calculate a per-atom vector
A fix used by fix ave/spatial must generate per-atom values.
Fix ave/spatial fix does not calculate per-atom values
A fix used by fix ave/spatial must generate per-atom values.
Fix ave/spatial fix vector is accessed out-of-range
The index for the vector is out of bounds.
Fix ave/spatial for triclinic boxes requires units reduced
Self-explanatory.
Fix ave/spatial settings invalid with changing box size
If the box size changes, only the units reduced option can be used.
Fix ave/spatial variable is not atom-style variable
A variable used by fix ave/spatial must generate per-atom values.
Fix ave/time cannot set output array intensive/extensive from these inputs
One of more of the vector inputs has individual elements which are flagged as intensive or extensive.
Such an input cannot be flagged as all intensive/extensive when turned into an array by fix ave/time.
Fix ave/time cannot use variable with vector mode
Variables produce scalar values.
Fix ave/time columns are inconsistent lengths
Self-explanatory.
Fix ave/time compute array is accessed out-of-range
An index for the array is out of bounds.
Fix ave/time compute does not calculate a scalar
Self-explantory.
Fix ave/time compute does not calculate a vector
Self-explantory.
Fix ave/time compute does not calculate an array
Self-explanatory.
Fix ave/time compute vector is accessed out-of-range
The index for the vector is out of bounds.
Fix ave/time fix array cannot be variable length

Self-explanatory.

Fix ave/time fix array is accessed out-of-range

An index for the array is out of bounds.

Fix ave/time fix does not calculate a scalar

Self-explanatory.

Fix ave/time fix does not calculate a vector

Self-explanatory.

Fix ave/time fix does not calculate an array

Self-explanatory.

Fix ave/time fix vector cannot be variable length

Self-explanatory.

Fix ave/time fix vector is accessed out-of-range

The index for the vector is out of bounds.

Fix ave/time variable is not equal-style variable

Self-explanatory.

Fix balance rcb cannot be used with comm_style brick

Comm_style tiled must be used instead.

Fix balance shift string is invalid

The string can only contain the characters "x", "y", or "z".

Fix bond/break needs ghost atoms from further away

This is because the fix needs to walk bonds to a certain distance to acquire needed info, The comm_modify cutoff command can be used to extend the communication range.

Fix bond/create angle type is invalid

Self-explanatory.

Fix bond/create cutoff is longer than pairwise cutoff

This is not allowed because bond creation is done using the pairwise neighbor list.

Fix bond/create dihedral type is invalid

Self-explanatory.

Fix bond/create improper type is invalid

Self-explanatory.

Fix bond/create induced too many angles/dihedrals/impropers per atom

See the read_data command for info on setting the "extra angle per atom", etc header values to allow for additional angles, etc to be formed.

Fix bond/create needs ghost atoms from further away

This is because the fix needs to walk bonds to a certain distance to acquire needed info, The comm_modify cutoff command can be used to extend the communication range.

Fix bond/swap cannot use dihedral or improper styles

These styles cannot be defined when using this fix.

Fix bond/swap requires pair and bond styles

Self-explanatory.

Fix bond/swap requires special_bonds = 0,1,1

Self-explanatory.

Fix box/relax generated negative box length

The pressure being applied is likely too large. Try applying it incrementally, to build to the high pressure.

Fix command before simulation box is defined

The fix command cannot be used before a read_data, read_restart, or create_box command.

Fix deform cannot use yz variable with xy

The yz setting cannot be a variable if xy deformation is also specified. This is because LAMMPS cannot determine if the yz setting will induce a box flip which would be invalid if xy is also changing.

Fix deform is changing yz too much with xy

When both yz and xy are changing, it induces changes in xz if the box must flip from one tilt extreme to another. Thus it is not allowed for yz to grow so much that a flip is induced.

Fix deform tilt factors require triclinic box
: Cannot deform the tilt factors of a simulation box unless it is a triclinic (non-orthogonal) box.

Fix deform volume setting is invalid
: Cannot use volume style unless other dimensions are being controlled.

Fix deposit and fix rigid/small not using same molecule template ID
: Self-explanatory.

Fix deposit and fix shake not using same molecule template ID
: Self-explanatory.

Fix deposit molecule must have atom types
: The defined molecule does not specify atom types.

Fix deposit molecule must have coordinates
: The defined molecule does not specify coordinates.

Fix deposit molecule template ID must be same as atom_style template ID
: When using atom_style template, you cannot deposit molecules that are not in that template.

Fix deposit region cannot be dynamic
: Only static regions can be used with fix deposit.

Fix deposit region does not support a bounding box
: Not all regions represent bounded volumes. You cannot use such a region with the fix deposit command.

Fix deposit shake fix does not exist
: Self-explanatory.

Fix efield requires atom attribute q or mu
: The atom style defined does not have this attribute.

Fix efield with dipoles cannot use atom-style variables
: This option is not supported.

Fix evaporate molecule requires atom attribute molecule
: The atom style being used does not define a molecule ID.

Fix external callback function not set
: This must be done by an external program in order to use this fix.

Fix for fix ave/atom not computed at compatible time
: Fixes generate their values on specific timesteps. Fix ave/atom is requesting a value on a non-allowed timestep.

Fix for fix ave/chunk not computed at compatible time
: Fixes generate their values on specific timesteps. Fix ave/chunk is requesting a value on a non-allowed timestep.

Fix for fix ave/correlate not computed at compatible time
: Fixes generate their values on specific timesteps. Fix ave/correlate is requesting a value on a non-allowed timestep.

Fix for fix ave/histo not computed at compatible time
: Fixes generate their values on specific timesteps. Fix ave/histo is requesting a value on a non-allowed timestep.

Fix for fix ave/spatial not computed at compatible time
: Fixes generate their values on specific timesteps. Fix ave/spatial is requesting a value on a non-allowed timestep.

Fix for fix ave/time not computed at compatible time
: Fixes generate their values on specific timesteps. Fix ave/time is requesting a value on a non-allowed timestep.

Fix for fix store/state not computed at compatible time
: Fixes generate their values on specific timesteps. Fix store/state is requesting a value on a non-allowed timestep.

Fix for fix vector not computed at compatible time
: Fixes generate their values on specific timesteps. Fix vector is requesting a value on a non-allowed timestep.

Fix freeze requires atom attribute torque
: The atom style defined does not have this attribute.

Fix gcmc and fix shake not using same molecule template ID
: Self-explanatory.

Fix gcmc atom has charge, but atom style does not
: Self-explanatory.

Fix gcmc cannot exchange individual atoms belonging to a molecule
: This is an error since you should not delete only one atom of a molecule. The user has specified atomic (non-molecular) gas exchanges, but an atom belonging to a molecule could be deleted.

Fix gcmc does not (yet) work with atom_style template
: Self-explanatory.

Fix gcmc molecule command requires that atoms have molecule attributes
: Should not choose the gcmc molecule feature if no molecules are being simulated. The general molecule flag is off, but gcmc's molecule flag is on.

Fix gcmc molecule has charges, but atom style does not
: Self-explanatory.

Fix gcmc molecule must have atom types
: The defined molecule does not specify atom types.

Fix gcmc molecule must have coordinates
: The defined molecule does not specify coordinates.

Fix gcmc molecule template ID must be same as atom_style template ID
: When using atom_style template, you cannot insert molecules that are not in that template.

Fix gcmc put atom outside box
: This should not normally happen. Contact the developers.

Fix gcmc ran out of available atom IDs
: See the setting for tagint in the src/lmptype.h file.

Fix gcmc ran out of available molecule IDs
: See the setting for tagint in the src/lmptype.h file.

Fix gcmc region cannot be dynamic
: Only static regions can be used with fix gcmc.

Fix gcmc region does not support a bounding box
: Not all regions represent bounded volumes. You cannot use such a region with the fix gcmc command.

Fix gcmc region extends outside simulation box
: Self-explanatory.

Fix gcmc shake fix does not exist
: Self-explanatory.

Fix gld c coefficients must be >= 0
: Self-explanatory.

Fix gld needs more prony series coefficients
: Self-explanatory.

Fix gld prony terms must be > 0
: Self-explanatory.

Fix gld series type must be pprony for now
: Self-explanatory.

Fix gld start temperature must be >= 0
: Self-explanatory.

Fix gld stop temperature must be >= 0
: Self-explanatory.

Fix gld tau coefficients must be > 0
: Self-explanatory.

Fix heat group has no atoms
: Self-explanatory.

Fix heat kinetic energy of an atom went negative
: This will cause the velocity rescaling about to be performed by fix heat to be invalid.

Fix heat kinetic energy went negative
: This will cause the velocity rescaling about to be performed by fix heat to be invalid.

Fix in variable not computed at compatible time
: Fixes generate their values on specific timesteps. The variable is requesting the values on a non-allowed timestep.

Fix langevin angmom is not yet implemented with kokkos
: This option is not yet available.

Fix langevin angmom requires atom style ellipsoid
: Self-explanatory.

Fix langevin angmom requires extended particles
: This fix option cannot be used with point paritlces.

Fix langevin omega is not yet implemented with kokkos
: This option is not yet available.

Fix langevin omega requires atom style sphere
: Self-explanatory.

Fix langevin omega requires extended particles
: One of the particles has radius 0.0.

Fix langevin period must be > 0.0
: The time window for temperature relaxation must be > 0

Fix langevin variable returned negative temperature
: Self-explanatory.

Fix momentum group has no atoms
: Self-explanatory.

Fix move cannot define z or vz variable for 2d problem
: Self-explanatory.

Fix move cannot rotate aroung non z-axis for 2d problem
: Self-explanatory.

Fix move cannot set linear z motion for 2d problem
: Self-explanatory.

Fix move cannot set wiggle z motion for 2d problem
: Self-explanatory.

Fix msst compute ID does not compute potential energy
: Self-explanatory.

Fix msst compute ID does not compute pressure
: Self-explanatory.

Fix msst compute ID does not compute temperature
: Self-explanatory.

Fix msst requires a periodic box
: Self-explanatory.

Fix msst tscale must satisfy 0 <= tscale < 1
: Self-explanatory.

Fix npt/nph has tilted box too far in one step - periodic cell is too far from equilibrium state
: Self-explanatory. The change in the box tilt is too extreme on a short timescale.

Fix nve/asphere requires extended particles
: This fix can only be used for particles with a shape setting.

Fix nve/asphere/noforce requires atom style ellipsoid
: Self-explanatory.

Fix nve/asphere/noforce requires extended particles
: One of the particles is not an ellipsoid.

Fix nve/body requires atom style body

Self-explanatory.

Fix nve/body requires bodies

This fix can only be used for particles that are bodies.

Fix nve/line can only be used for 2d simulations

Self-explanatory.

Fix nve/line requires atom style line

Self-explanatory.

Fix nve/line requires line particles

Self-explanatory.

Fix nve/sphere dipole requires atom attribute mu

An atom style with this attribute is needed.

Fix nve/sphere requires atom style sphere

Self-explanatory.

Fix nve/sphere requires extended particles

This fix can only be used for particles of a finite size.

Fix nve/tri can only be used for 3d simulations

Self-explanatory.

Fix nve/tri requires atom style tri

Self-explanatory.

Fix nve/tri requires tri particles

Self-explanatory.

Fix nvt/nph/npt asphere requires extended particles

The shape setting for a particle in the fix group has shape = 0.0, which means it is a point particle.

Fix nvt/nph/npt body requires bodies

Self-explanatory.

Fix nvt/nph/npt sphere requires atom style sphere

Self-explanatory.

Fix nvt/npt/nph damping parameters must be > 0.0

Self-explanatory.

Fix nvt/npt/nph dilate group ID does not exist

Self-explanatory.

Fix nvt/sphere requires extended particles

This fix can only be used for particles of a finite size.

Fix orient/fcc file open failed

The fix orient/fcc command could not open a specified file.

Fix orient/fcc file read failed

The fix orient/fcc command could not read the needed parameters from a specified file.

Fix orient/fcc found self twice

The neighbor lists used by fix orient/fcc are messed up. If this error occurs, it is likely a bug, so send an email to the developers.

Fix peri neigh does not exist

Somehow a fix that the pair style defines has been deleted.

Fix pour and fix rigid/small not using same molecule template ID

Self-explanatory.

Fix pour and fix shake not using same molecule template ID

Self-explanatory.

Fix pour insertion count per timestep is 0

Self-explanatory.

Fix pour molecule must have atom types

The defined molecule does not specify atom types.

Fix pour molecule must have coordinates

The defined molecule does not specify coordinates.

Fix pour molecule template ID must be same as atom style template ID
When using atom_style template, you cannot pour molecules that are not in that template.
Fix pour polydisperse fractions do not sum to 1.0
Self-explanatory.
Fix pour region ID does not exist
Self-explanatory.
Fix pour region cannot be dynamic
Only static regions can be used with fix pour.
Fix pour region does not support a bounding box
Not all regions represent bounded volumes. You cannot use such a region with the fix pour command.
Fix pour requires atom attributes radius, rmass
The atom style defined does not have these attributes.
Fix pour rigid fix does not exist
Self-explanatory.
Fix pour shake fix does not exist
Self-explanatory.
Fix press/berendsen damping parameters must be > 0.0
Self-explanatory.
Fix property/atom cannot specify mol twice
Self-explanatory.
Fix property/atom cannot specify q twice
Self-explanatory.
Fix property/atom mol when atom_style already has molecule attribute
Self-explanatory.
Fix property/atom q when atom_style already has charge attribute
Self-explanatory.
Fix property/atom vector name already exists
The name for an integer or floating-point vector must be unique.
Fix qeq has negative upper Taper radius cutoff
Self-explanatory.
Fix qeq/comb group has no atoms
Self-explanatory.
Fix qeq/comb requires atom attribute q
An atom style with charge must be used to perform charge equilibration.
Fix qeq/dynamic group has no atoms
Self-explanatory.
Fix qeq/dynamic requires atom attribute q
Self-explanatory.
Fix qeq/fire group has no atoms
Self-explanatory.
Fix qeq/fire requires atom attribute q
Self-explanatory.
Fix qeq/point group has no atoms
Self-explanatory.
Fix qeq/point has insufficient QEq matrix size
Occurs when number of neighbor atoms for an atom increased too much during a run. Increase SAFE_ZONE and MIN_CAP in fix_qeq.h and recompile.
Fix qeq/point requires atom attribute q
Self-explanatory.
Fix qeq/shielded group has no atoms
Self-explanatory.
Fix qeq/shielded has insufficient QEq matrix size

Occurs when number of neighbor atoms for an atom increased too much during a run. Increase SAFE_ZONE and MIN_CAP in fix_qeq.h and recompile.

Fix qeq/shielded requires atom attribute q

Self-explanatory.

Fix qeq/slater could not extract params from pair coul/streitz

This should not happen unless pair coul/streitz has been altered.

Fix qeq/slater group has no atoms

Self-explanatory.

Fix qeq/slater has insufficient QEq matrix size

Occurs when number of neighbor atoms for an atom increased too much during a run. Increase SAFE_ZONE and MIN_CAP in fix_qeq.h and recompile.

Fix qeq/slater requires atom attribute q

Self-explanatory.

Fix reax/bonds numbonds > nsbmax_most

The limit of the number of bonds expected by the ReaxFF force field was exceeded.

Fix recenter group has no atoms

Self-explanatory.

Fix restrain requires an atom map, see atom_modify

Self-explanatory.

Fix rigid atom has non-zero image flag in a non-periodic dimension

Image flags for non-periodic dimensions should not be set.

Fix rigid file has no lines

Self-explanatory.

Fix rigid langevin period must be > 0.0

Self-explanatory.

Fix rigid molecule requires atom attribute molecule

Self-explanatory.

Fix rigid npt/nph dilate group ID does not exist

Self-explanatory.

Fix rigid npt/nph does not yet allow triclinic box

This is a current restriction in LAMMPS.

Fix rigid npt/nph period must be > 0.0

Self-explanatory.

Fix rigid npt/small t_chain should not be less than 1

Self-explanatory.

Fix rigid npt/small t_order must be 3 or 5

Self-explanatory.

Fix rigid nvt/npt/nph damping parameters must be > 0.0

Self-explanatory.

Fix rigid nvt/small t_chain should not be less than 1

Self-explanatory.

Fix rigid nvt/small t_iter should not be less than 1

Self-explanatory.

Fix rigid nvt/small t_order must be 3 or 5

Self-explanatory.

Fix rigid xy torque cannot be on for 2d simulation

Self-explanatory.

Fix rigid z force cannot be on for 2d simulation

Self-explanatory.

Fix rigid/npt period must be > 0.0

Self-explanatory.

Fix rigid/npt temperature order must be 3 or 5

Self-explanatory.

Fix rigid/npt/small period must be > 0.0

Self-explanatory.

Fix rigid/nvt period must be > 0.0

Self-explanatory.

Fix rigid/nvt temperature order must be 3 or 5

Self-explanatory.

Fix rigid/nvt/small period must be > 0.0

Self-explanatory.

Fix rigid/small atom has non-zero image flag in a non-periodic dimension

Image flags for non-periodic dimensions should not be set.

Fix rigid/small langevin period must be > 0.0

Self-explanatory.

Fix rigid/small molecule must have atom types

The defined molecule does not specify atom types.

Fix rigid/small molecule must have coordinates

The defined molecule does not specify coordinates.

Fix rigid/small npt/nph period must be > 0.0

Self-explanatory.

Fix rigid/small nvt/npt/nph damping parameters must be > 0.0

Self-explanatory.

Fix rigid/small nvt/npt/nph dilate group ID does not exist

Self-explanatory.

Fix rigid/small requires an atom map, see atom_modify

Self-explanatory.

Fix rigid/small requires atom attribute molecule

Self-explanatory.

Fix rigid: Bad principal moments

The principal moments of inertia computed for a rigid body are not within the required tolerances.

Fix shake cannot be used with minimization

Cannot use fix shake while doing an energy minimization since it turns off bonds that should contribute to the energy.

Fix shake molecule template must have shake info

The defined molecule does not specify SHAKE information.

Fix spring couple group ID does not exist

Self-explanatory.

Fix srd can only currently be used with comm_style brick

This is a current restriction in LAMMPS.

Fix srd lamda must be >= 0.6 of SRD grid size

This is a requirement for accuracy reasons.

Fix srd no-slip requires atom attribute torque

This is because the SRD collisions will impart torque to the solute particles.

Fix srd requires SRD particles all have same mass

Self-explanatory.

Fix srd requires ghost atoms store velocity

Use the comm_modify vel yes command to enable this.

Fix srd requires newton pair on

Self-explanatory.

Fix store/state compute array is accessed out-of-range

Self-explanatory.

Fix store/state compute does not calculate a per-atom array

The compute calculates a per-atom vector.

Fix store/state compute does not calculate a per-atom vector
: The compute calculates a per-atom vector.

Fix store/state compute does not calculate per-atom values
: Computes that calculate global or local quantities cannot be used with fix store/state.

Fix store/state fix array is accessed out-of-range
: Self-explanatory.

Fix store/state fix does not calculate a per-atom array
: The fix calculates a per-atom vector.

Fix store/state fix does not calculate a per-atom vector
: The fix calculates a per-atom array.

Fix store/state fix does not calculate per-atom values
: Fixes that calculate global or local quantities cannot be used with fix store/state.

Fix store/state for atom property that isn't allocated
: Self-explanatory.

Fix store/state variable is not atom-style variable
: Only atom-style variables calculate per-atom quantities.

Fix temp/berendsen period must be > 0.0
: Self-explanatory.

Fix temp/berendsen variable returned negative temperature
: Self-explanatory.

Fix temp/csld is not compatible with fix rattle or fix shake
: These two commands cannot currently be used together with fix temp/csld.

Fix temp/csld variable returned negative temperature
: Self-explanatory.

Fix temp/csvr variable returned negative temperature
: Self-explanatory.

Fix temp/rescale variable returned negative temperature
: Self-explanatory.

Fix tfmc displacement length must be > 0
: Self-explanatory.

Fix tfmc is not compatible with fix shake
: These two commands cannot currently be used together.

Fix tfmc temperature must be > 0
: Self-explanatory.

Fix thermal/conductivity swap value must be positive
: Self-explanatory.

Fix tmd must come after integration fixes
: Any fix tmd command must appear in the input script after all time integration fixes (nve, nvt, npt). See the fix tmd documentation for details.

Fix ttm electron temperatures must be > 0.0
: Self-explanatory.

Fix ttm electronic_density must be > 0.0
: Self-explanatory.

Fix ttm electronic_specific_heat must be > 0.0
: Self-explanatory.

Fix ttm electronic_thermal_conductivity must be >= 0.0
: Self-explanatory.

Fix ttm gamma_p must be > 0.0
: Self-explanatory.

Fix ttm gamma_s must be >= 0.0
: Self-explanatory.

Fix ttm number of nodes must be > 0

Self-explanatory.

Fix ttm v_0 must be >= 0.0

Self-explanatory.

Fix used in compute chunk/atom not computed at compatible time

The chunk/atom compute cannot query the output of the fix on a timestep it is needed.

Fix used in compute reduce not computed at compatible time

Fixes generate their values on specific timesteps. Compute reduce is requesting a value on a non-allowed timestep.

Fix used in compute slice not computed at compatible time

Fixes generate their values on specific timesteps. Compute slice is requesting a value on a non-allowed timestep.

Fix vector cannot set output array intensive/extensive from these inputs

The inputs to the command have conflicting intensive/extensive attributes. You need to use more than one fix vector command.

Fix vector compute does not calculate a scalar

Self-explanatory.

Fix vector compute does not calculate a vector

Self-explanatory.

Fix vector compute vector is accessed out-of-range

Self-explanatory.

Fix vector fix does not calculate a scalar

Self-explanatory.

Fix vector fix does not calculate a vector

Self-explanatory.

Fix vector fix vector is accessed out-of-range

Self-explanatory.

Fix vector variable is not equal-style variable

Self-explanatory.

Fix viscosity swap value must be positive

Self-explanatory.

Fix viscosity vtarget value must be positive

Self-explanatory.

Fix wall cutoff <= 0.0

Self-explanatory.

Fix wall/colloid requires atom style sphere

Self-explanatory.

Fix wall/colloid requires extended particles

One of the particles has radius 0.0.

Fix wall/gran is incompatible with Pair style

Must use a granular pair style to define the parameters needed for this fix.

Fix wall/gran requires atom style sphere

Self-explanatory.

Fix wall/piston command only available at zlo

The face keyword must be zlo.

Fix wall/region colloid requires atom style sphere

Self-explanatory.

Fix wall/region colloid requires extended particles

One of the particles has radius 0.0.

Fix wall/region cutoff <= 0.0

Self-explanatory.

Fix_modify pressure ID does not compute pressure

The compute ID assigned to the fix must compute pressure.

Fix_modify temperature ID does not compute temperature
: The compute ID assigned to the fix must compute temperature.

For triclinic deformation, specified target stress must be hydrostatic
: Triclinic pressure control is allowed using the tri keyword, but non-hydrostatic pressure control can not be used in this case.

Found no restart file matching pattern
: When using a "*" in the restart file name, no matching file was found.

GPU library not compiled for this accelerator
: Self-explanatory.

GPU package does not (yet) work with atom_style template
: Self-explanatory.

GPU particle split must be set to 1 for this pair style.
: For this pair style, you cannot run part of the force calculation on the host. See the package command.

GPU split param must be positive for hybrid pair styles
: See the package gpu command.

GPUs are requested but Kokkos has not been compiled for CUDA
: Recompile Kokkos with CUDA support to use GPUs.

Ghost velocity forward comm not yet implemented with Kokkos
: This is a current restriction.

Gmask function in equal-style variable formula
: Gmask is per-atom operation.

Gravity changed since fix pour was created
: The gravity vector defined by fix gravity must be static.

Gravity must point in -y to use with fix pour in 2d
: Self-explanatory.

Gravity must point in -z to use with fix pour in 3d
: Self-explanatory.

Grmask function in equal-style variable formula
: Grmask is per-atom operation.

Group ID does not exist
: A group ID used in the group command does not exist.

Group ID in variable formula does not exist
: Self-explanatory.

Group all cannot be made dynamic
: This operation is not allowed.

Group command before simulation box is defined
: The group command cannot be used before a read_data, read_restart, or create_box command.

Group dynamic cannot reference itself
: Self-explanatory.

Group dynamic parent group cannot be dynamic
: Self-explanatory.

Group dynamic parent group does not exist
: Self-explanatory.

Group region ID does not exist
: A region ID used in the group command does not exist.

If read_dump purges it cannot replace or trim
: These operations are not compatible. See the read_dump doc page for details.

Illegal ... command
: Self-explanatory. Check the input script syntax and compare to the documentation for the command. You can use -echo screen as a command-line option when running LAMMPS to see the offending line.

Illegal COMB parameter
: One or more of the coefficients defined in the potential file is invalid.

Illegal COMB3 parameter
: One or more of the coefficients defined in the potential file is invalid.

Illegal Stillinger-Weber parameter
: One or more of the coefficients defined in the potential file is invalid.

Illegal Tersoff parameter
: One or more of the coefficients defined in the potential file is invalid.

Illegal Vashishta parameter
: One or more of the coefficients defined in the potential file is invalid.

Illegal compute voronoi/atom command (occupation and (surface or edges))
: Self-explanatory.

Illegal coul/streitz parameter
: One or more of the coefficients defined in the potential file is invalid.

Illegal dump_modify sfactor value (must be > 0.0)
: Self-explanatory.

Illegal dump_modify tfactor value (must be > 0.0)
: Self-explanatory.

Illegal fix gcmc gas mass <= 0
: The computed mass of the designated gas molecule or atom type was less than or equal to zero.

Illegal fix tfmc random seed
: Seeds can only be nonzero positive integers.

Illegal fix wall/piston velocity
: The piston velocity must be positive.

Illegal integrate style
: Self-explanatory.

Illegal nb3b/harmonic parameter
: One or more of the coefficients defined in the potential file is invalid.

Illegal number of angle table entries
: There must be at least 2 table entries.

Illegal number of bond table entries
: There must be at least 2 table entries.

Illegal number of pair table entries
: There must be at least 2 table entries.

Illegal or unset periodicity in restart
: This error should not normally occur unless the restart file is invalid.

Illegal range increment value
: The increment must be >= 1.

Illegal simulation box
: The lower bound of the simulation box is greater than the upper bound.

Illegal size double vector read requested
: This error should not normally occur unless the restart file is invalid.

Illegal size integer vector read requested
: This error should not normally occur unless the restart file is invalid.

Illegal size string or corrupt restart
: This error should not normally occur unless the restart file is invalid.

Imageint setting in lmptype.h is invalid
: Imageint must be as large or larger than smallint.

Imageint setting in lmptype.h is not compatible
: Format of imageint stored in restart file is not consistent with LAMMPS version you are running. See the settings in src/lmptype.h

Improper atom missing in delete_bonds
: The delete_bonds command cannot find one or more atoms in a particular improper on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid improper.

Improper atom missing in set command
: The set command cannot find one or more atoms in a particular improper on a particular processor. The pairwise cutoff is too short or the atoms are too far apart to make a valid improper.

Improper atoms %d %d %d %d missing on proc %d at step %ld
: One or more of 4 atoms needed to compute a particular improper are missing on this processor. Typically this is because the pairwise cutoff is set too short or the improper has blown apart and an atom is too far away.

Improper atoms missing on proc %d at step %ld
: One or more of 4 atoms needed to compute a particular improper are missing on this processor. Typically this is because the pairwise cutoff is set too short or the improper has blown apart and an atom is too far away.

Improper coeff for hybrid has invalid style
: Improper style hybrid uses another improper style as one of its coefficients. The improper style used in the improper_coeff command or read from a restart file is not recognized.

Improper coeffs are not set
: No improper coefficients have been assigned in the data file or via the improper_coeff command.

Improper style hybrid cannot have hybrid as an argument
: Self-explanatory.

Improper style hybrid cannot have none as an argument
: Self-explanatory.

Improper style hybrid cannot use same improper style twice
: Self-explanatory.

Improper_coeff command before improper_style is defined
: Coefficients cannot be set in the data file or via the improper_coeff command until an improper_style has been assigned.

Improper_coeff command before simulation box is defined
: The improper_coeff command cannot be used before a read_data, read_restart, or create_box command.

Improper_coeff command when no impropers allowed
: The chosen atom style does not allow for impropers to be defined.

Improper_style command when no impropers allowed
: The chosen atom style does not allow for impropers to be defined.

Impropers assigned incorrectly
: Impropers read in from the data file were not assigned correctly to atoms. This means there is something invalid about the topology definitions.

Impropers defined but no improper types
: The data file header lists improper but no improper types.

Incomplete use of variables in create_atoms command
: The var and set options must be used together.

Inconsistent iparam/jparam values in fix bond/create command
: If itype and jtype are the same, then their maxbond and newtype settings must also be the same.

Inconsistent line segment in data file
: The end points of the line segment are not equal distances from the center point which is the atom coordinate.

Inconsistent triangle in data file
: The centroid of the triangle as defined by the corner points is not the atom coordinate.

Inconsistent use of finite-size particles by molecule template molecules
: Not all of the molecules define a radius for their constituent particles.

Incorrect # of floating-point values in Bodies section of data file
: See doc page for body style.

Incorrect # of integer values in Bodies section of data file
: See doc page for body style.

Incorrect %s format in data file

A section of the data file being read by fix property/atom does not have the correct number of values per line.

Incorrect SNAP parameter file
The file cannot be parsed correctly, check its internal syntax.

Incorrect args for angle coefficients
Self-explanatory. Check the input script or data file.

Incorrect args for bond coefficients
Self-explanatory. Check the input script or data file.

Incorrect args for dihedral coefficients
Self-explanatory. Check the input script or data file.

Incorrect args for improper coefficients
Self-explanatory. Check the input script or data file.

Incorrect args for pair coefficients
Self-explanatory. Check the input script or data file.

Incorrect args in pair_style command
Self-explanatory.

Incorrect atom format in data file
Number of values per atom line in the data file is not consistent with the atom style.

Incorrect atom format in neb file
The number of fields per line is not what expected.

Incorrect bonus data format in data file
See the read_data doc page for a description of how various kinds of bonus data must be formatted for certain atom styles.

Incorrect boundaries with slab Ewald
Must have periodic x,y dimensions and non-periodic z dimension to use 2d slab option with Ewald.

Incorrect boundaries with slab EwaldDisp
Must have periodic x,y dimensions and non-periodic z dimension to use 2d slab option with Ewald.

Incorrect boundaries with slab PPPM
Must have periodic x,y dimensions and non-periodic z dimension to use 2d slab option with PPPM.

Incorrect boundaries with slab PPPMDisp
Must have periodic x,y dimensions and non-periodic z dimension to use 2d slab option with pppm/disp.

Incorrect element names in ADP potential file
The element names in the ADP file do not match those requested.

Incorrect element names in EAM potential file
The element names in the EAM file do not match those requested.

Incorrect format in COMB potential file
Incorrect number of words per line in the potential file.

Incorrect format in COMB3 potential file
Incorrect number of words per line in the potential file.

Incorrect format in MEAM potential file
Incorrect number of words per line in the potential file.

Incorrect format in SNAP coefficient file
Incorrect number of words per line in the coefficient file.

Incorrect format in SNAP parameter file
Incorrect number of words per line in the parameter file.

Incorrect format in Stillinger-Weber potential file
Incorrect number of words per line in the potential file.

Incorrect format in TMD target file
Format of file read by fix tmd command is incorrect.

Incorrect format in Tersoff potential file
Incorrect number of words per line in the potential file.

Incorrect format in Vashishta potential file

Incorrect number of words per line in the potential file.

Incorrect format in coul/streitz potential file

Incorrect number of words per line in the potential file.

Incorrect format in nb3b/harmonic potential file

Incorrect number of words per line in the potential file.

Incorrect integer value in Bodies section of data file

See doc page for body style.

Incorrect multiplicity arg for dihedral coefficients

Self-explanatory. Check the input script or data file.

Incorrect number of elements in potential file

Self-explanatory.

Incorrect rigid body format in fix rigid file

The number of fields per line is not what expected.

Incorrect rigid body format in fix rigid/small file

The number of fields per line is not what expected.

Incorrect sign arg for dihedral coefficients

Self-explanatory. Check the input script or data file.

Incorrect table format check for element types

Self-explanatory.

Incorrect velocity format in data file

Each atom style defines a format for the Velocity section of the data file. The read-in lines do not match.

Incorrect weight arg for dihedral coefficients

Self-explanatory. Check the input script or data file.

Index between variable brackets must be positive

Self-explanatory.

Indexed per-atom vector in variable formula without atom map

Accessing a value from an atom vector requires the ability to lookup an atom index, which is provided by an atom map. An atom map does not exist (by default) for non-molecular problems. Using the atom_modify map command will force an atom map to be created.

Initial temperatures not all set in fix ttm

Self-explantory.

Input line quote not followed by whitespace

An end quote must be followed by whitespace.

Insertion region extends outside simulation box

Self-explanatory.

Insufficient Jacobi rotations for POEMS body

Eigensolve for rigid body was not sufficiently accurate.

Insufficient Jacobi rotations for body nparticle

Eigensolve for rigid body was not sufficiently accurate.

Insufficient Jacobi rotations for rigid body

Eigensolve for rigid body was not sufficiently accurate.

Insufficient Jacobi rotations for rigid molecule

Eigensolve for rigid body was not sufficiently accurate.

Insufficient Jacobi rotations for triangle

The calculation of the intertia tensor of the triangle failed. This should not happen if it is a reasonably shaped triangle.

Insufficient memory on accelerator

There is insufficient memory on one of the devices specified for the gpu package

Internal error in atom_style body

This error should not occur. Contact the developers.

Invalid -reorder N value

Self-explanatory.

Invalid Angles section in molecule file
: Self-explanatory.

Invalid Bonds section in molecule file
: Self-explanatory.

Invalid Boolean syntax in if command
: Self-explanatory.

Invalid Charges section in molecule file
: Self-explanatory.

Invalid Coords section in molecule file
: Self-explanatory.

Invalid Diameters section in molecule file
: Self-explanatory.

Invalid Dihedrals section in molecule file
: Self-explanatory.

Invalid Impropers section in molecule file
: Self-explanatory.

Invalid Kokkos command-line args
: Self-explanatory. See Section 2.7 of the manual for details.

Invalid LAMMPS restart file
: The file does not appear to be a LAMMPS restart file since it doesn't contain the correct magic string at the beginning.

Invalid Masses section in molecule file
: Self-explanatory.

Invalid REAX atom type
: There is a mis-match between LAMMPS atom types and the elements listed in the ReaxFF force field file.

Invalid Special Bond Counts section in molecule file
: Self-explanatory.

Invalid Types section in molecule file
: Self-explanatory.

Invalid angle count in molecule file
: Self-explanatory.

Invalid angle table length
: Length must be 2 or greater.

Invalid angle type in Angles section of data file
: Angle type must be positive integer and within range of specified angle types.

Invalid angle type in Angles section of molecule file
: Self-explanatory.

Invalid angle type index for fix shake
: Self-explanatory.

Invalid args for non-hybrid pair coefficients
: "NULL" is only supported in pair_coeff calls when using pair hybrid

Invalid argument to factorial %d
: N must be >= 0 and <= 167, otherwise the factorial result is too large.

Invalid atom ID in %s section of data file
: An atom in a section of the data file being read by fix property/atom has an invalid atom ID that is <= 0 or > the maximum existing atom ID.

Invalid atom ID in Angles section of data file
: Atom IDs must be positive integers and within range of defined atoms.

Invalid atom ID in Angles section of molecule file
: Self-explanatory.

Invalid atom ID in Atoms section of data file

Atom IDs must be positive integers.

Invalid atom ID in Bodies section of data file

Atom IDs must be positive integers and within range of defined atoms.

Invalid atom ID in Bonds section of data file

Atom IDs must be positive integers and within range of defined atoms.

Invalid atom ID in Bonds section of molecule file

Self-explanatory.

Invalid atom ID in Bonus section of data file

Atom IDs must be positive integers and within range of defined atoms.

Invalid atom ID in Dihedrals section of data file

Atom IDs must be positive integers and within range of defined atoms.

Invalid atom ID in Impropers section of data file

Atom IDs must be positive integers and within range of defined atoms.

Invalid atom ID in Velocities section of data file

Atom IDs must be positive integers and within range of defined atoms.

Invalid atom ID in dihedrals section of molecule file

Self-explanatory.

Invalid atom ID in impropers section of molecule file

Self-explanatory.

Invalid atom ID in variable file

Self-explanatory.

Invalid atom IDs in neb file

An ID in the file was not found in the system.

Invalid atom diameter in molecule file

Diameters must be >= 0.0.

Invalid atom mass for fix shake

Mass specified in fix shake command must be > 0.0.

Invalid atom mass in molecule file

Masses must be > 0.0.

Invalid atom type in Atoms section of data file

Atom types must range from 1 to specified # of types.

Invalid atom type in create_atoms command

The create_box command specified the range of valid atom types. An invalid type is being requested.

Invalid atom type in create_atoms mol command

The atom types in the defined molecule are added to the value specified in the create_atoms command, as an offset. The final value for each atom must be between 1 to N, where N is the number of atom types.

Invalid atom type in fix atom/swap command

The atom type specified in the atom/swap command does not exist.

Invalid atom type in fix bond/create command

Self-explanatory.

Invalid atom type in fix deposit command

Self-explanatory.

Invalid atom type in fix deposit mol command

The atom types in the defined molecule are added to the value specified in the create_atoms command, as an offset. The final value for each atom must be between 1 to N, where N is the number of atom types.

Invalid atom type in fix gcmc command

The atom type specified in the gcmc command does not exist.

Invalid atom type in fix pour command

Self-explanatory.

Invalid atom type in fix pour mol command

The atom types in the defined molecule are added to the value specified in the create_atoms command, as an offset. The final value for each atom must be between 1 to N, where N is the number of atom types.

Invalid atom type in molecule file
: Atom types must range from 1 to specified # of types.

Invalid atom type in neighbor exclusion list
: Atom types must range from 1 to Ntypes inclusive.

Invalid atom type index for fix shake
: Atom types must range from 1 to Ntypes inclusive.

Invalid atom types in pair_write command
: Atom types must range from 1 to Ntypes inclusive.

Invalid atom vector in variable formula
: The atom vector is not recognized.

Invalid atom_style body command
: No body style argument was provided.

Invalid atom_style command
: Self-explanatory.

Invalid attribute in dump custom command
: Self-explantory.

Invalid attribute in dump local command
: Self-explantory.

Invalid attribute in dump modify command
: Self-explantory.

Invalid basis setting in create_atoms command
: The basis index must be between 1 to N where N is the number of basis atoms in the lattice. The type index must be between 1 to N where N is the number of atom types.

Invalid basis setting in fix append/atoms command
: The basis index must be between 1 to N where N is the number of basis atoms in the lattice. The type index must be between 1 to N where N is the number of atom types.

Invalid bin bounds in compute chunk/atom
: The lo/hi values are inconsistent.

Invalid bin bounds in fix ave/spatial
: The lo/hi values are inconsistent.

Invalid body nparticle command
: Arguments in atom-style command are not correct.

Invalid bond count in molecule file
: Self-explanatory.

Invalid bond table length
: Length must be 2 or greater.

Invalid bond type in Bonds section of data file
: Bond type must be positive integer and within range of specified bond types.

Invalid bond type in Bonds section of molecule file
: Self-explanatory.

Invalid bond type in create_bonds command
: Self-explanatory.

Invalid bond type in fix bond/break command
: Self-explanatory.

Invalid bond type in fix bond/create command
: Self-explanatory.

Invalid bond type index for fix shake
: Self-explanatory. Check the fix shake command in the input script.

Invalid coeffs for this dihedral style
: Cannot set class 2 coeffs in data file for this dihedral style.

Invalid color in dump_modify command
: The specified color name was not in the list of recognized colors. See the dump_modify doc page.

Invalid color map min/max values
: The min/max values are not consistent with either each other or with values in the color map.

Invalid command-line argument
: One or more command-line arguments is invalid. Check the syntax of the command you are using to launch LAMMPS.

Invalid compute ID in variable formula
: The compute is not recognized.

Invalid create_atoms rotation vector for 2d model
: The rotation vector can only have a z component.

Invalid custom OpenCL parameter string.
: There are not enough or too many parameters in the custom string for package GPU.

Invalid cutoff in comm_modify command
: Specified cutoff must be >= 0.0.

Invalid cutoffs in pair_write command
: Inner cutoff must be larger than 0.0 and less than outer cutoff.

Invalid d1 or d2 value for pair colloid coeff
: Neither d1 or d2 can be < 0.

Invalid data file section: Angle Coeffs
: Atom style does not allow angles.

Invalid data file section: AngleAngle Coeffs
: Atom style does not allow impropers.

Invalid data file section: AngleAngleTorsion Coeffs
: Atom style does not allow dihedrals.

Invalid data file section: AngleTorsion Coeffs
: Atom style does not allow dihedrals.

Invalid data file section: Angles
: Atom style does not allow angles.

Invalid data file section: Bodies
: Atom style does not allow bodies.

Invalid data file section: Bond Coeffs
: Atom style does not allow bonds.

Invalid data file section: BondAngle Coeffs
: Atom style does not allow angles.

Invalid data file section: BondBond Coeffs
: Atom style does not allow angles.

Invalid data file section: BondBond13 Coeffs
: Atom style does not allow dihedrals.

Invalid data file section: Bonds
: Atom style does not allow bonds.

Invalid data file section: Dihedral Coeffs
: Atom style does not allow dihedrals.

Invalid data file section: Dihedrals
: Atom style does not allow dihedrals.

Invalid data file section: Ellipsoids
: Atom style does not allow ellipsoids.

Invalid data file section: EndBondTorsion Coeffs
: Atom style does not allow dihedrals.

Invalid data file section: Improper Coeffs
: Atom style does not allow impropers.

Invalid data file section: Impropers
: Atom style does not allow impropers.

Invalid data file section: Lines

Atom style does not allow lines.

Invalid data file section: MiddleBondTorsion Coeffs

Atom style does not allow dihedrals.

Invalid data file section: Triangles

Atom style does not allow triangles.

Invalid delta_conf in tad command

The value must be between 0 and 1 inclusive.

Invalid density in Atoms section of data file

Density value cannot be <= 0.0.

Invalid density in set command

Density must be > 0.0.

Invalid diameter in set command

Self-explanatory.

Invalid dihedral count in molecule file

Self-explanatory.

Invalid dihedral type in Dihedrals section of data file

Dihedral type must be positive integer and within range of specified dihedral types.

Invalid dihedral type in dihedrals section of molecule file

Self-explanatory.

Invalid dipole length in set command

Self-explanatory.

Invalid displace_atoms rotate axis for 2d

Axis must be in z direction.

Invalid dump dcd filename

Filenames used with the dump dcd style cannot be binary or compressed or cause multiple files to be written.

Invalid dump frequency

Dump frequency must be 1 or greater.

Invalid dump image element name

The specified element name was not in the standard list of elements. See the dump_modify doc page.

Invalid dump image filename

The file produced by dump image cannot be binary and must be for a single processor.

Invalid dump image persp value

Persp value must be >= 0.0.

Invalid dump image theta value

Theta must be between 0.0 and 180.0 inclusive.

Invalid dump image zoom value

Zoom value must be > 0.0.

Invalid dump movie filename

The file produced by dump movie cannot be binary or compressed and must be a single file for a single processor.

Invalid dump xtc filename

Filenames used with the dump xtc style cannot be binary or compressed or cause multiple files to be written.

Invalid dump xyz filename

Filenames used with the dump xyz style cannot be binary or cause files to be written by each processor.

Invalid dump_modify threshhold operator

Operator keyword used for threshold specification in not recognized.

Invalid entry in -reorder file

Self-explanatory.

Invalid fix ID in variable formula

The fix is not recognized.

Invalid fix ave/time off column
: Self-explantory.

Invalid fix box/relax command for a 2d simulation
: Fix box/relax styles involving the z dimension cannot be used in a 2d simulation.

Invalid fix box/relax command pressure settings
: If multiple dimensions are coupled, those dimensions must be specified.

Invalid fix box/relax pressure settings
: Settings for coupled dimensions must be the same.

Invalid fix nvt/npt/nph command for a 2d simulation
: Cannot control z dimension in a 2d model.

Invalid fix nvt/npt/nph command pressure settings
: If multiple dimensions are coupled, those dimensions must be specified.

Invalid fix nvt/npt/nph pressure settings
: Settings for coupled dimensions must be the same.

Invalid fix press/berendsen for a 2d simulation
: The z component of pressure cannot be controlled for a 2d model.

Invalid fix press/berendsen pressure settings
: Settings for coupled dimensions must be the same.

Invalid fix qeq parameter file
: Element index > number of atom types.

Invalid fix rigid npt/nph command for a 2d simulation
: Cannot control z dimension in a 2d model.

Invalid fix rigid npt/nph command pressure settings
: If multiple dimensions are coupled, those dimensions must be specified.

Invalid fix rigid/small npt/nph command for a 2d simulation
: Cannot control z dimension in a 2d model.

Invalid fix rigid/small npt/nph command pressure settings
: If multiple dimensions are coupled, those dimensions must be specified.

Invalid flag in force field section of restart file
: Unrecognized entry in restart file.

Invalid flag in header section of restart file
: Unrecognized entry in restart file.

Invalid flag in peratom section of restart file
: The format of this section of the file is not correct.

Invalid flag in type arrays section of restart file
: Unrecognized entry in restart file.

Invalid frequency in temper command
: Nevery must be > 0.

Invalid group ID in neigh_modify command
: A group ID used in the neigh_modify command does not exist.

Invalid group function in variable formula
: Group function is not recognized.

Invalid group in comm_modify command
: Self-explanatory.

Invalid image up vector
: Up vector cannot be (0,0,0).

Invalid immediate variable
: Syntax of immediate value is incorrect.

Invalid improper count in molecule file
: Self-explanatory.

Invalid improper type in Impropers section of data file
: Improper type must be positive integer and within range of specified improper types.

Invalid improper type in impropers section of molecule file
Self-explanatory.
Invalid index for non-body particles in compute body/local command
Only indices 1,2,3 can be used for non-body particles.
Invalid index in compute body/local command
Self-explanatory.
Invalid is_active() function in variable formula
Self-explanatory.
Invalid is_available() function in variable formula
Self-explanatory.
Invalid is_defined() function in variable formula
Self-explanatory.
Invalid keyword in angle table parameters
Self-explanatory.
Invalid keyword in bond table parameters
Self-explanatory.
Invalid keyword in compute angle/local command
Self-explanatory.
Invalid keyword in compute bond/local command
Self-explanatory.
Invalid keyword in compute dihedral/local command
Self-explanatory.
Invalid keyword in compute improper/local command
Self-explanatory.
Invalid keyword in compute pair/local command
Self-explanatory.
Invalid keyword in compute property/atom command
Self-explanatory.
Invalid keyword in compute property/chunk command
Self-explanatory.
Invalid keyword in compute property/local command
Self-explanatory.
Invalid keyword in dump cfg command
Self-explanatory.
Invalid keyword in pair table parameters
Keyword used in list of table parameters is not recognized.
Invalid length in set command
Self-explanatory.
Invalid mass in set command
Self-explanatory.
Invalid mass line in data file
Self-explanatory.
Invalid mass value
Self-explanatory.
Invalid math function in variable formula
Self-explanatory.
Invalid math/group/special function in variable formula
Self-explanatory.
Invalid option in lattice command for non-custom style
Certain lattice keywords are not supported unless the lattice style is "custom".
Invalid order of forces within respa levels
For respa, ordering of force computations within respa levels must obey certain rules. E.g. bonds cannot

be compute less frequently than angles, pairwise forces cannot be computed less frequently than kspace, etc.

Invalid pair table cutoff
: Cutoffs in pair_coeff command are not valid with read-in pair table.

Invalid pair table length
: Length of read-in pair table is invalid

Invalid param file for fix qeq/shielded
: Invalid value of gamma.

Invalid param file for fix qeq/slater
: Zeta value is 0.0.

Invalid partitions in processors part command
: Valid partitions are numbered 1 to N and the sender and receiver cannot be the same partition.

Invalid python command
: Self-explanatory. Check the input script syntax and compare to the documentation for the command. You can use -echo screen as a command-line option when running LAMMPS to see the offending line.

Invalid radius in Atoms section of data file
: Radius must be >= 0.0.

Invalid random number seed in fix ttm command
: Random number seed must be > 0.

Invalid random number seed in set command
: Random number seed must be > 0.

Invalid replace values in compute reduce
: Self-explanatory.

Invalid rigid body ID in fix rigid file
: The ID does not match the number of an existing ID of rigid bodies that are defined by the fix rigid command.

Invalid rigid body ID in fix rigid/small file
: The ID does not match the number of an existing ID of rigid bodies that are defined by the fix rigid/small command.

Invalid run command N value
: The number of timesteps must fit in a 32-bit integer. If you want to run for more steps than this, perform multiple shorter runs.

Invalid run command start/stop value
: Self-explanatory.

Invalid run command upto value
: Self-explanatory.

Invalid seed for Marsaglia random # generator
: The initial seed for this random number generator must be a positive integer less than or equal to 900 million.

Invalid seed for Park random # generator
: The initial seed for this random number generator must be a positive integer.

Invalid shake angle type in molecule file
: Self-explanatory.

Invalid shake atom in molecule file
: Self-explanatory.

Invalid shake bond type in molecule file
: Self-explanatory.

Invalid shake flag in molecule file
: Self-explanatory.

Invalid shape in Ellipsoids section of data file
: Self-explanatory.

Invalid shape in Triangles section of data file

Two or more of the triangle corners are duplicate points.

Invalid shape in set command
Self-explanatory.

Invalid shear direction for fix wall/gran
Self-explanatory.

Invalid special atom index in molecule file
Self-explanatory.

Invalid special function in variable formula
Self-explanatory.

Invalid style in pair_write command
Self-explanatory. Check the input script.

Invalid syntax in variable formula
Self-explanatory.

Invalid t_event in prd command
Self-explanatory.

Invalid t_event in tad command
The value must be greater than 0.

Invalid template atom in Atoms section of data file
The atom indices must be between 1 to N, where N is the number of atoms in the template molecule the atom belongs to.

Invalid template index in Atoms section of data file
The template indices must be between 1 to N, where N is the number of molecules in the template.

Invalid thermo keyword in variable formula
The keyword is not recognized.

Invalid threads_per_atom specified.
For 3-body potentials on the GPU, the threads_per_atom setting cannot be greater than 4 for NVIDIA GPUs.

Invalid timestep reset for fix ave/atom
Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

Invalid timestep reset for fix ave/chunk
Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

Invalid timestep reset for fix ave/correlate
Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

Invalid timestep reset for fix ave/histo
Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

Invalid timestep reset for fix ave/spatial
Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

Invalid timestep reset for fix ave/time
Resetting the timestep has invalidated the sequence of timesteps this fix needs to process.

Invalid tmax in tad command
The value must be greater than 0.0.

Invalid type for mass set
Mass command must set a type from 1-N where N is the number of atom types.

Invalid use of library file() function
This function is called thru the library interface. This error should not occur. Contact the developers if it does.

Invalid value in set command
The value specified for the setting is invalid, likely because it is too small or too large.

Invalid variable evaluation in variable formula
A variable used in a formula could not be evaluated.

Invalid variable in next command
Self-explanatory.

Invalid variable name
: Variable name used in an input script line is invalid.

Invalid variable name in variable formula
: Variable name is not recognized.

Invalid variable style in special function next
: Only file-style or atomfile-style variables can be used with next().

Invalid variable style with next command
: Variable styles *equal* and *world* cannot be used in a next command.

Invalid volume in set command
: Volume must be > 0.0.

Invalid wiggle direction for fix wall/gran
: Self-explanatory.

Invoked angle equil angle on angle style none
: Self-explanatory.

Invoked angle single on angle style none
: Self-explanatory.

Invoked bond equil distance on bond style none
: Self-explanatory.

Invoked bond single on bond style none
: Self-explanatory.

Invoked pair single on pair style none
: A command (e.g. a dump) attempted to invoke the single() function on a pair style none, which is illegal. You are probably attempting to compute per-atom quantities with an undefined pair style.

Invoking coulombic in pair style lj/coul requires atom attribute q
: The atom style defined does not have this attribute.

Invoking coulombic in pair style lj/long/dipole/long requires atom attribute q
: The atom style defined does not have these attributes.

KIM neighbor iterator exceeded range
: This should not happen. It likely indicates a bug in the KIM implementation of the interatomic potential where it is requesting neighbors incorrectly.

KOKKOS package does not yet support comm_style tiled
: Self-explanatory.

KOKKOS package requires a kokkos enabled atom_style
: Self-explanatory.

KSpace accuracy must be > 0
: The kspace accuracy designated in the input must be greater than zero.

KSpace accuracy too large to estimate G vector
: Reduce the accuracy request or specify gwald explicitly via the kspace_modify command.

KSpace accuracy too low
: Requested accuracy must be less than 1.0.

KSpace solver requires a pair style
: No pair style is defined.

KSpace style does not yet support triclinic geometries
: The specified kspace style does not allow for non-orthogonal simulation boxes.

KSpace style has not yet been set
: Cannot use kspace_modify command until a kspace style is set.

KSpace style is incompatible with Pair style
: Setting a kspace style requires that a pair style with matching long-range Coulombic or dispersion components be used.

Keyword %s in MEAM parameter file not recognized
: Self-explanatory.

Kokkos has been compiled for CUDA but no GPUs are requested

One or more GPUs must be used when Kokkos is compiled for CUDA.

Kspace style does not support compute group/group

Self-explanatory.

Kspace style pppm/disp/tip4p requires newton on

Self-explanatory.

Kspace style pppm/tip4p requires newton on

Self-explanatory.

Kspace style requires atom attribute q

The atom style defined does not have these attributes.

Kspace_modify eigtol must be smaller than one

Self-explanatory.

LAMMPS is not built with Python embedded

This is done by including the PYTHON package before LAMMPS is built. This is required to use python-style variables.

LAMMPS unit_style lj not supported by KIM models

Self-explanatory. Check the input script or data file.

LJ6 off not supported in pair_style buck/long/coul/long

Self-exlanatory.

Label wasn't found in input script

Self-explanatory.

Lattice orient vectors are not orthogonal

The three specified lattice orientation vectors must be mutually orthogonal.

Lattice orient vectors are not right-handed

The three specified lattice orientation vectors must create a right-handed coordinate system such that a1 cross a2 = a3.

Lattice primitive vectors are collinear

The specified lattice primitive vectors do not for a unit cell with non-zero volume.

Lattice settings are not compatible with 2d simulation

One or more of the specified lattice vectors has a non-zero z component.

Lattice spacings are invalid

Each x,y,z spacing must be > 0.

Lattice style incompatible with simulation dimension

2d simulation can use sq, sq2, or hex lattice. 3d simulation can use sc, bcc, or fcc lattice.

Log of zero/negative value in variable formula

Self-explanatory.

Lost atoms via balance: original %ld current %ld

This should not occur. Report the problem to the developers.

Lost atoms: original %ld current %ld

Lost atoms are checked for each time thermo output is done. See the thermo_modify lost command for options. Lost atoms usually indicate bad dynamics, e.g. atoms have been blown far out of the simulation box, or moved futher than one processor's sub-domain away before reneighboring.

MEAM library error %d

A call to the MEAM Fortran library returned an error.

MPI_LMP_BIGINT and bigint in lmptype.h are not compatible

The size of the MPI datatype does not match the size of a bigint.

MPI_LMP_TAGINT and tagint in lmptype.h are not compatible

The size of the MPI datatype does not match the size of a tagint.

MSM can only currently be used with comm_style brick

This is a current restriction in LAMMPS.

MSM grid is too large

The global MSM grid is larger than OFFSET in one or more dimensions. OFFSET is currently set to 16384. You likely need to decrease the requested accuracy.

MSM order must be 4, 6, 8, or 10

This is a limitation of the MSM implementation in LAMMPS: the MSM order can only be 4, 6, 8, or 10.

Mass command before simulation box is defined

The mass command cannot be used before a read_data, read_restart, or create_box command.

Matrix factorization to split dispersion coefficients failed

This should not normally happen. Contact the developers.

Min_style command before simulation box is defined

The min_style command cannot be used before a read_data, read_restart, or create_box command.

Minimization could not find thermo_pe compute

This compute is created by the thermo command. It must have been explicitly deleted by a uncompute command.

Minimize command before simulation box is defined

The minimize command cannot be used before a read_data, read_restart, or create_box command.

Mismatched brackets in variable

Self-explanatory.

Mismatched compute in variable formula

A compute is referenced incorrectly or a compute that produces per-atom values is used in an equal-style variable formula.

Mismatched fix in variable formula

A fix is referenced incorrectly or a fix that produces per-atom values is used in an equal-style variable formula.

Mismatched variable in variable formula

A variable is referenced incorrectly or an atom-style variable that produces per-atom values is used in an equal-style variable formula.

Modulo 0 in variable formula

Self-explanatory.

Molecule IDs too large for compute chunk/atom

The IDs must not be larger than can be stored in a 32-bit integer since chunk IDs are 32-bit integers.

Molecule auto special bond generation overflow

Counts exceed maxspecial setting for other atoms in system.

Molecule file has angles but no nangles setting

Self-explanatory.

Molecule file has body params but no setting for them

Self-explanatory.

Molecule file has bonds but no nbonds setting

Self-explanatory.

Molecule file has dihedrals but no ndihedrals setting

Self-explanatory.

Molecule file has impropers but no nimpropers setting

Self-explanatory.

Molecule file has no Body Doubles section

Self-explanatory.

Molecule file has no Body Integers section

Self-explanatory.

Molecule file has special flags but no bonds

Self-explanatory.

Molecule file needs both Special Bond sections

Self-explanatory.

Molecule file requires atom style body

Self-explanatory.

Molecule file shake flags not before shake atoms

The order of the two sections is important.

Molecule file shake flags not before shake bonds
: The order of the two sections is important.

Molecule file shake info is incomplete
: All 3 SHAKE sections are needed.

Molecule file special list does not match special count
: The number of values in an atom's special list does not match count.

Molecule file z center-of-mass must be 0.0 for 2d
: Self-explanatory.

Molecule file z coord must be 0.0 for 2d
: Self-explanatory.

Molecule natoms must be 1 for body particle
: Self-explanatory.

Molecule sizescale must be 1.0 for body particle
: Self-explanatory.

Molecule template ID for atom_style template does not exist
: Self-explanatory.

Molecule template ID for create_atoms does not exist
: Self-explantory.

Molecule template ID for fix deposit does not exist
: Self-explanatory.

Molecule template ID for fix gcmc does not exist
: Self-explanatory.

Molecule template ID for fix pour does not exist
: Self-explanatory.

Molecule template ID for fix rigid/small does not exist
: Self-explanatory.

Molecule template ID for fix shake does not exist
: Self-explanatory.

Molecule template ID must be alphanumeric or underscore characters
: Self-explanatory.

Molecule toplogy/atom exceeds system topology/atom
: The number of bonds, angles, etc per-atom in the molecule exceeds the system setting. See the create_box command for how to specify these values.

Molecule topology type exceeds system topology type
: The number of bond, angle, etc types in the molecule exceeds the system setting. See the create_box command for how to specify these values.

More than one fix deform
: Only one fix deform can be defined at a time.

More than one fix freeze
: Only one of these fixes can be defined, since the granular pair potentials access it.

More than one fix shake
: Only one fix shake can be defined.

Mu not allowed when not using semi-grand in fix atom/swap command
: Self-explanatory.

Must define angle_style before Angle Coeffs
: Must use an angle_style command before reading a data file that defines Angle Coeffs.

Must define angle_style before BondAngle Coeffs
: Must use an angle_style command before reading a data file that defines Angle Coeffs.

Must define angle_style before BondBond Coeffs
: Must use an angle_style command before reading a data file that defines Angle Coeffs.

Must define bond_style before Bond Coeffs
: Must use a bond_style command before reading a data file that defines Bond Coeffs.

Must define dihedral_style before AngleAngleTorsion Coeffs
: Must use a dihedral_style command before reading a data file that defines AngleAngleTorsion Coeffs.

Must define dihedral_style before AngleTorsion Coeffs
: Must use a dihedral_style command before reading a data file that defines AngleTorsion Coeffs.

Must define dihedral_style before BondBond13 Coeffs
: Must use a dihedral_style command before reading a data file that defines BondBond13 Coeffs.

Must define dihedral_style before Dihedral Coeffs
: Must use a dihedral_style command before reading a data file that defines Dihedral Coeffs.

Must define dihedral_style before EndBondTorsion Coeffs
: Must use a dihedral_style command before reading a data file that defines EndBondTorsion Coeffs.

Must define dihedral_style before MiddleBondTorsion Coeffs
: Must use a dihedral_style command before reading a data file that defines MiddleBondTorsion Coeffs.

Must define improper_style before AngleAngle Coeffs
: Must use an improper_style command before reading a data file that defines AngleAngle Coeffs.

Must define improper_style before Improper Coeffs
: Must use an improper_style command before reading a data file that defines Improper Coeffs.

Must define pair_style before Pair Coeffs
: Must use a pair_style command before reading a data file that defines Pair Coeffs.

Must define pair_style before PairIJ Coeffs
: Must use a pair_style command before reading a data file that defines PairIJ Coeffs.

Must have more than one processor partition to temper
: Cannot use the temper command with only one processor partition. Use the -partition command-line option.

Must read Atoms before Angles
: The Atoms section of a data file must come before an Angles section.

Must read Atoms before Bodies
: The Atoms section of a data file must come before a Bodies section.

Must read Atoms before Bonds
: The Atoms section of a data file must come before a Bonds section.

Must read Atoms before Dihedrals
: The Atoms section of a data file must come before a Dihedrals section.

Must read Atoms before Ellipsoids
: The Atoms section of a data file must come before a Ellipsoids section.

Must read Atoms before Impropers
: The Atoms section of a data file must come before an Impropers section.

Must read Atoms before Lines
: The Atoms section of a data file must come before a Lines section.

Must read Atoms before Triangles
: The Atoms section of a data file must come before a Triangles section.

Must read Atoms before Velocities
: The Atoms section of a data file must come before a Velocities section.

Must set both respa inner and outer
: Cannot use just the inner or outer option with respa without using the other.

Must set number of threads via package omp command
: Because you are using the USER-OMP package, set the number of threads via its settings, not by the pair_style snap nthreads setting.

Must shrink-wrap piston boundary
: The boundary style of the face where the piston is applied must be of type s (shrink-wrapped).

Must specify a region in fix deposit
: The region keyword must be specified with this fix.

Must specify a region in fix pour
: Self-explanatory.

Must specify at least 2 types in fix atom/swap command
: Self-explanatory.

Must use 'kspace_modify pressure/scalar no' for rRESPA with kspace_style MSM
: The kspace scalar pressure option cannot (yet) be used with rRESPA.

Must use 'kspace_modify pressure/scalar no' for tensor components with kspace_style msm
: Otherwise MSM will compute only a scalar pressure. See the kspace_modify command for details on this setting.

Must use 'kspace_modify pressure/scalar no' to obtain per-atom virial with kspace_style MSM
: The kspace scalar pressure option cannot be used to obtain per-atom virial.

Must use 'kspace_modify pressure/scalar no' with GPU MSM Pair styles
: The kspace scalar pressure option is not (yet) compatible with GPU MSM Pair styles.

Must use 'kspace_modify pressure/scalar no' with kspace_style msm/cg
: The kspace scalar pressure option is not compatible with kspace_style msm/cg.

Must use -in switch with multiple partitions
: A multi-partition simulation cannot read the input script from stdin. The -in command-line option must be used to specify a file.

Must use Kokkos half/thread or full neighbor list with threads or GPUs
: Using Kokkos half-neighbor lists with threading is not allowed.

Must use a block or cylinder region with fix pour
: Self-explanatory.

Must use a block region with fix pour for 2d simulations
: Self-explanatory.

Must use a bond style with TIP4P potential
: TIP4P potentials assume bond lengths in water are constrained by a fix shake command.

Must use a molecular atom style with fix poems molecule
: Self-explanatory.

Must use a z-axis cylinder region with fix pour
: Self-explanatory.

Must use an angle style with TIP4P potential
: TIP4P potentials assume angles in water are constrained by a fix shake command.

Must use atom map style array with Kokkos
: See the atom_modify map command.

Must use atom style with molecule IDs with fix bond/swap
: Self-explanatory.

Must use pair_style comb or comb3 with fix qeq/comb
: Self-explanatory.

Must use variable energy with fix addforce
: Must define an energy vartiable when applyting a dynamic force during minimization.

Must use variable energy with fix efield
: You must define an energy when performing a minimization with a variable E-field.

NEB command before simulation box is defined
: Self-explanatory.

NEB requires damped dynamics minimizer
: Use a different minimization style.

NEB requires use of fix neb
: Self-explanatory.

NL ramp in wall/piston only implemented in zlo for now
: The ramp keyword can only be used for piston applied to face zlo.

Need nswaptypes mu values in fix atom/swap command
: Self-explanatory.

Needed bonus data not in data file
: Some atom styles require bonus data. See the read_data doc page for details.

Needed molecular topology not in data file
: The header of the data file indicated bonds, angles, etc would be included, but they are not present.

Neigh_modify exclude molecule requires atom attribute molecule
: Self-explanatory.

Neigh_modify include group != atom_modify first group
: Self-explanatory.

Neighbor delay must be 0 or multiple of every setting
: The delay and every parameters set via the neigh_modify command are inconsistent. If the delay setting is non-zero, then it must be a multiple of the every setting.

Neighbor include group not allowed with ghost neighbors
: This is a current restriction within LAMMPS.

Neighbor list overflow, boost neigh_modify one
: There are too many neighbors of a single atom. Use the neigh_modify command to increase the max number of neighbors allowed for one atom. You may also want to boost the page size.

Neighbor multi not yet enabled for ghost neighbors
: This is a current restriction within LAMMPS.

Neighbor multi not yet enabled for granular
: Self-explanatory.

Neighbor multi not yet enabled for rRESPA
: Self-explanatory.

Neighbor page size must be >= 10x the one atom setting
: This is required to prevent wasting too much memory.

New atom IDs exceed maximum allowed ID
: See the setting for tagint in the src/lmptype.h file.

New bond exceeded bonds per atom in create_bonds
: See the read_data command for info on setting the "extra bond per atom" header value to allow for additional bonds to be formed.

New bond exceeded bonds per atom in fix bond/create
: See the read_data command for info on setting the "extra bond per atom" header value to allow for additional bonds to be formed.

New bond exceeded special list size in fix bond/create
: See the special_bonds extra command for info on how to leave space in the special bonds list to allow for additional bonds to be formed.

Newton bond change after simulation box is defined
: The newton command cannot be used to change the newton bond value after a read_data, read_restart, or create_box command.

Next command must list all universe and uloop variables
: This is to insure they stay in sync.

No Kspace style defined for compute group/group
: Self-explanatory.

No OpenMP support compiled in
: An OpenMP flag is set, but LAMMPS was not built with OpenMP support.

No angle style is defined for compute angle/local
: Self-explanatory.

No angles allowed with this atom style
: Self-explanatory.

No atoms in data file
: The header of the data file indicated that atoms would be included, but they are not present.

No basis atoms in lattice
: Basis atoms must be defined for lattice style user.

No bodies allowed with this atom style
: Self-explanatory. Check data file.

No bond style is defined for compute bond/local
: Self-explanatory.

No bonds allowed with this atom style
: Self-explanatory.

No box information in dump. You have to use 'box no'
: Self-explanatory.

No count or invalid atom count in molecule file
: The number of atoms must be specified.

No dihedral style is defined for compute dihedral/local
: Self-explanatory.

No dihedrals allowed with this atom style
: Self-explanatory.

No dump custom arguments specified
: The dump custom command requires that atom quantities be specified to output to dump file.

No dump local arguments specified
: Self-explanatory.

No ellipsoids allowed with this atom style
: Self-explanatory. Check data file.

No fix gravity defined for fix pour
: Gravity is required to use fix pour.

No improper style is defined for compute improper/local
: Self-explanatory.

No impropers allowed with this atom style
: Self-explanatory.

No input values for fix ave/spatial
: Self-explanatory.

No lines allowed with this atom style
: Self-explanatory. Check data file.

No matching element in ADP potential file
: The ADP potential file does not contain elements that match the requested elements.

No matching element in EAM potential file
: The EAM potential file does not contain elements that match the requested elements.

No molecule topology allowed with atom style template
: The data file cannot specify the number of bonds, angles, etc, because this info if inferred from the molecule templates.

No overlap of box and region for create_atoms
: Self-explanatory.

No pair coul/streitz for fix qeq/slater
: These commands must be used together.

No pair hbond/dreiding coefficients set
: Self-explanatory.

No pair style defined for compute group/group
: Cannot calculate group interactions without a pair style defined.

No pair style is defined for compute pair/local
: Self-explanatory.

No pair style is defined for compute property/local
: Self-explanatory.

No rigid bodies defined
: The fix specification did not end up defining any rigid bodies.

No triangles allowed with this atom style
: Self-explanatory. Check data file.

No values in fix ave/chunk command

Self-explanatory.

No values in fix ave/time command

Self-explanatory.

Non digit character between brackets in variable

Self-explantory.

Non integer # of swaps in temper command

Swap frequency in temper command must evenly divide the total # of timesteps.

Non-numeric box dimensions - simulation unstable

The box size has apparently blown up.

Non-zero atom IDs with atom_modify id = no

Self-explanatory.

Non-zero read_data shift z value for 2d simulation

Self-explanatory.

Nprocs not a multiple of N for -reorder

Self-explanatory.

Number of core atoms != number of shell atoms

There must be a one-to-one pairing of core and shell atoms.

Numeric index is out of bounds

A command with an argument that specifies an integer or range of integers is using a value that is less than 1 or greater than the maximum allowed limit.

One or more Atom IDs is negative

Atom IDs must be positive integers.

One or more atom IDs is too big

The limit on atom IDs is set by the SMALLBIG, BIGBIG, SMALLSMALL setting in your Makefile. See Section_start 2.2 of the manual for more details.

One or more atom IDs is zero

Either all atoms IDs must be zero or none of them.

One or more atoms belong to multiple rigid bodies

Two or more rigid bodies defined by the fix rigid command cannot contain the same atom.

One or more rigid bodies are a single particle

Self-explanatory.

One or zero atoms in rigid body

Any rigid body defined by the fix rigid command must contain 2 or more atoms.

Only 2 types allowed when not using semi-grand in fix atom/swap command

Self-explanatory.

Only one cut-off allowed when requesting all long

Self-explanatory.

Only one cutoff allowed when requesting all long

Self-explanatory.

Only zhi currently implemented for fix append/atoms

Self-explanatory.

Out of range atoms - cannot compute MSM

One or more atoms are attempting to map their charge to a MSM grid point that is not owned by a processor. This is likely for one of two reasons, both of them bad. First, it may mean that an atom near the boundary of a processor's sub-domain has moved more than 1/2 the neighbor skin distance without neighbor lists being rebuilt and atoms being migrated to new processors. This also means you may be missing pairwise interactions that need to be computed. The solution is to change the re-neighboring criteria via the neigh_modify command. The safest settings are "delay 0 every 1 check yes". Second, it may mean that an atom has moved far outside a processor's sub-domain or even the entire simulation box. This indicates bad physics, e.g. due to highly overlapping atoms, too large a timestep, etc.

Out of range atoms - cannot compute PPPM

One or more atoms are attempting to map their charge to a PPPM grid point that is not owned by a

processor. This is likely for one of two reasons, both of them bad. First, it may mean that an atom near the boundary of a processor's sub-domain has moved more than 1/2 the neighbor skin distance without neighbor lists being rebuilt and atoms being migrated to new processors. This also means you may be missing pairwise interactions that need to be computed. The solution is to change the re-neighboring criteria via the neigh_modify command. The safest settings are "delay 0 every 1 check yes". Second, it may mean that an atom has moved far outside a processor's sub-domain or even the entire simulation box. This indicates bad physics, e.g. due to highly overlapping atoms, too large a timestep, etc.

Out of range atoms - cannot compute PPPMDisp

One or more atoms are attempting to map their charge to a PPPM grid point that is not owned by a processor. This is likely for one of two reasons, both of them bad. First, it may mean that an atom near the boundary of a processor's sub-domain has moved more than 1/2 the neighbor skin distance without neighbor lists being rebuilt and atoms being migrated to new processors. This also means you may be missing pairwise interactions that need to be computed. The solution is to change the re-neighboring criteria via the neigh_modify command. The safest settings are "delay 0 every 1 check yes". Second, it may mean that an atom has moved far outside a processor's sub-domain or even the entire simulation box. This indicates bad physics, e.g. due to highly overlapping atoms, too large a timestep, etc.

Overflow of allocated fix vector storage

This should not normally happen if the fix correctly calculated how long the vector will grow to. Contact the developers.

Overlapping large/large in pair colloid

This potential is infinite when there is an overlap.

Overlapping small/large in pair colloid

This potential is infinite when there is an overlap.

POEMS fix must come before NPT/NPH fix

NPT/NPH fix must be defined in input script after all poems fixes, else the fix contribution to the pressure virial is incorrect.

PPPM can only currently be used with comm_style brick

This is a current restriction in LAMMPS.

PPPM grid is too large

The global PPPM grid is larger than OFFSET in one or more dimensions. OFFSET is currently set to 4096. You likely need to decrease the requested accuracy.

PPPM grid stencil extends beyond nearest neighbor processor

This is not allowed if the kspace_modify overlap setting is no.

PPPM order < minimum allowed order

The default minimum order is 2. This can be reset by the kspace_modify minorder command.

PPPM order cannot be < 2 or > than %d

This is a limitation of the PPPM implementation in LAMMPS.

PPPMDisp Coulomb grid is too large

The global PPPM grid is larger than OFFSET in one or more dimensions. OFFSET is currently set to 4096. You likely need to decrease the requested accuracy.

PPPMDisp Dispersion grid is too large

The global PPPM grid is larger than OFFSET in one or more dimensions. OFFSET is currently set to 4096. You likely need to decrease the requested accuracy.

PPPMDisp can only currently be used with comm_style brick

This is a current restriction in LAMMPS.

PPPMDisp coulomb order cannot be greater than %d

This is a limitation of the PPPM implementation in LAMMPS.

PPPMDisp used but no parameters set, for further information please see the pppm/disp documentation

An efficient and accurate usage of the pppm/disp requires settings via the kspace_modify command. Please see the pppm/disp documentation for further instructions.

PRD command before simulation box is defined

The prd command cannot be used before a read_data, read_restart, or create_box command.

PRD nsteps must be multiple of t_event
: Self-explanatory.

PRD t_corr must be multiple of t_event
: Self-explanatory.

Package command after simulation box is defined
: The package command cannot be used afer a read_data, read_restart, or create_box command.

Package cuda command without USER-CUDA package enabled
: The USER-CUDA package must be installed via "make yes-user-cuda" before LAMMPS is built, and the "-c on" must be used to enable the package.

Package gpu command without GPU package installed
: The GPU package must be installed via "make yes-gpu" before LAMMPS is built.

Package intel command without USER-INTEL package installed
: The USER-INTEL package must be installed via "make yes-user-intel" before LAMMPS is built.

Package kokkos command without KOKKOS package enabled
: The KOKKOS package must be installed via "make yes-kokkos" before LAMMPS is built, and the "-k on" must be used to enable the package.

Package omp command without USER-OMP package installed
: The USER-OMP package must be installed via "make yes-user-omp" before LAMMPS is built.

Pair body requires atom style body
: Self-explanatory.

Pair body requires body style nparticle
: This pair style is specific to the nparticle body style.

Pair brownian requires atom style sphere
: Self-explanatory.

Pair brownian requires extended particles
: One of the particles has radius 0.0.

Pair brownian requires monodisperse particles
: All particles must be the same finite size.

Pair brownian/poly requires atom style sphere
: Self-explanatory.

Pair brownian/poly requires extended particles
: One of the particles has radius 0.0.

Pair brownian/poly requires newton pair off
: Self-explanatory.

Pair coeff for hybrid has invalid style
: Style in pair coeff must have been listed in pair_style command.

Pair coul/wolf requires atom attribute q
: The atom style defined does not have this attribute.

Pair cutoff < Respa interior cutoff
: One or more pairwise cutoffs are too short to use with the specified rRESPA cutoffs.

Pair dipole/cut requires atom attributes q, mu, torque
: The atom style defined does not have these attributes.

Pair dipole/cut/gpu requires atom attributes q, mu, torque
: The atom style defined does not have this attribute.

Pair dipole/long requires atom attributes q, mu, torque
: The atom style defined does not have these attributes.

Pair dipole/sf/gpu requires atom attributes q, mu, torque
: The atom style defined does not one or more of these attributes.

Pair distance < table inner cutoff
: Two atoms are closer together than the pairwise table allows.

Pair distance > table outer cutoff
: Two atoms are further apart than the pairwise table allows.

Pair dpd requires ghost atoms store velocity
: Use the comm_modify vel yes command to enable this.

Pair gayberne epsilon a,b,c coeffs are not all set
: Each atom type involved in pair_style gayberne must have these 3 coefficients set at least once.

Pair gayberne requires atom style ellipsoid
: Self-explanatory.

Pair gayberne requires atoms with same type have same shape
: Self-explanatory.

Pair gayberne/gpu requires atom style ellipsoid
: Self-explanatory.

Pair gayberne/gpu requires atoms with same type have same shape
: Self-explanatory.

Pair granular requires atom attributes radius, rmass
: The atom style defined does not have these attributes.

Pair granular requires ghost atoms store velocity
: Use the comm_modify vel yes command to enable this.

Pair granular with shear history requires newton pair off
: This is a current restriction of the implementation of pair granular styles with history.

Pair hybrid single calls do not support per sub-style special bond values
: Self-explanatory.

Pair hybrid sub-style does not support single call
: You are attempting to invoke a single() call on a pair style that doesn't support it.

Pair hybrid sub-style is not used
: No pair_coeff command used a sub-style specified in the pair_style command.

Pair inner cutoff < Respa interior cutoff
: One or more pairwise cutoffs are too short to use with the specified rRESPA cutoffs.

Pair inner cutoff >= Pair outer cutoff
: The specified cutoffs for the pair style are inconsistent.

Pair line/lj requires atom style line
: Self-explanatory.

Pair lj/long/dipole/long requires atom attributes mu, torque
: The atom style defined does not have these attributes.

Pair lubricate requires atom style sphere
: Self-explanatory.

Pair lubricate requires ghost atoms store velocity
: Use the comm_modify vel yes command to enable this.

Pair lubricate requires monodisperse particles
: All particles must be the same finite size.

Pair lubricate/poly requires atom style sphere
: Self-explanatory.

Pair lubricate/poly requires extended particles
: One of the particles has radius 0.0.

Pair lubricate/poly requires ghost atoms store velocity
: Use the comm_modify vel yes command to enable this.

Pair lubricate/poly requires newton pair off
: Self-explanatory.

Pair lubricateU requires atom style sphere
: Self-explanatory.

Pair lubricateU requires ghost atoms store velocity
: Use the comm_modify vel yes command to enable this.

Pair lubricateU requires monodisperse particles
: All particles must be the same finite size.

Pair lubricateU/poly requires ghost atoms store velocity
: Use the comm_modify vel yes command to enable this.

Pair lubricateU/poly requires newton pair off
: Self-explanatory.

Pair peri lattice is not identical in x, y, and z
: The lattice defined by the lattice command must be cubic.

Pair peri requires a lattice be defined
: Use the lattice command for this purpose.

Pair peri requires an atom map, see atom_modify
: Even for atomic systems, an atom map is required to find Peridynamic bonds. Use the atom_modify command to define one.

Pair resquared epsilon a,b,c coeffs are not all set
: Self-explanatory.

Pair resquared epsilon and sigma coeffs are not all set
: Self-explanatory.

Pair resquared requires atom style ellipsoid
: Self-explanatory.

Pair resquared requires atoms with same type have same shape
: Self-explanatory.

Pair resquared/gpu requires atom style ellipsoid
: Self-explanatory.

Pair resquared/gpu requires atoms with same type have same shape
: Self-explanatory.

Pair style AIREBO requires atom IDs
: This is a requirement to use the AIREBO potential.

Pair style AIREBO requires newton pair on
: See the newton command. This is a restriction to use the AIREBO potential.

Pair style BOP requires atom IDs
: This is a requirement to use the BOP potential.

Pair style BOP requires newton pair on
: See the newton command. This is a restriction to use the BOP potential.

Pair style COMB requires atom IDs
: This is a requirement to use the AIREBO potential.

Pair style COMB requires atom attribute q
: Self-explanatory.

Pair style COMB requires newton pair on
: See the newton command. This is a restriction to use the COMB potential.

Pair style COMB3 requires atom IDs
: This is a requirement to use the COMB3 potential.

Pair style COMB3 requires atom attribute q
: Self-explanatory.

Pair style COMB3 requires newton pair on
: See the newton command. This is a restriction to use the COMB3 potential.

Pair style LCBOP requires atom IDs
: This is a requirement to use the LCBOP potential.

Pair style LCBOP requires newton pair on
: See the newton command. This is a restriction to use the Tersoff potential.

Pair style MEAM requires newton pair on
: See the newton command. This is a restriction to use the MEAM potential.

Pair style SNAP requires newton pair on
: See the newton command. This is a restriction to use the SNAP potential.

Pair style Stillinger-Weber requires atom IDs

This is a requirement to use the SW potential.

Pair style Stillinger-Weber requires newton pair on

See the newton command. This is a restriction to use the SW potential.

Pair style Tersoff requires atom IDs

This is a requirement to use the Tersoff potential.

Pair style Tersoff requires newton pair on

See the newton command. This is a restriction to use the Tersoff potential.

Pair style Vashishta requires atom IDs

This is a requirement to use the Vashishta potential.

Pair style Vashishta requires newton pair on

See the newton command. This is a restriction to use the Vashishta potential.

Pair style bop requires comm ghost cutoff at least 3x larger than %g

Use the communicate ghost command to set this. See the pair bop doc page for more details.

Pair style born/coul/long requires atom attribute q

An atom style that defines this attribute must be used.

Pair style born/coul/long/gpu requires atom attribute q

The atom style defined does not have this attribute.

Pair style born/coul/wolf requires atom attribute q

The atom style defined does not have this attribute.

Pair style buck/coul/cut requires atom attribute q

The atom style defined does not have this attribute.

Pair style buck/coul/long requires atom attribute q

The atom style defined does not have these attributes.

Pair style buck/coul/long/gpu requires atom attribute q

The atom style defined does not have this attribute.

Pair style buck/long/coul/long requires atom attribute q

The atom style defined does not have this attribute.

Pair style coul/cut requires atom attribute q

The atom style defined does not have these attributes.

Pair style coul/cut/gpu requires atom attribute q

The atom style defined does not have this attribute.

Pair style coul/debye/gpu requires atom attribute q

The atom style defined does not have this attribute.

Pair style coul/dsf requires atom attribute q

The atom style defined does not have this attribute.

Pair style coul/dsf/gpu requires atom attribute q

The atom style defined does not have this attribute.

Pair style coul/long/gpu requires atom attribute q

The atom style defined does not have these attributes.

Pair style coul/streitz requires atom attribute q

Self-explanatory.

Pair style does not have extra field requested by compute pair/local

The pair style does not support the pN value requested by the compute pair/local command.

Pair style does not support bond_style quartic

The pair style does not have a single() function, so it can not be invoked by bond_style quartic.

Pair style does not support compute group/group

The pair_style does not have a single() function, so it cannot be invokded by the compute group/group command.

Pair style does not support compute pair/local

The pair style does not have a single() function, so it can not be invoked by compute pair/local.

Pair style does not support compute property/local

The pair style does not have a single() function, so it can not be invoked by fix bond/swap.

Pair style does not support fix bond/swap
: The pair style does not have a single() function, so it can not be invoked by fix bond/swap.

Pair style does not support pair_write
: The pair style does not have a single() function, so it can not be invoked by pair write.

Pair style does not support rRESPA inner/middle/outer
: You are attempting to use rRESPA options with a pair style that does not support them.

Pair style granular with history requires atoms have IDs
: Atoms in the simulation do not have IDs, so history effects cannot be tracked by the granular pair potential.

Pair style hbond/dreiding requires an atom map, see atom_modify
: Self-explanatory.

Pair style hbond/dreiding requires atom IDs
: Self-explanatory.

Pair style hbond/dreiding requires molecular system
: Self-explanatory.

Pair style hbond/dreiding requires newton pair on
: See the newton command for details.

Pair style hybrid cannot have hybrid as an argument
: Self-explanatory.

Pair style hybrid cannot have none as an argument
: Self-explanatory.

Pair style is incompatible with KSpace style
: If a pair style with a long-range Coulombic component is selected, then a kspace style must also be used.

Pair style is incompatible with TIP4P KSpace style
: The pair style does not have the requires TIP4P settings.

Pair style lj/charmm/coul/charmm requires atom attribute q
: The atom style defined does not have these attributes.

Pair style lj/charmm/coul/long requires atom attribute q
: The atom style defined does not have these attributes.

Pair style lj/charmm/coul/long/gpu requires atom attribute q
: The atom style defined does not have this attribute.

Pair style lj/class2/coul/cut requires atom attribute q
: The atom style defined does not have this attribute.

Pair style lj/class2/coul/long requires atom attribute q
: The atom style defined does not have this attribute.

Pair style lj/class2/coul/long/gpu requires atom attribute q
: The atom style defined does not have this attribute.

Pair style lj/cut/coul/cut requires atom attribute q
: The atom style defined does not have this attribute.

Pair style lj/cut/coul/cut/gpu requires atom attribute q
: The atom style defined does not have this attribute.

Pair style lj/cut/coul/debye/gpu requires atom attribute q
: The atom style defined does not have this attribute.

Pair style lj/cut/coul/dsf requires atom attribute q
: The atom style defined does not have these attributes.

Pair style lj/cut/coul/dsf/gpu requires atom attribute q
: The atom style defined does not have this attribute.

Pair style lj/cut/coul/long requires atom attribute q
: The atom style defined does not have this attribute.

Pair style lj/cut/coul/long/gpu requires atom attribute q
: The atom style defined does not have this attribute.

Pair style lj/cut/tip4p/cut requires atom IDs

This is a requirement to use this potential.

Pair style lj/cut/tip4p/cut requires atom attribute q

The atom style defined does not have this attribute.

Pair style lj/cut/tip4p/cut requires newton pair on

See the newton command. This is a restriction to use this potential.

Pair style lj/cut/tip4p/long requires atom IDs

There are no atom IDs defined in the system and the TIP4P potential requires them to find O,H atoms with a water molecule.

Pair style lj/cut/tip4p/long requires atom attribute q

The atom style defined does not have these attributes.

Pair style lj/cut/tip4p/long requires newton pair on

This is because the computation of constraint forces within a water molecule adds forces to atoms owned by other processors.

Pair style lj/gromacs/coul/gromacs requires atom attribute q

An atom_style with this attribute is needed.

Pair style lj/long/dipole/long does not currently support respa

This feature is not yet supported.

Pair style lj/long/tip4p/long requires atom IDs

There are no atom IDs defined in the system and the TIP4P potential requires them to find O,H atoms with a water molecule.

Pair style lj/long/tip4p/long requires atom attribute q

The atom style defined does not have these attributes.

Pair style lj/long/tip4p/long requires newton pair on

This is because the computation of constraint forces within a water molecule adds forces to atoms owned by other processors.

Pair style lj/sdk/coul/long/gpu requires atom attribute q

The atom style defined does not have this attribute.

Pair style nb3b/harmonic requires atom IDs

This is a requirement to use this potential.

Pair style nb3b/harmonic requires newton pair on

See the newton command. This is a restriction to use this potential.

Pair style nm/cut/coul/cut requires atom attribute q

The atom style defined does not have this attribute.

Pair style nm/cut/coul/long requires atom attribute q

The atom style defined does not have this attribute.

Pair style peri requires atom style peri

Self-explanatory.

Pair style polymorphic requires atom IDs

This is a requirement to use the polymorphic potential.

Pair style polymorphic requires newton pair on

See the newton command. This is a restriction to use the polymorphic potential.

Pair style reax requires atom IDs

This is a requirement to use the ReaxFF potential.

Pair style reax requires atom attribute q

The atom style defined does not have this attribute.

Pair style reax requires newton pair on

This is a requirement to use the ReaxFF potential.

Pair style requires a KSpace style

No kspace style is defined.

Pair style requires use of kspace_style ewald/disp

Self-explanatory.

Pair style sw/gpu requires atom IDs

This is a requirement to use this potential.

Pair style sw/gpu requires newton pair off

See the newton command. This is a restriction to use this potential.

Pair style tersoff/gpu requires atom IDs

This is a requirement to use the tersoff/gpu potential.

Pair style tersoff/gpu requires newton pair off

See the newton command. This is a restriction to use this pair style.

Pair style tip4p/cut requires atom IDs

This is a requirement to use this potential.

Pair style tip4p/cut requires atom attribute q

The atom style defined does not have this attribute.

Pair style tip4p/cut requires newton pair on

See the newton command. This is a restriction to use this potential.

Pair style tip4p/long requires atom IDs

There are no atom IDs defined in the system and the TIP4P potential requires them to find O,H atoms with a water molecule.

Pair style tip4p/long requires atom attribute q

The atom style defined does not have these attributes.

Pair style tip4p/long requires newton pair on

This is because the computation of constraint forces within a water molecule adds forces to atoms owned by other processors.

Pair table cutoffs must all be equal to use with KSpace

When using pair style table with a long-range KSpace solver, the cutoffs for all atom type pairs must all be the same, since the long-range solver starts at that cutoff.

Pair table parameters did not set N

List of pair table parameters must include N setting.

Pair tersoff/zbl requires metal or real units

This is a current restriction of this pair potential.

Pair tersoff/zbl/kk requires metal or real units

This is a current restriction of this pair potential.

Pair tri/lj requires atom style tri

Self-explanatory.

Pair yukawa/colloid requires atom style sphere

Self-explantory.

Pair yukawa/colloid requires atoms with same type have same radius

Self-explantory.

Pair yukawa/colloid/gpu requires atom style sphere

Self-explanatory.

PairKIM only works with 3D problems

This is a current limitation.

Pair_coeff command before pair_style is defined

Self-explanatory.

Pair_coeff command before simulation box is defined

The pair_coeff command cannot be used before a read_data, read_restart, or create_box command.

Pair_modify command before pair_style is defined

Self-explanatory.

Pair_modify special setting for pair hybrid incompatible with global special_bonds setting

Cannot override a setting of 0.0 or 1.0 or change a setting between 0.0 and 1.0.

Pair_write command before pair_style is defined

Self-explanatory.

Particle on or inside fix wall surface

Particles must be "exterior" to the wall in order for energy/force to be calculated.

Particle outside surface of region used in fix wall/region
: Particles must be inside the region for energy/force to be calculated. A particle outside the region generates an error.

Per-atom compute in equal-style variable formula
: Equal-style variables cannot use per-atom quantities.

Per-atom energy was not tallied on needed timestep
: You are using a thermo keyword that requires potentials to have tallied energy, but they didn't on this timestep. See the variable doc page for ideas on how to make this work.

Per-atom fix in equal-style variable formula
: Equal-style variables cannot use per-atom quantities.

Per-atom virial was not tallied on needed timestep
: You are using a thermo keyword that requires potentials to have tallied the virial, but they didn't on this timestep. See the variable doc page for ideas on how to make this work.

Per-processor system is too big
: The number of owned atoms plus ghost atoms on a single processor must fit in 32-bit integer.

Potential energy ID for fix neb does not exist
: Self-explanatory.

Potential energy ID for fix nvt/nph/npt does not exist
: A compute for potential energy must be defined.

Potential file has duplicate entry
: The potential file has more than one entry for the same element.

Potential file is missing an entry
: The potential file does not have a needed entry.

Power by 0 in variable formula
: Self-explanatory.

Pressure ID for fix box/relax does not exist
: The compute ID needed to compute pressure for the fix does not exist.

Pressure ID for fix modify does not exist
: Self-explanatory.

Pressure ID for fix npt/nph does not exist
: Self-explanatory.

Pressure ID for fix press/berendsen does not exist
: The compute ID needed to compute pressure for the fix does not exist.

Pressure ID for fix rigid npt/nph does not exist
: Self-explanatory.

Pressure ID for thermo does not exist
: The compute ID needed to compute pressure for thermodynamics does not exist.

Pressure control can not be used with fix nvt
: Self-explanatory.

Pressure control can not be used with fix nvt/asphere
: Self-explanatory.

Pressure control can not be used with fix nvt/body
: Self-explanatory.

Pressure control can not be used with fix nvt/sllod
: Self-explanatory.

Pressure control can not be used with fix nvt/sphere
: Self-explanatory.

Pressure control must be used with fix nph
: Self-explanatory.

Pressure control must be used with fix nph/asphere
: Self-explanatory.

Pressure control must be used with fix nph/body

Self-explanatory.

Pressure control must be used with fix nph/small

Self-explanatory.

Pressure control must be used with fix nph/sphere

Self-explanatory.

Pressure control must be used with fix nphug

A pressure control keyword (iso, aniso, tri, x, y, or z) must be provided.

Pressure control must be used with fix npt

Self-explanatory.

Pressure control must be used with fix npt/asphere

Self-explanatory.

Pressure control must be used with fix npt/body

Self-explanatory.

Pressure control must be used with fix npt/sphere

Self-explanatory.

Processor count in z must be 1 for 2d simulation

Self-explanatory.

Processor partitions do not match number of allocated processors

The total number of processors in all partitions must match the number of processors LAMMPS is running on.

Processors command after simulation box is defined

The processors command cannot be used after a read_data, read_restart, or create_box command.

Processors custom grid file is inconsistent

The vales in the custom file are not consistent with the number of processors you are running on or the Px,Py,Pz settings of the processors command. Or there was not a setting for every processor.

Processors grid numa and map style are incompatible

Using numa for gstyle in the processors command requires using cart for the map option.

Processors part option and grid style are incompatible

Cannot use gstyle numa or custom with the part option.

Processors twogrid requires proc count be a multiple of core count

Self-explanatory.

Pstart and Pstop must have the same value

Self-explanatory.

Python function evaluation failed

The Python function did not run succesfully and/or did not return a value (if it is supposed to return a value). This is probably due to some error condition in the function.

Python function is not callable

The provided Python code was run successfully, but it not define a callable function with the required name.

Python invoke of undefined function

Cannot invoke a function that has not been previously defined.

Python variable does not match Python function

This matching is defined by the python-style variable and the python command.

Python variable has no function

No python command was used to define the function associated with the python-style variable.

QEQ with 'newton pair off' not supported

See the newton command. This is a restriction to use the QEQ fixes.

R0 < 0 for fix spring command

Equilibrium spring length is invalid.

RATTLE coordinate constraints are not satisfied up to desired tolerance

Self-explanatory.

RATTLE determinant = 0.0

The determinant of the matrix being solved for a single cluster specified by the fix rattle command is numerically invalid.

RATTLE failed

Certain constraints were not satisfied.

RATTLE velocity constraints are not satisfied up to desired tolerance

Self-explanatory.

Read data add offset is too big

It cannot be larger than the size of atom IDs, e.g. the maximum 32-bit integer.

Read dump of atom property that isn't allocated

Self-explanatory.

Read rerun dump file timestep > specified stop

Self-explanatory.

Read restart MPI-IO input not allowed with % in filename

This is because a % signifies one file per processor and MPI-IO creates one large file for all processors.

Read_data shrink wrap did not assign all atoms correctly

This is typically because the box-size specified in the data file is large compared to the actual extent of atoms in a shrink-wrapped dimension. When LAMMPS shrink-wraps the box atoms will be lost if the processor they are re-assigned to is too far away. Choose a box size closer to the actual extent of the atoms.

Read_dump command before simulation box is defined

The read_dump command cannot be used before a read_data, read_restart, or create_box command.

Read_dump field not found in dump file

Self-explanatory.

Read_dump triclinic status does not match simulation

Both the dump snapshot and the current LAMMPS simulation must be using either an orthogonal or triclinic box.

Read_dump xyz fields do not have consistent scaling/wrapping

Self-explanatory.

Reading from MPI-IO filename when MPIIO package is not installed

Self-explanatory.

Reax_defs.h setting for NATDEF is too small

Edit the setting in the ReaxFF library and re-compile the library and re-build LAMMPS.

Reax_defs.h setting for NNEIGHMAXDEF is too small

Edit the setting in the ReaxFF library and re-compile the library and re-build LAMMPS.

Receiving partition in processors part command is already a receiver

Cannot specify a partition to be a receiver twice.

Region ID for compute chunk/atom does not exist

Self-explanatory.

Region ID for compute reduce/region does not exist

Self-explanatory.

Region ID for compute temp/region does not exist

Self-explanatory.

Region ID for dump custom does not exist

Self-explanatory.

Region ID for fix addforce does not exist

Self-explanatory.

Region ID for fix atom/swap does not exist

Self-explanatory.

Region ID for fix ave/spatial does not exist

Self-explanatory.

Region ID for fix aveforce does not exist

Self-explanatory.

Region ID for fix deposit does not exist
: Self-explanatory.

Region ID for fix efield does not exist
: Self-explanatory.

Region ID for fix evaporate does not exist
: Self-explanatory.

Region ID for fix gcmc does not exist
: Self-explanatory.

Region ID for fix heat does not exist
: Self-explanatory.

Region ID for fix setforce does not exist
: Self-explanatory.

Region ID for fix wall/region does not exist
: Self-explanatory.

Region ID for group dynamic does not exist
: Self-explanatory.

Region ID in variable formula does not exist
: Self-explanatory.

Region cannot have 0 length rotation vector
: Self-explanatory.

Region for fix oneway does not exist
: Self-explanatory.

Region intersect region ID does not exist
: Self-explanatory.

Region union or intersect cannot be dynamic
: The sub-regions can be dynamic, but not the combined region.

Region union region ID does not exist
: One or more of the region IDs specified by the region union command does not exist.

Replacing a fix, but new style != old style
: A fix ID can be used a 2nd time, but only if the style matches the previous fix. In this case it is assumed you with to reset a fix's parameters. This error may mean you are mistakenly re-using a fix ID when you do not intend to.

Replicate command before simulation box is defined
: The replicate command cannot be used before a read_data, read_restart, or create_box command.

Replicate did not assign all atoms correctly
: Atoms replicated by the replicate command were not assigned correctly to processors. This is likely due to some atom coordinates being outside a non-periodic simulation box.

Replicated system atom IDs are too big
: See the setting for tagint in the src/lmptype.h file.

Replicated system is too big
: See the setting for bigint in the src/lmptype.h file.

Required border comm not yet implemented with Kokkos
: There are various limitations in the communication options supported by Kokkos.

Rerun command before simulation box is defined
: The rerun command cannot be used before a read_data, read_restart, or create_box command.

Rerun dump file does not contain requested snapshot
: Self-explanatory.

Resetting timestep size is not allowed with fix move
: This is because fix move is moving atoms based on elapsed time.

Respa inner cutoffs are invalid
: The first cutoff must be <= the second cutoff.

Respa levels must be >= 1

Self-explanatory.

Respa middle cutoffs are invalid

The first cutoff must be <= the second cutoff.

Restart file MPI-IO output not allowed with % in filename

This is because a % signifies one file per processor and MPI-IO creates one large file for all processors.

Restart file byte ordering is not recognized

The file does not appear to be a LAMMPS restart file since it doesn't contain a recognized byte-orderomg flag at the beginning.

Restart file byte ordering is swapped

The file was written on a machine with different byte-ordering than the machine you are reading it on. Convert it to a text data file instead, on the machine you wrote it on.

Restart file incompatible with current version

This is probably because you are trying to read a file created with a version of LAMMPS that is too old compared to the current version. Use your older version of LAMMPS and convert the restart file to a data file.

Restart file is a MPI-IO file

The file is inconsistent with the filename you specified for it.

Restart file is a multi-proc file

The file is inconsistent with the filename you specified for it.

Restart file is not a MPI-IO file

The file is inconsistent with the filename you specified for it.

Restart file is not a multi-proc file

The file is inconsistent with the filename you specified for it.

Restart variable returned a bad timestep

The variable must return a timestep greater than the current timestep.

Restrain atoms %d %d %d %d missing on proc %d at step %ld

The 4 atoms in a restrain dihedral specified by the fix restrain command are not all accessible to a processor. This probably means an atom has moved too far.

Restrain atoms %d %d %d missing on proc %d at step %ld

The 3 atoms in a restrain angle specified by the fix restrain command are not all accessible to a processor. This probably means an atom has moved too far.

Restrain atoms %d %d missing on proc %d at step %ld

The 2 atoms in a restrain bond specified by the fix restrain command are not all accessible to a processor. This probably means an atom has moved too far.

Reuse of compute ID

A compute ID cannot be used twice.

Reuse of dump ID

A dump ID cannot be used twice.

Reuse of molecule template ID

The template IDs must be unique.

Reuse of region ID

A region ID cannot be used twice.

Rigid body atoms %d %d missing on proc %d at step %ld

This means that an atom cannot find the atom that owns the rigid body it is part of, or vice versa. The solution is to use the communicate cutoff command to insure ghost atoms are acquired from far enough away to encompass the max distance printed when the fix rigid/small command was invoked.

Rigid body has degenerate moment of inertia

Fix poems will only work with bodies (collections of atoms) that have non-zero principal moments of inertia. This means they must be 3 or more non-collinear atoms, even with joint atoms removed.

Rigid fix must come before NPT/NPH fix

NPT/NPH fix must be defined in input script after all rigid fixes, else the rigid fix contribution to the pressure virial is incorrect.

Rmask function in equal-style variable formula
: Rmask is per-atom operation.

Run command before simulation box is defined
: The run command cannot be used before a read_data, read_restart, or create_box command.

Run command start value is after start of run
: Self-explanatory.

Run command stop value is before end of run
: Self-explanatory.

Run_style command before simulation box is defined
: The run_style command cannot be used before a read_data, read_restart, or create_box command.

SRD bin size for fix srd differs from user request
: Fix SRD had to adjust the bin size to fit the simulation box. See the cubic keyword if you want this message to be an error vs warning.

SRD bins for fix srd are not cubic enough
: The bin shape is not within tolerance of cubic. See the cubic keyword if you want this message to be an error vs warning.

SRD particle %d started inside big particle %d on step %ld bounce %d
: See the inside keyword if you want this message to be an error vs warning.

SRD particle %d started inside wall %d on step %ld bounce %d
: See the inside keyword if you want this message to be an error vs warning.

Same dimension twice in fix ave/spatial
: Self-explanatory.

Sending partition in processors part command is already a sender
: Cannot specify a partition to be a sender twice.

Set command before simulation box is defined
: The set command cannot be used before a read_data, read_restart, or create_box command.

Set command floating point vector does not exist
: Self-explanatory.

Set command integer vector does not exist
: Self-explanatory.

Set command with no atoms existing
: No atoms are yet defined so the set command cannot be used.

Set region ID does not exist
: Region ID specified in set command does not exist.

Shake angles have different bond types
: All 3-atom angle-constrained SHAKE clusters specified by the fix shake command that are the same angle type, must also have the same bond types for the 2 bonds in the angle.

Shake atoms %d %d %d %d missing on proc %d at step %ld
: The 4 atoms in a single shake cluster specified by the fix shake command are not all accessible to a processor. This probably means an atom has moved too far.

Shake atoms %d %d %d missing on proc %d at step %ld
: The 3 atoms in a single shake cluster specified by the fix shake command are not all accessible to a processor. This probably means an atom has moved too far.

Shake atoms %d %d missing on proc %d at step %ld
: The 2 atoms in a single shake cluster specified by the fix shake command are not all accessible to a processor. This probably means an atom has moved too far.

Shake cluster of more than 4 atoms
: A single cluster specified by the fix shake command can have no more than 4 atoms.

Shake clusters are connected
: A single cluster specified by the fix shake command must have a single central atom with up to 3 other atoms bonded to it.

Shake determinant = 0.0

The determinant of the matrix being solved for a single cluster specified by the fix shake command is numerically invalid.

Shake fix must come before NPT/NPH fix

NPT fix must be defined in input script after SHAKE fix, else the SHAKE fix contribution to the pressure virial is incorrect.

Shear history overflow, boost neigh_modify one

There are too many neighbors of a single atom. Use the neigh_modify command to increase the max number of neighbors allowed for one atom. You may also want to boost the page size.

Small to big integers are not sized correctly

This error occurs whenthe sizes of smallint, imageint, tagint, bigint, as defined in src/lmptype.h are not what is expected. Contact the developers if this occurs.

Smallint setting in lmptype.h is invalid

It has to be the size of an integer.

Smallint setting in lmptype.h is not compatible

Smallint stored in restart file is not consistent with LAMMPS version you are running.

Special list size exceeded in fix bond/create

See the read_data command for info on setting the "extra special per atom" header value to allow for additional special values to be stored.

Specified processors != physical processors

The 3d grid of processors defined by the processors command does not match the number of processors LAMMPS is being run on.

Specified target stress must be uniaxial or hydrostatic

Self-explanatory.

Sqrt of negative value in variable formula

Self-explanatory.

Subsequent read data induced too many angles per atom

See the create_box extra/angle/per/atom or read_data "extra angle per atom" header value to set this limit larger.

Subsequent read data induced too many bonds per atom

See the create_box extra/bond/per/atom or read_data "extra bond per atom" header value to set this limit larger.

Subsequent read data induced too many dihedrals per atom

See the create_box extra/dihedral/per/atom or read_data "extra dihedral per atom" header value to set this limit larger.

Subsequent read data induced too many impropers per atom

See the create_box extra/improper/per/atom or read_data "extra improper per atom" header value to set this limit larger.

Substitution for illegal variable

Input script line contained a variable that could not be substituted for.

Support for writing images in JPEG format not included

LAMMPS was not built with the -DLAMMPS_JPEG switch in the Makefile.

Support for writing images in PNG format not included

LAMMPS was not built with the -DLAMMPS_PNG switch in the Makefile.

Support for writing movies not included

LAMMPS was not built with the -DLAMMPS_FFMPEG switch in the Makefile

System in data file is too big

See the setting for bigint in the src/lmptype.h file.

System is not charge neutral, net charge = %g

The total charge on all atoms on the system is not 0.0. For some KSpace solvers this is an error.

TAD nsteps must be multiple of t_event

Self-explanatory.

TIP4P hydrogen has incorrect atom type

The TIP4P pairwise computation found an H atom whose type does not agree with the specified H type.

TIP4P hydrogen is missing

The TIP4P pairwise computation failed to find the correct H atom within a water molecule.

TMD target file did not list all group atoms

The target file for the fix tmd command did not list all atoms in the fix group.

Tad command before simulation box is defined

Self-explanatory.

Tagint setting in lmptype.h is invalid

Tagint must be as large or larger than smallint.

Tagint setting in lmptype.h is not compatible

Format of tagint stored in restart file is not consistent with LAMMPS version you are running. See the settings in src/lmptype.h

Target pressure for fix rigid/nph cannot be < 0.0

Self-explanatory.

Target pressure for fix rigid/npt/small cannot be < 0.0

Self-explanatory.

Target temperature for fix nvt/npt/nph cannot be 0.0

Self-explanatory.

Target temperature for fix rigid/npt cannot be 0.0

Self-explanatory.

Target temperature for fix rigid/npt/small cannot be 0.0

Self-explanatory.

Target temperature for fix rigid/nvt cannot be 0.0

Self-explanatory.

Target temperature for fix rigid/nvt/small cannot be 0.0

Self-explanatory.

Temper command before simulation box is defined

The temper command cannot be used before a read_data, read_restart, or create_box command.

Temperature ID for fix bond/swap does not exist

Self-explanatory.

Temperature ID for fix box/relax does not exist

Self-explanatory.

Temperature ID for fix nvt/npt does not exist

Self-explanatory.

Temperature ID for fix press/berendsen does not exist

Self-explanatory.

Temperature ID for fix rigid nvt/npt/nph does not exist

Self-explanatory.

Temperature ID for fix temp/berendsen does not exist

Self-explanatory.

Temperature ID for fix temp/csld does not exist

Self-explanatory.

Temperature ID for fix temp/csvr does not exist

Self-explanatory.

Temperature ID for fix temp/rescale does not exist

Self-explanatory.

Temperature compute degrees of freedom < 0

This should not happen if you are calculating the temperature on a valid set of atoms.

Temperature control can not be used with fix nph

Self-explanatory.

Temperature control can not be used with fix nph/asphere

Self-explanatory.

Temperature control can not be used with fix nph/body
: Self-explanatory.

Temperature control can not be used with fix nph/sphere
: Self-explanatory.

Temperature control must be used with fix nphug
: The temp keyword must be provided.

Temperature control must be used with fix npt
: Self-explanatory.

Temperature control must be used with fix npt/asphere
: Self-explanatory.

Temperature control must be used with fix npt/body
: Self-explanatory.

Temperature control must be used with fix npt/sphere
: Self-explanatory.

Temperature control must be used with fix nvt
: Self-explanatory.

Temperature control must be used with fix nvt/asphere
: Self-explanatory.

Temperature control must be used with fix nvt/body
: Self-explanatory.

Temperature control must be used with fix nvt/sllod
: Self-explanatory.

Temperature control must be used with fix nvt/sphere
: Self-explanatory.

Temperature control must not be used with fix nph/small
: Self-explanatory.

Temperature for fix nvt/sllod does not have a bias
: The specified compute must compute temperature with a bias.

Tempering could not find thermo_pe compute
: This compute is created by the thermo command. It must have been explicitly deleted by a uncompute command.

Tempering fix ID is not defined
: The fix ID specified by the temper command does not exist.

Tempering temperature fix is not valid
: The fix specified by the temper command is not one that controls temperature (nvt or langevin).

Test_descriptor_string already allocated
: This is an internal error. Contact the developers.

The package gpu command is required for gpu styles
: Self-explanatory.

Thermo and fix not computed at compatible times
: Fixes generate values on specific timesteps. The thermo output does not match these timesteps.

Thermo compute array is accessed out-of-range
: Self-explanatory.

Thermo compute does not compute array
: Self-explanatory.

Thermo compute does not compute scalar
: Self-explanatory.

Thermo compute does not compute vector
: Self-explanatory.

Thermo compute vector is accessed out-of-range
: Self-explanatory.

Thermo custom variable cannot be indexed

Self-explanatory.

Thermo custom variable is not equal-style variable

Only equal-style variables can be output with thermodynamics, not atom-style variables.

Thermo every variable returned a bad timestep

The variable must return a timestep greater than the current timestep.

Thermo fix array is accessed out-of-range

Self-explanatory.

Thermo fix does not compute array

Self-explanatory.

Thermo fix does not compute scalar

Self-explanatory.

Thermo fix does not compute vector

Self-explanatory.

Thermo fix vector is accessed out-of-range

Self-explanatory.

Thermo keyword in variable requires thermo to use/init pe

You are using a thermo keyword in a variable that requires potential energy to be calculated, but your thermo output does not use it. Add it to your thermo output.

Thermo keyword in variable requires thermo to use/init press

You are using a thermo keyword in a variable that requires pressure to be calculated, but your thermo output does not use it. Add it to your thermo output.

Thermo keyword in variable requires thermo to use/init temp

You are using a thermo keyword in a variable that requires temperature to be calculated, but your thermo output does not use it. Add it to your thermo output.

Thermo style does not use press

Cannot use thermo_modify to set this parameter since the thermo_style is not computing this quantity.

Thermo style does not use temp

Cannot use thermo_modify to set this parameter since the thermo_style is not computing this quantity.

Thermo_modify every variable returned a bad timestep

The returned timestep is less than or equal to the current timestep.

Thermo_modify int format does not contain d character

Self-explanatory.

Thermo_modify pressure ID does not compute pressure

The specified compute ID does not compute pressure.

Thermo_modify temperature ID does not compute temperature

The specified compute ID does not compute temperature.

Thermo_style command before simulation box is defined

The thermo_style command cannot be used before a read_data, read_restart, or create_box command.

This variable thermo keyword cannot be used between runs

Keywords that refer to time (such as cpu, elapsed) do not make sense in between runs.

Threshhold for an atom property that isn't allocated

A dump threshhold has been requested on a quantity that is not defined by the atom style used in this simulation.

Timestep must be >= 0

Specified timestep is invalid.

Too big a problem to use velocity create loop all

The system size must fit in a 32-bit integer to use this option.

Too big a timestep for dump dcd

The timestep must fit in a 32-bit integer to use this dump style.

Too big a timestep for dump xtc

The timestep must fit in a 32-bit integer to use this dump style.

Too few bits for lookup table

Table size specified via pair_modify command does not work with your machine's floating point representation.

Too few lines in %s section of data file
Self-explanatory.

Too few values in body lines in data file
Self-explanatory.

Too few values in body section of molecule file
Self-explanatory.

Too many -pk arguments in command line
The string formed by concatenating the arguments is too long. Use a package command in the input script instead.

Too many MSM grid levels
The max number of MSM grid levels is hardwired to 10.

Too many args in variable function
More args are used than any variable function allows.

Too many atom pairs for pair bop
The number of atomic pairs exceeds the expected number. Check your atomic structure to ensure that it is realistic.

Too many atom sorting bins
This is likely due to an immense simulation box that has blown up to a large size.

Too many atom triplets for pair bop
The number of three atom groups for angle determinations exceeds the expected number. Check your atomic structrure to ensure that it is realistic.

Too many atoms for dump dcd
The system size must fit in a 32-bit integer to use this dump style.

Too many atoms for dump xtc
The system size must fit in a 32-bit integer to use this dump style.

Too many atoms to dump sort
Cannot sort when running with more than 2^31 atoms.

Too many exponent bits for lookup table
Table size specified via pair_modify command does not work with your machine's floating point representation.

Too many groups
The maximum number of atom groups (including the "all" group) is given by MAX_GROUP in group.cpp and is 32.

Too many iterations
You must use a number of iterations that fit in a 32-bit integer for minimization.

Too many lines in one body in data file - boost MAXBODY
MAXBODY is a setting at the top of the src/read_data.cpp file. Set it larger and re-compile the code.

Too many local+ghost atoms for neighbor list
The number of nlocal + nghost atoms on a processor is limited by the size of a 32-bit integer with 2 bits removed for masking 1-2, 1-3, 1-4 neighbors.

Too many mantissa bits for lookup table
Table size specified via pair_modify command does not work with your machine's floating point representation.

Too many masses for fix shake
The fix shake command cannot list more masses than there are atom types.

Too many molecules for fix poems
The limit is 2^31 = ~2 billion molecules.

Too many molecules for fix rigid
The limit is 2^31 = ~2 billion molecules.

Too many neighbor bins

This is likely due to an immense simulation box that has blown up to a large size.

Too many timesteps

The cummulative timesteps must fit in a 64-bit integer.

Too many timesteps for NEB

You must use a number of timesteps that fit in a 32-bit integer for NEB.

Too many total atoms

See the setting for bigint in the src/lmptype.h file.

Too many total bits for bitmapped lookup table

Table size specified via pair_modify command is too large. Note that a value of N generates a 2^N size table.

Too many values in body lines in data file

Self-explanatory.

Too many values in body section of molecule file

Self-explanatory.

Too much buffered per-proc info for dump

The size of the buffered string must fit in a 32-bit integer for a dump.

Too much per-proc info for dump

Number of local atoms times number of columns must fit in a 32-bit integer for dump.

Tree structure in joint connections

Fix poems cannot (yet) work with coupled bodies whose joints connect the bodies in a tree structure.

Triclinic box skew is too large

The displacement in a skewed direction must be less than half the box length in that dimension. E.g. the xy tilt must be between -half and +half of the x box length. This constraint can be relaxed by using the box tilt command.

Tried to convert a double to int, but input_double > INT_MAX

Self-explanatory.

Trying to build an occasional neighbor list before initialization completed

This is not allowed. Source code caller needs to be modified.

Two fix ave commands using same compute chunk/atom command in incompatible ways

They are both attempting to "lock" the chunk/atom command so that the chunk assignments persist for some number of timesteps, but are doing it in different ways.

Two groups cannot be the same in fix spring couple

Self-explanatory.

USER-CUDA mode requires CUDA variant of min style

CUDA mode is enabled, so the min style must include a cuda suffix.

USER-CUDA mode requires CUDA variant of run style

CUDA mode is enabled, so the run style must include a cuda suffix.

USER-CUDA package does not yet support comm_style tiled

Self-explanatory.

USER-CUDA package requires a cuda enabled atom_style

Self-explanatory.

Unable to initialize accelerator for use

There was a problem initializing an accelerator for the gpu package

Unbalanced quotes in input line

No matching end double quote was found following a leading double quote.

Unexpected end of -reorder file

Self-explanatory.

Unexpected end of AngleCoeffs section

Read a blank line.

Unexpected end of BondCoeffs section

Read a blank line.

Unexpected end of DihedralCoeffs section

Read a blank line.

Unexpected end of ImproperCoeffs section

Read a blank line.

Unexpected end of PairCoeffs section

Read a blank line.

Unexpected end of custom file

Self-explanatory.

Unexpected end of data file

LAMMPS hit the end of the data file while attempting to read a section. Something is wrong with the format of the data file.

Unexpected end of dump file

A read operation from the file failed.

Unexpected end of fix rigid file

A read operation from the file failed.

Unexpected end of fix rigid/small file

A read operation from the file failed.

Unexpected end of molecule file

Self-explanatory.

Unexpected end of neb file

A read operation from the file failed.

Units command after simulation box is defined

The units command cannot be used after a read_data, read_restart, or create_box command.

Universe/uloop variable count < # of partitions

A universe or uloop style variable must specify a number of values >= to the number of processor partitions.

Unknown angle style

The choice of angle style is unknown.

Unknown atom style

The choice of atom style is unknown.

Unknown body style

The choice of body style is unknown.

Unknown bond style

The choice of bond style is unknown.

Unknown category for info is_active()

Self-explanatory.

Unknown category for info is_available()

Self-explanatory.

Unknown category for info is_defined()

Self-explanatory.

Unknown command: %s

The command is not known to LAMMPS. Check the input script.

Unknown compute style

The choice of compute style is unknown.

Unknown dihedral style

The choice of dihedral style is unknown.

Unknown dump reader style

The choice of dump reader style via the format keyword is unknown.

Unknown dump style

The choice of dump style is unknown.

Unknown error in GPU library

Self-explanatory.

Unknown fix style

The choice of fix style is unknown.

Unknown identifier in data file: %s
A section of the data file cannot be read by LAMMPS.

Unknown improper style
The choice of improper style is unknown.

Unknown keyword in thermo_style custom command
One or more specified keywords are not recognized.

Unknown kspace style
The choice of kspace style is unknown.

Unknown name for info newton category
Self-explanatory.

Unknown name for info package category
Self-explanatory.

Unknown name for info pair category
Self-explanatory.

Unknown pair style
The choice of pair style is unknown.

Unknown pair_modify hybrid sub-style
The choice of sub-style is unknown.

Unknown region style
The choice of region style is unknown.

Unknown section in molecule file
Self-explanatory.

Unknown table style in angle style table
Self-explanatory.

Unknown table style in bond style table
Self-explanatory.

Unknown table style in pair_style command
Style of table is invalid for use with pair_style table command.

Unknown unit_style
Self-explanatory. Check the input script or data file.

Unrecognized lattice type in MEAM file 1
The lattice type in an entry of the MEAM library file is not valid.

Unrecognized lattice type in MEAM file 2
The lattice type in an entry of the MEAM parameter file is not valid.

Unrecognized pair style in compute pair command
Self-explanatory.

Unrecognized virial argument in pair_style command
Only two options are supported: LAMMPSvirial and KIMvirial

Unsupported mixing rule in kspace_style ewald/disp
Only geometric mixing is supported.

Unsupported order in kspace_style ewald/disp
Only 1/r^6 dispersion or dipole terms are supported.

Unsupported order in kspace_style pppm/disp, pair_style %s
Only pair styles with 1/r and 1/r^6 dependence are currently supported.

Use cutoff keyword to set cutoff in single mode
Mode is single so cutoff/multi keyword cannot be used.

Use cutoff/multi keyword to set cutoff in multi mode
Mode is multi so cutoff keyword cannot be used.

Using fix nvt/sllod with inconsistent fix deform remap option
Fix nvt/sllod requires that deforming atoms have a velocity profile provided by "remap v" as a fix deform option.

Using fix nvt/sllod with no fix deform defined
: Self-explanatory.

Using fix srd with inconsistent fix deform remap option
: When shearing the box in an SRD simulation, the remap v option for fix deform needs to be used.

Using pair lubricate with inconsistent fix deform remap option
: Must use remap v option with fix deform with this pair style.

Using pair lubricate/poly with inconsistent fix deform remap option
: If fix deform is used, the remap v option is required.

Using suffix cuda without USER-CUDA package enabled
: Self-explanatory.

Using suffix gpu without GPU package installed
: Self-explanatory.

Using suffix intel without USER-INTEL package installed
: Self-explanatory.

Using suffix kk without KOKKOS package enabled
: Self-explanatory.

Using suffix omp without USER-OMP package installed
: Self-explanatory.

Using update dipole flag requires atom attribute mu
: Self-explanatory.

Using update dipole flag requires atom style sphere
: Self-explanatory.

Variable ID in variable formula does not exist
: Self-explanatory.

Variable atom ID is too large
: Specified ID is larger than the maximum allowed atom ID.

Variable evaluation before simulation box is defined
: Cannot evaluate a compute or fix or atom-based value in a variable before the simulation has been setup.

Variable evaluation in fix wall gave bad value
: The returned value for epsilon or sigma < 0.0.

Variable evaluation in region gave bad value
: Variable returned a radius < 0.0.

Variable for compute ti is invalid style
: Self-explanatory.

Variable for create_atoms is invalid style
: The variables must be equal-style variables.

Variable for displace_atoms is invalid style
: It must be an equal-style or atom-style variable.

Variable for dump every is invalid style
: Only equal-style variables can be used.

Variable for dump image center is invalid style
: Must be an equal-style variable.

Variable for dump image persp is invalid style
: Must be an equal-style variable.

Variable for dump image phi is invalid style
: Must be an equal-style variable.

Variable for dump image theta is invalid style
: Must be an equal-style variable.

Variable for dump image zoom is invalid style
: Must be an equal-style variable.

Variable for fix adapt is invalid style
: Only equal-style variables can be used.

Variable for fix addforce is invalid style
: Self-explanatory.

Variable for fix aveforce is invalid style
: Only equal-style variables can be used.

Variable for fix deform is invalid style
: The variable must be an equal-style variable.

Variable for fix efield is invalid style
: The variable must be an equal- or atom-style variable.

Variable for fix gravity is invalid style
: Only equal-style variables can be used.

Variable for fix heat is invalid style
: Only equal-style or atom-style variables can be used.

Variable for fix indent is invalid style
: Only equal-style variables can be used.

Variable for fix indent is not equal style
: Only equal-style variables can be used.

Variable for fix langevin is invalid style
: It must be an equal-style variable.

Variable for fix move is invalid style
: Only equal-style variables can be used.

Variable for fix setforce is invalid style
: Only equal-style variables can be used.

Variable for fix temp/berendsen is invalid style
: Only equal-style variables can be used.

Variable for fix temp/csld is invalid style
: Only equal-style variables can be used.

Variable for fix temp/csvr is invalid style
: Only equal-style variables can be used.

Variable for fix temp/rescale is invalid style
: Only equal-style variables can be used.

Variable for fix wall is invalid style
: Only equal-style variables can be used.

Variable for fix wall/reflect is invalid style
: Only equal-style variables can be used.

Variable for fix wall/srd is invalid style
: Only equal-style variables can be used.

Variable for group dynamic is invalid style
: The variable must be an atom-style variable.

Variable for group is invalid style
: Only atom-style variables can be used.

Variable for region cylinder is invalid style
: Only equal-style varaibles are allowed.

Variable for region is invalid style
: Only equal-style variables can be used.

Variable for region is not equal style
: Self-explanatory.

Variable for region sphere is invalid style
: Only equal-style varaibles are allowed.

Variable for restart is invalid style
: Only equal-style variables can be used.

Variable for set command is invalid style
: Only atom-style variables can be used.

Variable for thermo every is invalid style
: Only equal-style variables can be used.

Variable for velocity set is invalid style
: Only atom-style variables can be used.

Variable for voronoi radius is not atom style
: Self-explanatory.

Variable formula compute array is accessed out-of-range
: Self-explanatory.

Variable formula compute vector is accessed out-of-range
: Self-explanatory.

Variable formula fix array is accessed out-of-range
: Self-explanatory.

Variable formula fix vector is accessed out-of-range
: Self-explanatory.

Variable has circular dependency
: A circular dependency is when variable "a" in used by variable "b" and variable "b" is also used by varaible "a". Circular dependencies with longer chains of dependence are also not allowed.

Variable name between brackets must be alphanumeric or underscore characters
: Self-explanatory.

Variable name for compute chunk/atom does not exist
: Self-explanatory.

Variable name for compute reduce does not exist
: Self-explanatory.

Variable name for compute ti does not exist
: Self-explanatory.

Variable name for create_atoms does not exist
: Self-explanatory.

Variable name for displace_atoms does not exist
: Self-explanatory.

Variable name for dump every does not exist
: Self-explanatory.

Variable name for dump image center does not exist
: Self-explanatory.

Variable name for dump image persp does not exist
: Self-explanatory.

Variable name for dump image phi does not exist
: Self-explanatory.

Variable name for dump image theta does not exist
: Self-explanatory.

Variable name for dump image zoom does not exist
: Self-explanatory.

Variable name for fix adapt does not exist
: Self-explanatory.

Variable name for fix addforce does not exist
: Self-explanatory.

Variable name for fix ave/atom does not exist
: Self-explanatory.

Variable name for fix ave/chunk does not exist
: Self-explanatory.

Variable name for fix ave/correlate does not exist
: Self-explanatory.

Variable name for fix ave/histo does not exist

Self-explanatory.

Variable name for fix ave/spatial does not exist

Self-explanatory.

Variable name for fix ave/time does not exist

Self-explanatory.

Variable name for fix aveforce does not exist

Self-explanatory.

Variable name for fix deform does not exist

Self-explantory.

Variable name for fix efield does not exist

Self-explanatory.

Variable name for fix gravity does not exist

Self-explanatory.

Variable name for fix heat does not exist

Self-explanatory.

Variable name for fix indent does not exist

Self-explanatory.

Variable name for fix langevin does not exist

Self-explanatory.

Variable name for fix move does not exist

Self-explanatory.

Variable name for fix setforce does not exist

Self-explanatory.

Variable name for fix store/state does not exist

Self-explanatory.

Variable name for fix temp/berendsen does not exist

Self-explanatory.

Variable name for fix temp/csld does not exist

Self-explanatory.

Variable name for fix temp/csvr does not exist

Self-explanatory.

Variable name for fix temp/rescale does not exist

Self-explanatory.

Variable name for fix vector does not exist

Self-explanatory.

Variable name for fix wall does not exist

Self-explanatory.

Variable name for fix wall/reflect does not exist

Self-explanatory.

Variable name for fix wall/srd does not exist

Self-explanatory.

Variable name for group does not exist

Self-explanatory.

Variable name for group dynamic does not exist

Self-explanatory.

Variable name for region cylinder does not exist

Self-explanatory.

Variable name for region does not exist

Self-explanatory.

Variable name for region sphere does not exist

Self-explanatory.

Variable name for restart does not exist

Self-explanatory.

Variable name for set command does not exist

Self-explanatory.

Variable name for thermo every does not exist

Self-explanatory.

Variable name for velocity set does not exist

Self-explanatory.

Variable name for voronoi radius does not exist

Self-explanatory.

Variable name must be alphanumeric or underscore characters

Self-explanatory.

Variable uses atom property that isn't allocated

Self-explanatory.

Velocity command before simulation box is defined

The velocity command cannot be used before a read_data, read_restart, or create_box command.

Velocity command with no atoms existing

A velocity command has been used, but no atoms yet exist.

Velocity ramp in z for a 2d problem

Self-explanatory.

Velocity rigid used with non-rigid fix-ID

Self-explanatory.

Velocity temperature ID does calculate a velocity bias

The specified compute must compute a bias for temperature.

Velocity temperature ID does not compute temperature

The compute ID given to the velocity command must compute temperature.

Verlet/split can only currently be used with comm_style brick

This is a current restriction in LAMMPS.

Verlet/split does not yet support TIP4P

This is a current limitation.

Verlet/split requires 2 partitions

See the -partition command-line switch.

Verlet/split requires Rspace partition layout be multiple of Kspace partition layout in each dim

This is controlled by the processors command.

Verlet/split requires Rspace partition size be multiple of Kspace partition size

This is so there is an equal number of Rspace processors for every Kspace processor.

Virial was not tallied on needed timestep

You are using a thermo keyword that requires potentials to have tallied the virial, but they didn't on this timestep. See the variable doc page for ideas on how to make this work.

Voro++ error: narea and neigh have a different size

This error is returned by the Voro++ library.

Wall defined twice in fix wall command

Self-explanatory.

Wall defined twice in fix wall/reflect command

Self-explanatory.

Wall defined twice in fix wall/srd command

Self-explanatory.

Water H epsilon must be 0.0 for pair style lj/cut/tip4p/cut

This is because LAMMPS does not compute the Lennard-Jones interactions with these particles for efficiency reasons.

Water H epsilon must be 0.0 for pair style lj/cut/tip4p/long

This is because LAMMPS does not compute the Lennard-Jones interactions with these particles for efficiency reasons.

Water H epsilon must be 0.0 for pair style lj/long/tip4p/long
: This is because LAMMPS does not compute the Lennard-Jones interactions with these particles for efficiency reasons.

World variable count doesn't match # of partitions
: A world-style variable must specify a number of values equal to the number of processor partitions.

Write_data command before simulation box is defined
: Self-explanatory.

Write_restart command before simulation box is defined
: The write_restart command cannot be used before a read_data, read_restart, or create_box command.

Writing to MPI-IO filename when MPIIO package is not installed
: Self-explanatory.

Zero length rotation vector with displace_atoms
: Self-explanatory.

Zero length rotation vector with fix move
: Self-explanatory.

Zero-length lattice orient vector
: Self-explanatory.

Warnings:

Adjusting Coulombic cutoff for MSM, new cutoff = %g
: The adjust/cutoff command is turned on and the Coulombic cutoff has been adjusted to match the user-specified accuracy.

Angle atoms missing at step %ld
: One or more of 3 atoms needed to compute a particular angle are missing on this processor. Typically this is because the pairwise cutoff is set too short or the angle has blown apart and an atom is too far away.

Angle style in data file differs from currently defined angle style
: Self-explanatory.

Atom style in data file differs from currently defined atom style
: Self-explanatory.

Bond atom missing in box size check
: The 2nd atoms needed to compute a particular bond is missing on this processor. Typically this is because the pairwise cutoff is set too short or the bond has blown apart and an atom is too far away.

Bond atom missing in image check
: The 2nd atom in a particular bond is missing on this processor. Typically this is because the pairwise cutoff is set too short or the bond has blown apart and an atom is too far away.

Bond atoms missing at step %ld
: The 2nd atom needed to compute a particular bond is missing on this processor. Typically this is because the pairwise cutoff is set too short or the bond has blown apart and an atom is too far away.

Bond style in data file differs from currently defined bond style
: Self-explanatory.

Bond/angle/dihedral extent > half of periodic box length
: This is a restriction because LAMMPS can be confused about which image of an atom in the bonded interaction is the correct one to use. "Extent" in this context means the maximum end-to-end length of the bond/angle/dihedral. LAMMPS computes this by taking the maximum bond length, multiplying by the number of bonds in the interaction (e.g. 3 for a dihedral) and adding a small amount of stretch.

Both groups in compute group/group have a net charge; the Kspace boundary correction to energy will be non-zero
: Self-explantory.

Calling write_dump before a full system init.
: The write_dump command is used before the system has been fully initialized as part of a 'run' or 'minimize' command. Not all dump styles and features are fully supported at this point and thus the

command may fail or produce incomplete or incorrect output. Insert a "run 0" command, if a full system init is required.

Cannot count rigid body degrees-of-freedom before bodies are fully initialized
This means the temperature associated with the rigid bodies may be incorrect on this timestep.

Cannot count rigid body degrees-of-freedom before bodies are initialized
This means the temperature associated with the rigid bodies may be incorrect on this timestep.

Cannot include log terms without 1/r terms; setting flagHI to 1
Self-explanatory.

Cannot include log terms without 1/r terms; setting flagHI to 1.
Self-explanatory.

Charges are set, but coulombic solver is not used
Self-explanatory.

Charges did not converge at step %ld: %lg
Self-explanatory.

Communication cutoff is too small for SNAP micro load balancing, increased to %lf
Self-explanatory.

Compute cna/atom cutoff may be too large to find ghost atom neighbors
The neighbor cutoff used may not encompass enough ghost atoms to perform this operation correctly.

Computing temperature of portions of rigid bodies
The group defined by the temperature compute does not encompass all the atoms in one or more rigid bodies, so the change in degrees-of-freedom for the atoms in those partial rigid bodies will not be accounted for.

Create_bonds max distance > minimum neighbor cutoff
This means atom pairs for some atom types may not be in the neighbor list and thus no bond can be created between them.

Delete_atoms cutoff > minimum neighbor cutoff
This means atom pairs for some atom types may not be in the neighbor list and thus an atom in that pair cannot be deleted.

Dihedral atoms missing at step %ld
One or more of 4 atoms needed to compute a particular dihedral are missing on this processor. Typically this is because the pairwise cutoff is set too short or the dihedral has blown apart and an atom is too far away.

Dihedral problem
Conformation of the 4 listed dihedral atoms is extreme; you may want to check your simulation geometry.

Dihedral problem: %d %ld %d %d %d %d
Conformation of the 4 listed dihedral atoms is extreme; you may want to check your simulation geometry.

Dihedral style in data file differs from currently defined dihedral style
Self-explanatory.

Dump dcd/xtc timestamp may be wrong with fix dt/reset
If the fix changes the timestep, the dump dcd file will not reflect the change.

Energy tally does not account for 'zero yes'
The energy removed by using the 'zero yes' flag is not accounted for in the energy tally and thus energy conservation cannot be monitored in this case.

Estimated error in splitting of dispersion coeffs is %g
Error is greater than 0.0001 percent.

Ewald/disp Newton solver failed, using old method to estimate g_ewald
Self-explanatory. Choosing a different cutoff value may help.

FENE bond too long
A FENE bond has stretched dangerously far. It's interaction strength will be truncated to attempt to prevent the bond from blowing up.

FENE bond too long: %ld %d %d %g
A FENE bond has stretched dangerously far. It's interaction strength will be truncated to attempt to

prevent the bond from blowing up.

FENE bond too long: %ld %g

A FENE bond has stretched dangerously far. It's interaction strength will be truncated to attempt to prevent the bond from blowing up.

Fix SRD walls overlap but fix srd overlap not set

You likely want to set this in your input script.

Fix bond/swap will ignore defined angles

See the doc page for fix bond/swap for more info on this restriction.

Fix deposit near setting < possible overlap separation %g

This test is performed for finite size particles with a diameter, not for point particles. The near setting is smaller than the particle diameter which can lead to overlaps.

Fix evaporate may delete atom with non-zero molecule ID

This is probably an error, since you should not delete only one atom of a molecule.

Fix gcmc using full_energy option

Fix gcmc has automatically turned on the full_energy option since it is required for systems like the one specified by the user. User input included one or more of the following: kspace, triclinic, a hybrid pair style, an eam pair style, or no "single" function for the pair style.

Fix property/atom mol or charge w/out ghost communication

A model typically needs these properties defined for ghost atoms.

Fix qeq CG convergence failed (%g) after %d iterations at %ld step

Self-explanatory.

Fix qeq has non-zero lower Taper radius cutoff

Absolute value must be <= 0.01.

Fix qeq has very low Taper radius cutoff

Value should typically be >= 5.0.

Fix qeq/dynamic tolerance may be too small for damped dynamics

Self-explanatory.

Fix qeq/fire tolerance may be too small for damped fires

Self-explanatory.

Fix rattle should come after all other integration fixes

This fix is designed to work after all other integration fixes change atom positions. Thus it should be the last integration fix specified. If not, it will not satisfy the desired constraints as well as it otherwise would.

Fix recenter should come after all other integration fixes

Other fixes may change the position of the center-of-mass, so fix recenter should come last.

Fix srd SRD moves may trigger frequent reneighboring

This is because the SRD particles may move long distances.

Fix srd grid size > 1/4 of big particle diameter

This may cause accuracy problems.

Fix srd particle moved outside valid domain

This may indicate a problem with your simulation parameters.

Fix srd particles may move > big particle diameter

This may cause accuracy problems.

Fix srd viscosity < 0.0 due to low SRD density

This may cause accuracy problems.

Fix thermal/conductivity comes before fix ave/spatial

The order of these 2 fixes in your input script is such that fix thermal/conductivity comes first. If you are using fix ave/spatial to measure the temperature profile induced by fix viscosity, then this may cause a glitch in the profile since you are averaging immediately after swaps have occurred. Flipping the order of the 2 fixes typically helps.

Fix viscosity comes before fix ave/spatial

The order of these 2 fixes in your input script is such that fix viscosity comes first. If you are using fix ave/spatial to measure the velocity profile induced by fix viscosity, then this may cause a glitch in the

profile since you are averaging immediately after swaps have occurred. Flipping the order of the 2 fixes typically helps.

Fixes cannot send data in Kokkos communication, switching to classic communication
This is current restriction with Kokkos.

For better accuracy use 'pair_modify table 0'
The user-specified force accuracy cannot be achieved unless the table feature is disabled by using 'pair_modify table 0'.

Geometric mixing assumed for 1/r^6 coefficients
Self-explanatory.

Group for fix_modify temp != fix group
The fix_modify command is specifying a temperature computation that computes a temperature on a different group of atoms than the fix itself operates on. This is probably not what you want to do.

H matrix size has been exceeded: m_fill=%d H.m=%d\n
This is the size of the matrix.

Ignoring unknown or incorrect info command flag
Self-explanatory. An unknown argument was given to the info command. Compare your input with the documentation.

Improper atoms missing at step %ld
One or more of 4 atoms needed to compute a particular improper are missing on this processor. Typically this is because the pairwise cutoff is set too short or the improper has blown apart and an atom is too far away.

Improper problem: %d %ld %d %d %d %d
Conformation of the 4 listed improper atoms is extreme; you may want to check your simulation geometry.

Improper style in data file differs from currently defined improper style
Self-explanatory.

Inconsistent image flags
The image flags for a pair on bonded atoms appear to be inconsistent. Inconsistent means that when the coordinates of the two atoms are unwrapped using the image flags, the two atoms are far apart. Specifically they are further apart than half a periodic box length. Or they are more than a box length apart in a non-periodic dimension. This is usually due to the initial data file not having correct image flags for the 2 atoms in a bond that straddles a periodic boundary. They should be different by 1 in that case. This is a warning because inconsistent image flags will not cause problems for dynamics or most LAMMPS simulations. However they can cause problems when such atoms are used with the fix rigid or replicate commands.

KIM Model does not provide `energy'; Potential energy will be zero
Self-explanatory.

KIM Model does not provide `forces'; Forces will be zero
Self-explanatory.

KIM Model does not provide `particleEnergy'; energy per atom will be zero
Self-explanatory.

KIM Model does not provide `particleVirial'; virial per atom will be zero
Self-explanatory.

Kspace_modify slab param < 2.0 may cause unphysical behavior
The kspace_modify slab parameter should be larger to insure periodic grids padded with empty space do not overlap.

Less insertions than requested
The fix pour command was unsuccessful at finding open space for as many particles as it tried to insert.

Library error in lammps_gather_atoms
This library function cannot be used if atom IDs are not defined or are not consecutively numbered.

Library error in lammps_scatter_atoms
This library function cannot be used if atom IDs are not defined or are not consecutively numbered, or if

no atom map is defined. See the atom_modify command for details about atom maps.

Lost atoms via change_box: original %ld current %ld

The command options you have used caused atoms to be lost.

Lost atoms via displace_atoms: original %ld current %ld

The command options you have used caused atoms to be lost.

Lost atoms: original %ld current %ld

Lost atoms are checked for each time thermo output is done. See the thermo_modify lost command for options. Lost atoms usually indicate bad dynamics, e.g. atoms have been blown far out of the simulation box, or moved futher than one processor's sub-domain away before reneighboring.

MSM mesh too small, increasing to 2 points in each direction

Self-explanatory.

Mismatch between velocity and compute groups

The temperature computation used by the velocity command will not be on the same group of atoms that velocities are being set for.

Mixing forced for lj coefficients

Self-explanatory.

Molecule attributes do not match system attributes

An attribute is specified (e.g. diameter, charge) that is not defined for the specified atom style.

Molecule has bond topology but no special bond settings

This means the bonded atoms will not be excluded in pair-wise interactions.

Molecule template for create_atoms has multiple molecules

The create_atoms command will only create molecules of a single type, i.e. the first molecule in the template.

Molecule template for fix gcmc has multiple molecules

The fix gcmc command will only create molecules of a single type, i.e. the first molecule in the template.

Molecule template for fix shake has multiple molecules

The fix shake command will only recoginze molecules of a single type, i.e. the first molecule in the template.

More than one compute centro/atom

It is not efficient to use compute centro/atom more than once.

More than one compute cluster/atom

It is not efficient to use compute cluster/atom more than once.

More than one compute cna/atom defined

It is not efficient to use compute cna/atom more than once.

More than one compute contact/atom

It is not efficient to use compute contact/atom more than once.

More than one compute coord/atom

It is not efficient to use compute coord/atom more than once.

More than one compute damage/atom

It is not efficient to use compute ke/atom more than once.

More than one compute dilatation/atom

Self-explanatory.

More than one compute erotate/sphere/atom

It is not efficient to use compute erorate/sphere/atom more than once.

More than one compute hexorder/atom

It is not efficient to use compute hexorder/atom more than once.

More than one compute ke/atom

It is not efficient to use compute ke/atom more than once.

More than one compute orientorder/atom

It is not efficient to use compute orientorder/atom more than once.

More than one compute plasticity/atom

Self-explanatory.

More than one compute sna/atom
: Self-explanatory.

More than one compute snad/atom
: Self-explanatory.

More than one compute snav/atom
: Self-explanatory.

More than one fix poems
: It is not efficient to use fix poems more than once.

More than one fix rigid
: It is not efficient to use fix rigid more than once.

Neighbor exclusions used with KSpace solver may give inconsistent Coulombic energies
: This is because excluding specific pair interactions also excludes them from long-range interactions which may not be the desired effect. The special_bonds command handles this consistently by insuring excluded (or weighted) 1-2, 1-3, 1-4 interactions are treated consistently by both the short-range pair style and the long-range solver. This is not done for exclusions of charged atom pairs via the neigh_modify exclude command.

New thermo_style command, previous thermo_modify settings will be lost
: If a thermo_style command is used after a thermo_modify command, the settings changed by the thermo_modify command will be reset to their default values. This is because the thermo_modify commmand acts on the currently defined thermo style, and a thermo_style command creates a new style.

No Kspace calculation with verlet/split
: The 2nd partition performs a kspace calculation so the kspace_style command must be used.

No automatic unit conversion to XTC file format conventions possible for units lj
: This means no scaling will be performed.

No fixes defined, atoms won't move
: If you are not using a fix like nve, nvt, npt then atom velocities and coordinates will not be updated during timestepping.

No joints between rigid bodies, use fix rigid instead
: The bodies defined by fix poems are not connected by joints. POEMS will integrate the body motion, but it would be more efficient to use fix rigid.

Not using real units with pair reax
: This is most likely an error, unless you have created your own ReaxFF parameter file in a different set of units.

Number of MSM mesh points changed to be a multiple of 2
: MSM requires that the number of grid points in each direction be a multiple of two and the number of grid points in one or more directions have been adjusted to meet this requirement.

OMP_NUM_THREADS environment is not set.
: This environment variable must be set appropriately to use the USER-OMP pacakge.

One or more atoms are time integrated more than once
: This is probably an error since you typically do not want to advance the positions or velocities of an atom more than once per timestep.

One or more chunks do not contain all atoms in molecule
: This may not be what you intended.

One or more dynamic groups may not be updated at correct point in timestep
: If there are other fixes that act immediately after the intitial stage of time integration within a timestep (i.e. after atoms move), then the command that sets up the dynamic group should appear after those fixes. This will insure that dynamic group assignements are made after all atoms have moved.

One or more respa levels compute no forces
: This is computationally inefficient.

Pair COMB charge %.10f with force %.10f hit max barrier
: Something is possibly wrong with your model.

Pair COMB charge %.10f with force %.10f hit min barrier

Something is possibly wrong with your model.

Pair brownian needs newton pair on for momentum conservation

Self-explanatory.

Pair dpd needs newton pair on for momentum conservation

Self-explanatory.

Pair dsmc: num_of_collisions > number_of_A

Collision model in DSMC is breaking down.

Pair dsmc: num_of_collisions > number_of_B

Collision model in DSMC is breaking down.

Pair style in data file differs from currently defined pair style

Self-explanatory.

Particle deposition was unsuccessful

The fix deposit command was not able to insert as many atoms as needed. The requested volume fraction may be too high, or other atoms may be in the insertion region.

Proc sub-domain size < neighbor skin, could lead to lost atoms

The decomposition of the physical domain (likely due to load balancing) has led to a processor's sub-domain being smaller than the neighbor skin in one or more dimensions. Since reneighboring is triggered by atoms moving the skin distance, this may lead to lost atoms, if an atom moves all the way across a neighboring processor's sub-domain before reneighboring is triggered.

Reducing PPPM order b/c stencil extends beyond nearest neighbor processor

This may lead to a larger grid than desired. See the kspace_modify overlap command to prevent changing of the PPPM order.

Reducing PPPMDisp Coulomb order b/c stencil extends beyond neighbor processor

This may lead to a larger grid than desired. See the kspace_modify overlap command to prevent changing of the PPPM order.

Reducing PPPMDisp dispersion order b/c stencil extends beyond neighbor processor

This may lead to a larger grid than desired. See the kspace_modify overlap command to prevent changing of the PPPM order.

Replacing a fix, but new group != old group

The ID and style of a fix match for a fix you are changing with a fix command, but the new group you are specifying does not match the old group.

Replicating in a non-periodic dimension

The parameters for a replicate command will cause a non-periodic dimension to be replicated; this may cause unwanted behavior.

Resetting reneighboring criteria during PRD

A PRD simulation requires that neigh_modify settings be delay = 0, every = 1, check = yes. Since these settings were not in place, LAMMPS changed them and will restore them to their original values after the PRD simulation.

Resetting reneighboring criteria during TAD

A TAD simulation requires that neigh_modify settings be delay = 0, every = 1, check = yes. Since these settings were not in place, LAMMPS changed them and will restore them to their original values after the PRD simulation.

Resetting reneighboring criteria during minimization

Minimization requires that neigh_modify settings be delay = 0, every = 1, check = yes. Since these settings were not in place, LAMMPS changed them and will restore them to their original values after the minimization.

Restart file used different # of processors

The restart file was written out by a LAMMPS simulation running on a different number of processors. Due to round-off, the trajectories of your restarted simulation may diverge a little more quickly than if you ran on the same # of processors.

Restart file used different 3d processor grid

The restart file was written out by a LAMMPS simulation running on a different 3d grid of processors.

Due to round-off, the trajectories of your restarted simulation may diverge a little more quickly than if you ran on the same # of processors.

Restart file used different boundary settings, using restart file values

Your input script cannot change these restart file settings.

Restart file used different newton bond setting, using restart file value

The restart file value will override the setting in the input script.

Restart file used different newton pair setting, using input script value

The input script value will override the setting in the restart file.

Restrain problem: %d %ld %d %d %d %d

Conformation of the 4 listed dihedral atoms is extreme; you may want to check your simulation geometry.

Running PRD with only one replica

This is allowed, but you will get no parallel speed-up.

SRD bin shifting turned on due to small lamda

This is done to try to preserve accuracy.

SRD bin size for fix srd differs from user request

Fix SRD had to adjust the bin size to fit the simulation box. See the cubic keyword if you want this message to be an error vs warning.

SRD bins for fix srd are not cubic enough

The bin shape is not within tolerance of cubic. See the cubic keyword if you want this message to be an error vs warning.

SRD particle %d started inside big particle %d on step %ld bounce %d

See the inside keyword if you want this message to be an error vs warning.

SRD particle %d started inside wall %d on step %ld bounce %d

See the inside keyword if you want this message to be an error vs warning.

Shake determinant < 0.0

The determinant of the quadratic equation being solved for a single cluster specified by the fix shake command is numerically suspect. LAMMPS will set it to 0.0 and continue.

Shell command '%s' failed with error '%s'

Self-explanatory.

Shell command returned with non-zero status

This may indicate the shell command did not operate as expected.

Should not allow rigid bodies to bounce off relecting walls

LAMMPS allows this, but their dynamics are not computed correctly.

Should not use fix nve/limit with fix shake or fix rattle

This will lead to invalid constraint forces in the SHAKE/RATTLE computation.

Simulations might be very slow because of large number of structure factors

Self-explanatory.

Slab correction not needed for MSM

Slab correction is intended to be used with Ewald or PPPM and is not needed by MSM.

System is not charge neutral, net charge = %g

The total charge on all atoms on the system is not 0.0. For some KSpace solvers this is only a warning.

Table inner cutoff >= outer cutoff

You specified an inner cutoff for a Coulombic table that is longer than the global cutoff. Probably not what you wanted.

Temperature for MSST is not for group all

User-assigned temperature to MSST fix does not compute temperature for all atoms. Since MSST computes a global pressure, the kinetic energy contribution from the temperature is assumed to also be for all atoms. Thus the pressure used by MSST could be inaccurate.

Temperature for NPT is not for group all

User-assigned temperature to NPT fix does not compute temperature for all atoms. Since NPT computes a global pressure, the kinetic energy contribution from the temperature is assumed to also be for all atoms. Thus the pressure used by NPT could be inaccurate.

Temperature for fix modify is not for group all

The temperature compute is being used with a pressure calculation which does operate on group all, so this may be inconsistent.

Temperature for thermo pressure is not for group all

User-assigned temperature to thermo via the thermo_modify command does not compute temperature for all atoms. Since thermo computes a global pressure, the kinetic energy contribution from the temperature is assumed to also be for all atoms. Thus the pressure printed by thermo could be inaccurate.

The fix ave/spatial command has been replaced by the more flexible fix ave/chunk and compute chunk/atom commands -- fix ave/spatial will be removed in the summer of 2015

Self-explanatory.

The minimizer does not re-orient dipoles when using fix efield

This means that only the atom coordinates will be minimized, not the orientation of the dipoles.

Too many common neighbors in CNA %d times

More than the maximum # of neighbors was found multiple times. This was unexpected.

Too many inner timesteps in fix ttm

Self-explanatory.

Too many neighbors in CNA for %d atoms

More than the maximum # of neighbors was found multiple times. This was unexpected.

Triclinic box skew is large

The displacement in a skewed direction is normally required to be less than half the box length in that dimension. E.g. the xy tilt must be between -half and +half of the x box length. You have relaxed the constraint using the box tilt command, but the warning means that a LAMMPS simulation may be inefficient as a result.

Use special bonds = 0,1,1 with bond style fene

Most FENE models need this setting for the special_bonds command.

Use special bonds = 0,1,1 with bond style fene/expand

Most FENE models need this setting for the special_bonds command.

Using a manybody potential with bonds/angles/dihedrals and special_bond exclusions

This is likely not what you want to do. The exclusion settings will eliminate neighbors in the neighbor list, which the manybody potential needs to calculated its terms correctly.

Using compute temp/deform with inconsistent fix deform remap option

Fix nvt/sllod assumes deforming atoms have a velocity profile provided by "remap v" or "remap none" as a fix deform option.

Using compute temp/deform with no fix deform defined

This is probably an error, since it makes little sense to use compute temp/deform in this case.

Using fix srd with box deformation but no SRD thermostat

The deformation will heat the SRD particles so this can be dangerous.

Using kspace solver on system with no charge

Self-explanatory.

Using largest cut-off for lj/long/dipole/long long long

Self-explanatory.

Using largest cutoff for buck/long/coul/long

Self-exlanatory.

Using largest cutoff for lj/long/coul/long

Self-explanatory.

Using largest cutoff for pair_style lj/long/tip4p/long

Self-explanatory.

Using package gpu without any pair style defined

Self-explanatory.

Using pair potential shift with pair_modify compute no

The shift effects will thus not be computed.

Using pair tail corrections with nonperiodic system

This is probably a bogus thing to do, since tail corrections are computed by integrating the density of a periodic system out to infinity.

Using pair tail corrections with pair_modify compute no

The tail corrections will thus not be computed.

pair style reax is now deprecated and will soon be retired. Users should switch to pair_style reax/c

Self-explanatory.

13. Future and history

This section lists features we plan to add to LAMMPS, features of previous versions of LAMMPS, and features of other parallel molecular dynamics codes our group has distributed.

13.1 Coming attractions

The Wish list link on the LAMMPS WWW page gives a list of features we are hoping to add to LAMMPS in the future, including contact names of individuals you can email if you are interested in contributing to the developement or would be a future user of that feature.

You can also send email to the developers if you want to add your wish to the list.

13.2 Past versions

LAMMPS development began in the mid 1990s under a cooperative research & development agreement (CRADA) between two DOE labs (Sandia and LLNL) and 3 companies (Cray, Bristol Myers Squibb, and Dupont). The goal was to develop a large-scale parallel classical MD code; the coding effort was led by Steve Plimpton at Sandia.

After the CRADA ended, a final F77 version, LAMMPS 99, was released. As development of LAMMPS continued at Sandia, its memory management was converted to F90; a final F90 version was released as LAMMPS 2001.

The current LAMMPS is a rewrite in C++ and was first publicly released as an open source code in 2004. It includes many new features beyond those in LAMMPS 99 or 2001. It also includes features from older parallel MD codes written at Sandia, namely ParaDyn, Warp, and GranFlow (see below).

In late 2006 we began merging new capabilities into LAMMPS that were developed by Aidan Thompson at Sandia for his MD code GRASP, which has a parallel framework similar to LAMMPS. Most notably, these have included many-body potentials - Stillinger-Weber, Tersoff, ReaxFF - and the associated charge-equilibration routines needed for ReaxFF.

The History link on the LAMMPS WWW page gives a timeline of features added to the C++ open-source version of LAMMPS over the last several years.

These older codes are available for download from the LAMMPS WWW site, except for Warp & GranFlow which were primarily used internally. A brief listing of their features is given here.

LAMMPS 2001

- F90 + MPI
- dynamic memory
- spatial-decomposition parallelism
- NVE, NVT, NPT, NPH, rRESPA integrators

- LJ and Coulombic pairwise force fields
- all-atom, united-atom, bead-spring polymer force fields
- CHARMM-compatible force fields
- class 2 force fields
- 3d/2d Ewald & PPPM
- various force and temperature constraints
- SHAKE
- Hessian-free truncated-Newton minimizer
- user-defined diagnostics

LAMMPS 99

- F77 + MPI
- static memory allocation
- spatial-decomposition parallelism
- most of the LAMMPS 2001 features with a few exceptions
- no 2d Ewald & PPPM
- molecular force fields are missing a few CHARMM terms
- no SHAKE

Warp

- F90 + MPI
- spatial-decomposition parallelism
- embedded atom method (EAM) metal potentials + LJ
- lattice and grain-boundary atom creation
- NVE, NVT integrators
- boundary conditions for applying shear stresses
- temperature controls for actively sheared systems
- per-atom energy and centro-symmetry computation and output

ParaDyn

- F77 + MPI
- atom- and force-decomposition parallelism
- embedded atom method (EAM) metal potentials
- lattice atom creation
- NVE, NVT, NPT integrators
- all serial DYNAMO features for controls and constraints

GranFlow

- F90 + MPI
- spatial-decomposition parallelism
- frictional granular potentials
- NVE integrator
- boundary conditions for granular flow and packing and walls
- particle insertion

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5.3.1 USER-CUDA package

The USER-CUDA package was developed by Christian Trott (Sandia) while at U Technology Ilmenau in Germany. It provides NVIDIA GPU versions of many pair styles, many fixes, a few computes, and for long-range Coulombics via the PPPM command. It has the following general features:

- The package is designed to allow an entire LAMMPS calculation, for many timesteps, to run entirely on the GPU (except for inter-processor MPI communication), so that atom-based data (e.g. coordinates, forces) do not have to move back-and-forth between the CPU and GPU.
- The speed-up advantage of this approach is typically better when the number of atoms per GPU is large
- Data will stay on the GPU until a timestep where a non-USER-CUDA fix or compute is invoked. Whenever a non-GPU operation occurs (fix, compute, output), data automatically moves back to the CPU as needed. This may incur a performance penalty, but should otherwise work transparently.
- Neighbor lists are constructed on the GPU.
- The package only supports use of a single MPI task, running on a single CPU (core), assigned to each GPU.

Here is a quick overview of how to use the USER-CUDA package:

- build the library in lib/cuda for your GPU hardware with desired precision
- include the USER-CUDA package and build LAMMPS
- use the mpirun command to specify 1 MPI task per GPU (on each node)
- enable the USER-CUDA package via the "-c on" command-line switch
- specify the # of GPUs per node
- use USER-CUDA styles in your input script

The latter two steps can be done using the "-pk cuda" and "-sf cuda" command-line switches respectively. Or the effect of the "-pk" or "-sf" switches can be duplicated by adding the package cuda or suffix cuda commands respectively to your input script.

Required hardware/software:

To use this package, you need to have one or more NVIDIA GPUs and install the NVIDIA Cuda software on your system:

Your NVIDIA GPU needs to support Compute Capability 1.3. This list may help you to find out the Compute Capability of your card:

http://en.wikipedia.org/wiki/Comparison_of_Nvidia_graphics_processing_units

Install the Nvidia Cuda Toolkit (version 3.2 or higher) and the corresponding GPU drivers. The Nvidia Cuda SDK is not required, but we recommend it also be installed. You can then make sure its sample projects can be compiled without problems.

Building LAMMPS with the USER-CUDA package:

This requires two steps (a,b): build the USER-CUDA library, then build LAMMPS with the USER-CUDA package.

You can do both these steps in one line, using the src/Make.py script, described in Section 2.4 of the manual. Type "Make.py -h" for help. If run from the src directory, this command will create src/lmp_cuda using src/MAKE/Makefile.mpi as the starting Makefile.machine:

```
Make.py -p cuda -cuda mode=single arch=20 -o cuda -a lib-cuda file mpi
```

Or you can follow these two (a,b) steps:

(a) Build the USER-CUDA library

The USER-CUDA library is in lammps/lib/cuda. If your *CUDA* toolkit is not installed in the default system directoy */usr/local/cuda* edit the file *lib/cuda/Makefile.common* accordingly.

To build the library with the settings in lib/cuda/Makefile.default, simply type:

```
make
```

To set options when the library is built, type "make OPTIONS", where *OPTIONS* are one or more of the following. The settings will be written to the *lib/cuda/Makefile.defaults* before the build.

```
precision=N to set the precision level
  N = 1 for single precision (default)
  N = 2 for double precision
  N = 3 for positions in double precision
  N = 4 for positions and velocities in double precision
arch=M to set GPU compute capability
  M = 35 for Kepler GPUs
  M = 20 for CC2.0 (GF100/110, e.g. C2050,GTX580,GTX470) (default)
  M = 21 for CC2.1 (GF104/114,  e.g. GTX560, GTX460, GTX450)
  M = 13 for CC1.3 (GF200, e.g. C1060, GTX285)
prec_timer=0/1 to use hi-precision timers
  0 = do not use them (default)
  1 = use them
  this is usually only useful for Mac machines
dbg=0/1 to activate debug mode
  0 = no debug mode (default)
  1 = yes debug mode
  this is only useful for developers
cufft=1 for use of the CUDA FFT library
  0 = no CUFFT support (default)
  in the future other CUDA-enabled FFT libraries might be supported
```

If the build is successful, it will produce the files liblammpscuda.a and Makefile.lammps.

Note that if you change any of the options (like precision), you need to re-build the entire library. Do a "make clean" first, followed by "make".

(b) Build LAMMPS with the USER-CUDA package

```
cd lammps/src
make yes-user-cuda
make machine
```

No additional compile/link flags are needed in Makefile.machine.

Note that if you change the USER-CUDA library precision (discussed above) and rebuild the USER-CUDA library, then you also need to re-install the USER-CUDA package and re-build LAMMPS, so that all affected

files are re-compiled and linked to the new USER-CUDA library.

Run with the USER-CUDA package from the command line:

The mpirun or mpiexec command sets the total number of MPI tasks used by LAMMPS (one or multiple per compute node) and the number of MPI tasks used per node. E.g. the mpirun command in MPICH does this via its -np and -ppn switches. Ditto for OpenMPI via -np and -npernode.

When using the USER-CUDA package, you must use exactly one MPI task per physical GPU.

You must use the "-c on" command-line switch to enable the USER-CUDA package. The "-c on" switch also issues a default package cuda 1 command which sets various USER-CUDA options to default values, as discussed on the package command doc page.

Use the "-sf cuda" command-line switch, which will automatically append "cuda" to styles that support it. Use the "-pk cuda Ng" command-line switch to set Ng = # of GPUs per node to a different value than the default set by the "-c on" switch (1 GPU) or change other package cuda options.

```
lmp_machine -c on -sf cuda -pk cuda 1 -in in.script                       # 1 MPI task uses 1 GPU
mpirun -np 2 lmp_machine -c on -sf cuda -pk cuda 2 -in in.script          # 2 MPI tasks use 2 GPUs o
mpirun -np 24 -ppn 2 lmp_machine -c on -sf cuda -pk cuda 2 -in in.script  # ditto on 12 16-core node
```

The syntax for the "-pk" switch is the same as same as the "package cuda" command. See the package command doc page for details, including the default values used for all its options if it is not specified.

Note that the default for the package cuda command is to set the Newton flag to "off" for both pairwise and bonded interactions. This typically gives fastest performance. If the newton command is used in the input script, it can override these defaults.

Or run with the USER-CUDA package by editing an input script:

The discussion above for the mpirun/mpiexec command and the requirement of one MPI task per GPU is the same.

You must still use the "-c on" command-line switch to enable the USER-CUDA package.

Use the suffix cuda command, or you can explicitly add a "cuda" suffix to individual styles in your input script, e.g.

```
pair_style lj/cut/cuda 2.5
```

You only need to use the package cuda command if you wish to change any of its option defaults, including the number of GPUs/node (default = 1), as set by the "-c on" command-line switch.

Speed-ups to expect:

The performance of a GPU versus a multi-core CPU is a function of your hardware, which pair style is used, the number of atoms/GPU, and the precision used on the GPU (double, single, mixed).

See the Benchmark page of the LAMMPS web site for performance of the USER-CUDA package on different hardware.

Guidelines for best performance:

- The USER-CUDA package offers more speed-up relative to CPU performance when the number of atoms per GPU is large, e.g. on the order of tens or hundreds of 1000s.
- As noted above, this package will continue to run a simulation entirely on the GPU(s) (except for inter-processor MPI communication), for multiple timesteps, until a CPU calculation is required, either by a fix or compute that is non-GPU-ized, or until output is performed (thermo or dump snapshot or restart file). The less often this occurs, the faster your simulation will run.

Restrictions:

None.

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5.3.2 GPU package

The GPU package was developed by Mike Brown at ORNL and his collaborators, particularly Trung Nguyen (ORNL). It provides GPU versions of many pair styles, including the 3-body Stillinger-Weber pair style, and for kspace_style pppm for long-range Coulombics. It has the following general features:

- It is designed to exploit common GPU hardware configurations where one or more GPUs are coupled to many cores of one or more multi-core CPUs, e.g. within a node of a parallel machine.
- Atom-based data (e.g. coordinates, forces) moves back-and-forth between the CPU(s) and GPU every timestep.
- Neighbor lists can be built on the CPU or on the GPU
- The charge assignement and force interpolation portions of PPPM can be run on the GPU. The FFT portion, which requires MPI communication between processors, runs on the CPU.
- Asynchronous force computations can be performed simultaneously on the CPU(s) and GPU.
- It allows for GPU computations to be performed in single or double precision, or in mixed-mode precision, where pairwise forces are computed in single precision, but accumulated into double-precision force vectors.
- LAMMPS-specific code is in the GPU package. It makes calls to a generic GPU library in the lib/gpu directory. This library provides NVIDIA support as well as more general OpenCL support, so that the same functionality can eventually be supported on a variety of GPU hardware.

Here is a quick overview of how to use the GPU package:

- build the library in lib/gpu for your GPU hardware wity desired precision
- include the GPU package and build LAMMPS
- use the mpirun command to set the number of MPI tasks/node which determines the number of MPI tasks/GPU
- specify the # of GPUs per node
- use GPU styles in your input script

The latter two steps can be done using the "-pk gpu" and "-sf gpu" command-line switches respectively. Or the effect of the "-pk" or "-sf" switches can be duplicated by adding the package gpu or suffix gpu commands respectively to your input script.

Required hardware/software:

To use this package, you currently need to have an NVIDIA GPU and install the NVIDIA Cuda software on your system:

- Check if you have an NVIDIA GPU: cat /proc/driver/nvidia/gpus/0/information
- Go to http://www.nvidia.com/object/cuda_get.html
- Install a driver and toolkit appropriate for your system (SDK is not necessary)
- Run lammps/lib/gpu/nvc_get_devices (after building the GPU library, see below) to list supported devices and properties

Building LAMMPS with the GPU package:

This requires two steps (a,b): build the GPU library, then build LAMMPS with the GPU package.

You can do both these steps in one line, using the src/Make.py script, described in Section 2.4 of the manual. Type "Make.py -h" for help. If run from the src directory, this command will create src/lmp_gpu using src/MAKE/Makefile.mpi as the starting Makefile.machine:

```
Make.py -p gpu -gpu mode=single arch=31 -o gpu -a lib-gpu file mpi
```

Or you can follow these two (a,b) steps:

(a) Build the GPU library

The GPU library is in lammps/lib/gpu. Select a Makefile.machine (in lib/gpu) appropriate for your system. You should pay special attention to 3 settings in this makefile.

- CUDA_HOME = needs to be where NVIDIA Cuda software is installed on your system
- CUDA_ARCH = needs to be appropriate to your GPUs
- CUDA_PREC = precision (double, mixed, single) you desire

See lib/gpu/Makefile.linux.double for examples of the ARCH settings for different GPU choices, e.g. Fermi vs Kepler. It also lists the possible precision settings:

```
CUDA_PREC = -D_SINGLE_SINGLE  # single precision for all calculations
CUDA_PREC = -D_DOUBLE_DOUBLE  # double precision for all calculations
CUDA_PREC = -D_SINGLE_DOUBLE  # accumulation of forces, etc, in double
```

The last setting is the mixed mode referred to above. Note that your GPU must support double precision to use either the 2nd or 3rd of these settings.

To build the library, type:

```
make -f Makefile.machine
```

If successful, it will produce the files libgpu.a and Makefile.lammps.

The latter file has 3 settings that need to be appropriate for the paths and settings for the CUDA system software on your machine. Makefile.lammps is a copy of the file specified by the EXTRAMAKE setting in Makefile.machine. You can change EXTRAMAKE or create your own Makefile.lammps.machine if needed.

Note that to change the precision of the GPU library, you need to re-build the entire library. Do a "clean" first, e.g. "make -f Makefile.linux clean", followed by the make command above.

(b) Build LAMMPS with the GPU package

```
cd lammps/src
make yes-gpu
make machine
```

No additional compile/link flags are needed in Makefile.machine.

Note that if you change the GPU library precision (discussed above) and rebuild the GPU library, then you also need to re-install the GPU package and re-build LAMMPS, so that all affected files are re-compiled and linked to the new GPU library.

Run with the GPU package from the command line:

The mpirun or mpiexec command sets the total number of MPI tasks used by LAMMPS (one or multiple per compute node) and the number of MPI tasks used per node. E.g. the mpirun command in MPICH does this via its -np and -ppn switches. Ditto for OpenMPI via -np and -npernode.

When using the GPU package, you cannot assign more than one GPU to a single MPI task. However multiple MPI tasks can share the same GPU, and in many cases it will be more efficient to run this way. Likewise it may be more efficient to use less MPI tasks/node than the available # of CPU cores. Assignment of multiple MPI tasks to a GPU will happen automatically if you create more MPI tasks/node than there are GPUs/mode. E.g. with 8 MPI tasks/node and 2 GPUs, each GPU will be shared by 4 MPI tasks.

Use the "-sf gpu" command-line switch, which will automatically append "gpu" to styles that support it. Use the "-pk gpu Ng" command-line switch to set Ng = # of GPUs/node to use.

```
lmp_machine -sf gpu -pk gpu 1 -in in.script                         # 1 MPI task uses 1 GPU
mpirun -np 12 lmp_machine -sf gpu -pk gpu 2 -in in.script           # 12 MPI tasks share 2 GPUs on a
mpirun -np 48 -ppn 12 lmp_machine -sf gpu -pk gpu 2 -in in.script   # ditto on 4 16-core nodes
```

Note that if the "-sf gpu" switch is used, it also issues a default package gpu 1 command, which sets the number of GPUs/node to 1.

Using the "-pk" switch explicitly allows for setting of the number of GPUs/node to use and additional options. Its syntax is the same as same as the "package gpu" command. See the package command doc page for details, including the default values used for all its options if it is not specified.

Note that the default for the package gpu command is to set the Newton flag to "off" pairwise interactions. It does not affect the setting for bonded interactions (LAMMPS default is "on"). The "off" setting for pairwise interaction is currently required for GPU package pair styles.

Or run with the GPU package by editing an input script:

The discussion above for the mpirun/mpiexec command, MPI tasks/node, and use of multiple MPI tasks/GPU is the same.

Use the suffix gpu command, or you can explicitly add an "gpu" suffix to individual styles in your input script, e.g.

```
pair_style lj/cut/gpu 2.5
```

You must also use the package gpu command to enable the GPU package, unless the "-sf gpu" or "-pk gpu" command-line switches were used. It specifies the number of GPUs/node to use, as well as other options.

Speed-ups to expect:

The performance of a GPU versus a multi-core CPU is a function of your hardware, which pair style is used, the number of atoms/GPU, and the precision used on the GPU (double, single, mixed).

See the Benchmark page of the LAMMPS web site for performance of the GPU package on various hardware, including the Titan HPC platform at ORNL.

You should also experiment with how many MPI tasks per GPU to use to give the best performance for your problem and machine. This is also a function of the problem size and the pair style being using. Likewise, you should experiment with the precision setting for the GPU library to see if single or mixed precision will give accurate results, since they will typically be faster.

Guidelines for best performance:

- Using multiple MPI tasks per GPU will often give the best performance, as allowed my most multi-core CPU/GPU configurations.
- If the number of particles per MPI task is small (e.g. 100s of particles), it can be more efficient to run with fewer MPI tasks per GPU, even if you do not use all the cores on the compute node.
- The package gpu command has several options for tuning performance. Neighbor lists can be built on the GPU or CPU. Force calculations can be dynamically balanced across the CPU cores and GPUs. GPU-specific settings can be made which can be optimized for different hardware. See the packakge command doc page for details.
- As described by the package gpu command, GPU accelerated pair styles can perform computations asynchronously with CPU computations. The "Pair" time reported by LAMMPS will be the maximum of the time required to complete the CPU pair style computations and the time required to complete the GPU pair style computations. Any time spent for GPU-enabled pair styles for computations that run simultaneously with bond, angle, dihedral, improper, and long-range calculations will not be included in the "Pair" time.
- When the *mode* setting for the package gpu command is force/neigh, the time for neighbor list calculations on the GPU will be added into the "Pair" time, not the "Neigh" time. An additional breakdown of the times required for various tasks on the GPU (data copy, neighbor calculations, force computations, etc) are output only with the LAMMPS screen output (not in the log file) at the end of each run. These timings represent total time spent on the GPU for each routine, regardless of asynchronous CPU calculations.
- The output section "GPU Time Info (average)" reports "Max Mem / Proc". This is the maximum memory used at one time on the GPU for data storage by a single MPI process.

Restrictions:

None.

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5.3.3 USER-INTEL package

The USER-INTEL package was developed by Mike Brown at Intel Corporation. It provides two methods for accelerating simulations, depending on the hardware you have. The first is acceleration on Intel(R) CPUs by running in single, mixed, or double precision with vectorization. The second is acceleration on Intel(R) Xeon Phi(TM) coprocessors via offloading neighbor list and non-bonded force calculations to the Phi. The same C++ code is used in both cases. When offloading to a coprocessor from a CPU, the same routine is run twice, once on the CPU and once with an offload flag.

Note that the USER-INTEL package supports use of the Phi in "offload" mode, not "native" mode like the KOKKOS package.

Also note that the USER-INTEL package can be used in tandem with the USER-OMP package. This is useful when offloading pair style computations to the Phi, so that other styles not supported by the USER-INTEL package, e.g. bond, angle, dihedral, improper, and long-range electrostatics, can run simultaneously in threaded mode on the CPU cores. Since less MPI tasks than CPU cores will typically be invoked when running with coprocessors, this enables the extra CPU cores to be used for useful computation.

As illustrated below, if LAMMPS is built with both the USER-INTEL and USER-OMP packages, this dual mode of operation is made easier to use, via the "-suffix hybrid intel omp" command-line switch or the suffix hybrid intel omp command. Both set a second-choice suffix to "omp" so that styles from the USER-INTEL package will be used if available, with styles from the USER-OMP package as a second choice.

Here is a quick overview of how to use the USER-INTEL package for CPU acceleration, assuming one or more 16-core nodes. More details follow.

```
use an Intel compiler
use these CCFLAGS settings in Makefile.machine: -fopenmp, -DLAMMPS_MEMALIGN=64, -restrict, -xHost, -
use these LINKFLAGS settings in Makefile.machine: -fopenmp, -xHost
make yes-user-intel yes-user-omp     # including user-omp is optional
make mpi                             # build with the USER-INTEL package, if settings (including com
make intel_cpu                       # or Makefile.intel_cpu already has settings, uses Intel MPI wr
Make.py -v -p intel omp -intel cpu -a file mpich_icc   # or one-line build via Make.py for MPICH
Make.py -v -p intel omp -intel cpu -a file ompi_icc    # or for OpenMPI
Make.py -v -p intel omp -intel cpu -a file intel_cpu   # or for Intel MPI wrapper

lmp_machine -sf intel -pk intel 0 omp 16 -in in.script    # 1 node, 1 MPI task/node, 16 threads/task
mpirun -np 32 lmp_machine -sf intel -in in.script         # 2 nodess, 16 MPI tasks/node, no threads,
lmp_machine -sf hybrid intel omp -pk intel 0 omp 16 -pk omp 16 -in in.script         # 1 node, 1 MPI
mpirun -np 32 -ppn 4 lmp_machine -sf hybrid intel omp -pk omp 4 -pk omp 4 -in in.script      # 8 nod
```

Here is a quick overview of how to use the USER-INTEL package for the same CPUs as above (16 cores/node), with an additional Xeon Phi(TM) coprocessor per node. More details follow.

```
Same as above for building, with these additions/changes:
add the flag -DLMP_INTEL_OFFLOAD to CCFLAGS in Makefile.machine
add the flag -offload to LINKFLAGS in Makefile.machine
for Make.py change "-intel cpu" to "-intel phi", and "file intel_cpu" to "file intel_phi"

mpirun -np 32 lmp_machine -sf intel -pk intel 1 -in in.script                # 2 nodes, 16 MPI task
mpirun -np 16 -ppn 8 lmp_machine -sf intel -pk intel 1 omp 2 -in in.script           # 2 nodes, 8 M
mpirun -np 32 -ppn 8 lmp_machine -sf hybrid intel omp -pk intel 1 omp 2 -pk omp 2 -in in.script # 4
```

Required hardware/software:

Your compiler must support the OpenMP interface. Use of an Intel(R) C++ compiler is recommended, but not required. However, g++ will not recognize some of the settings listed above, so they cannot be used. Optimizations for vectorization have only been tested with the Intel(R) compiler. Use of other compilers may not result in vectorization, or give poor performance.

The recommended version of the Intel(R) compiler is 14.0.1.106. Versions 15.0.1.133 and later are also supported. If using Intel(R) MPI, versions 15.0.2.044 and later are recommended.

To use the offload option, you must have one or more Intel(R) Xeon Phi(TM) coprocessors and use an Intel(R) C++ compiler.

Building LAMMPS with the USER-INTEL package:

The lines above illustrate how to include/build with the USER-INTEL package, for either CPU or Phi support, in two steps, using the "make" command. Or how to do it with one command via the src/Make.py script, described in Section 2.4 of the manual. Type "Make.py -h" for help. Because the mechanism for specifing what compiler to use (Intel in this case) is different for different MPI wrappers, 3 versions of the Make.py command are shown.

Note that if you build with support for a Phi coprocessor, the same binary can be used on nodes with or without coprocessors installed. However, if you do not have coprocessors on your system, building without offload support will produce a smaller binary.

If you also build with the USER-OMP package, you can use styles from both packages, as described below.

Note that the CCFLAGS and LINKFLAGS settings in Makefile.machine must include "-fopenmp". Likewise, if you use an Intel compiler, the CCFLAGS setting must include "-restrict". For Phi support, the "-DLMP_INTEL_OFFLOAD" (CCFLAGS) and "-offload" (LINKFLAGS) settings are required. The other settings listed above are optional, but will typically improve performance. The Make.py command will add all of these automatically.

If you are compiling on the same architecture that will be used for the runs, adding the flag *-xHost* to CCFLAGS enables vectorization with the Intel(R) compiler. Otherwise, you must provide the correct compute node architecture to the -x option (e.g. -xAVX).

Example machines makefiles Makefile.intel_cpu and Makefile.intel_phi are included in the src/MAKE/OPTIONS directory with settings that perform well with the Intel(R) compiler. The latter has support for offload to Phi coprocessors; the former does not.

Run with the USER-INTEL package from the command line:

The mpirun or mpiexec command sets the total number of MPI tasks used by LAMMPS (one or multiple per compute node) and the number of MPI tasks used per node. E.g. the mpirun command in MPICH does this via its -np and -ppn switches. Ditto for OpenMPI via -np and -npernode.

If you compute (any portion of) pairwise interactions using USER-INTEL pair styles on the CPU, or use USER-OMP styles on the CPU, you need to choose how many OpenMP threads per MPI task to use. If both packages are used, it must be done for both packages, and the same thread count value should be used for both. Note that the product of MPI tasks * threads/task should not exceed the physical number of cores (on a node), otherwise performance will suffer.

When using the USER-INTEL package for the Phi, you also need to specify the number of coprocessor/node and optionally the number of coprocessor threads per MPI task to use. Note that coprocessor threads (which run on the coprocessor) are totally independent from OpenMP threads (which run on the CPU). The default values for the settings that affect coprocessor threads are typically fine, as discussed below.

As in the lines above, use the "-sf intel" or "-sf hybrid intel omp" command-line switch, which will automatically append "intel" to styles that support it. In the second case, "omp" will be appended if an "intel" style does not exist.

Note that if either switch is used, it also invokes a default command: package intel 1. If the "-sf hybrid intel omp" switch is used, the default USER-OMP command package omp 0 is also invoked (if LAMMPS was built with USER-OMP). Both set the number of OpenMP threads per MPI task via the OMP_NUM_THREADS environment variable. The first command sets the number of Xeon Phi(TM) coprocessors/node to 1 (ignored if USER-INTEL is built for CPU-only), and the precision mode to "mixed" (default value).

You can also use the "-pk intel Nphi" command-line switch to explicitly set Nphi = # of Xeon Phi(TM) coprocessors/node, as well as additional options. Nphi should be >= 1 if LAMMPS was built with coprocessor support, otherswise Nphi = 0 for a CPU-only build. All the available coprocessor threads on each Phi will be divided among MPI tasks, unless the *tptask* option of the "-pk intel" command-line switch is used to limit the coprocessor threads per MPI task. See the package intel command for details, including the default values used for all its options if not specified, and how to set the number of OpenMP threads via the OMP_NUM_THREADS environment variable if desired.

If LAMMPS was built with the USER-OMP package, you can also use the "-pk omp Nt" command-line switch to explicitly set Nt = # of OpenMP threads per MPI task to use, as well as additional options. Nt should be the same threads per MPI task as set for the USER-INTEL package, e.g. via the "-pk intel Nphi omp Nt" command. Again, see the package omp command for details, including the default values used for all its options if not specified, and how to set the number of OpenMP threads via the OMP_NUM_THREADS environment variable if desired.

Or run with the USER-INTEL package by editing an input script:

The discussion above for the mpirun/mpiexec command, MPI tasks/node, OpenMP threads per MPI task, and coprocessor threads per MPI task is the same.

Use the suffix intel or suffix hybrid intel omp commands, or you can explicitly add an "intel" or "omp" suffix to individual styles in your input script, e.g.

```
pair_style lj/cut/intel 2.5
```

You must also use the package intel command, unless the "-sf intel" or "-pk intel" command-line switches were used. It specifies how many coprocessors/node to use, as well as other OpenMP threading and coprocessor options. The package doc page explains how to set the number of OpenMP threads via an environment variable if desired.

If LAMMPS was also built with the USER-OMP package, you must also use the package omp command to enable that package, unless the "-sf hybrid intel omp" or "-pk omp" command-line switches were used. It specifies how many OpenMP threads per MPI task to use (should be same as the setting for the USER-INTEL package), as well as other options. Its doc page explains how to set the number of OpenMP threads via an environment variable if desired.

Speed-ups to expect:

If LAMMPS was not built with coprocessor support (CPU only) when including the USER-INTEL package, then acclerated styles will run on the CPU using vectorization optimizations and the specified precision. This may give a substantial speed-up for a pair style, particularly if mixed or single precision is used.

If LAMMPS was built with coproccesor support, the pair styles will run on one or more Intel(R) Xeon Phi(TM) coprocessors (per node). The performance of a Xeon Phi versus a multi-core CPU is a function of your hardware, which pair style is used, the number of atoms/coprocessor, and the precision used on the coprocessor (double, single, mixed).

See the Benchmark page of the LAMMPS web site for performance of the USER-INTEL package on different hardware.

NOTE: Setting core affinity is often used to pin MPI tasks and OpenMP threads to a core or group of cores so that memory access can be uniform. Unless disabled at build time, affinity for MPI tasks and OpenMP threads on the host (CPU) will be set by default on the host when using offload to a coprocessor. In this case, it is unnecessary to use other methods to control affinity (e.g. taskset, numactl, I_MPI_PIN_DOMAIN, etc.). This can be disabled in an input script with the *no_affinity* option to the package intel command or by disabling the option at build time (by adding -DINTEL_OFFLOAD_NOAFFINITY to the CCFLAGS line of your Makefile). Disabling this option is not recommended, especially when running on a machine with hyperthreading disabled.

Guidelines for best performance on an Intel(R) Xeon Phi(TM) coprocessor:

- The default for the package intel command is to have all the MPI tasks on a given compute node use a single Xeon Phi(TM) coprocessor. In general, running with a large number of MPI tasks on each node will perform best with offload. Each MPI task will automatically get affinity to a subset of the hardware threads available on the coprocessor. For example, if your card has 61 cores, with 60 cores available for offload and 4 hardware threads per core (240 total threads), running with 24 MPI tasks per node will cause each MPI task to use a subset of 10 threads on the coprocessor. Fine tuning of the number of threads to use per MPI task or the number of threads to use per core can be accomplished with keyword settings of the package intel command.
- If desired, only a fraction of the pair style computation can be offloaded to the coprocessors. This is accomplished by using the *balance* keyword in the package intel command. A balance of 0 runs all calculations on the CPU. A balance of 1 runs all calculations on the coprocessor. A balance of 0.5 runs half of the calculations on the coprocessor. Setting the balance to -1 (the default) will enable dynamic load balancing that continously adjusts the fraction of offloaded work throughout the simulation. This option typically produces results within 5 to 10 percent of the optimal fixed balance.
- When using offload with CPU hyperthreading disabled, it may help performance to use fewer MPI tasks and OpenMP threads than available cores. This is due to the fact that additional threads are generated internally to handle the asynchronous offload tasks.
- If running short benchmark runs with dynamic load balancing, adding a short warm-up run (10-20 steps) will allow the load-balancer to find a near-optimal setting that will carry over to additional runs.
- If pair computations are being offloaded to an Intel(R) Xeon Phi(TM) coprocessor, a diagnostic line is printed to the screen (not to the log file), during the setup phase of a run, indicating that offload mode is being used and indicating the number of coprocessor threads per MPI task. Additionally, an offload timing summary is printed at the end of each run. When offloading, the frequency for atom sorting is changed to 1 so that the per-atom data is effectively sorted at every rebuild of the neighbor lists.
- For simulations with long-range electrostatics or bond, angle, dihedral, improper calculations, computation and data transfer to the coprocessor will run concurrently with computations and MPI communications for these calculations on the host CPU. The USER-INTEL package has two modes for deciding which atoms will be handled by the coprocessor. This choice is controlled with the *ghost* keyword of the package intel command. When set to 0, ghost atoms (atoms at the borders between MPI tasks) are not offloaded to the card. This allows for overlap of MPI communication of forces with

computation on the coprocessor when the newton setting is "on". The default is dependent on the style being used, however, better performance may be achieved by setting this option explictly.

Restrictions:

When offloading to a coprocessor, hybrid styles that require skip lists for neighbor builds cannot be offloaded. Using hybrid/overlay is allowed. Only one intel accelerated style may be used with hybrid styles. Special_bonds exclusion lists are not currently supported with offload, however, the same effect can often be accomplished by setting cutoffs for excluded atom types to 0. None of the pair styles in the USER-INTEL package currently support the "inner", "middle", "outer" options for rRESPA integration via the run_style respa command; only the "pair" option is supported.

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5.3.4 KOKKOS package

The KOKKOS package was developed primarily by Christian Trott (Sandia) with contributions of various styles by others, including Sikandar Mashayak (UIUC), Stan Moore (Sandia), and Ray Shan (Sandia). The underlying Kokkos library was written primarily by Carter Edwards, Christian Trott, and Dan Sunderland (all Sandia).

The KOKKOS package contains versions of pair, fix, and atom styles that use data structures and macros provided by the Kokkos library, which is included with LAMMPS in lib/kokkos.

The Kokkos library is part of Trilinos and can also be downloaded from Github. Kokkos is a templated C++ library that provides two key abstractions for an application like LAMMPS. First, it allows a single implementation of an application kernel (e.g. a pair style) to run efficiently on different kinds of hardware, such as a GPU, Intel Phi, or many-core CPU.

The Kokkos library also provides data abstractions to adjust (at compile time) the memory layout of basic data structures like 2d and 3d arrays and allow the transparent utilization of special hardware load and store operations. Such data structures are used in LAMMPS to store atom coordinates or forces or neighbor lists. The layout is chosen to optimize performance on different platforms. Again this functionality is hidden from the developer, and does not affect how the kernel is coded.

These abstractions are set at build time, when LAMMPS is compiled with the KOKKOS package installed. All Kokkos operations occur within the context of an individual MPI task running on a single node of the machine. The total number of MPI tasks used by LAMMPS (one or multiple per compute node) is set in the usual manner via the mpirun or mpiexec commands, and is independent of Kokkos.

Kokkos currently provides support for 3 modes of execution (per MPI task). These are OpenMP (for many-core CPUs), Cuda (for NVIDIA GPUs), and OpenMP (for Intel Phi). Note that the KOKKOS package supports running on the Phi in native mode, not offload mode like the USER-INTEL package supports. You choose the mode at build time to produce an executable compatible with specific hardware.

Here is a quick overview of how to use the KOKKOS package for CPU acceleration, assuming one or more 16-core nodes. More details follow.

use a C++11 compatible compiler make yes-kokkos make mpi KOKKOS_DEVICES=OpenMP # build with the KOKKOS package make kokkos_omp # or Makefile.kokkos_omp already has variable set Make.py -v -p kokkos -kokkos omp -o mpi -a file mpi # or one-line build via Make.py

```
mpirun -np 16 lmp_mpi -k on -sf kk -in in.lj              # 1 node, 16 MPI tasks/node, no threads
mpirun -np 2 -ppn 1 lmp_mpi -k on t 16 -sf kk -in in.lj   # 2 nodes, 1 MPI task/node, 16 threads/tas
mpirun -np 2 lmp_mpi -k on t 8 -sf kk -in in.lj           # 1 node, 2 MPI tasks/node, 8 threads/task
mpirun -np 32 -ppn 4 lmp_mpi -k on t 4 -sf kk -in in.lj   # 8 nodes, 4 MPI tasks/node, 4 threads/tas
```

- specify variables and settings in your Makefile.machine that enable OpenMP, GPU, or Phi support
- include the KOKKOS package and build LAMMPS
- enable the KOKKOS package and its hardware options via the "-k on" command-line switch use KOKKOS styles in your input script

Here is a quick overview of how to use the KOKKOS package for GPUs, assuming one or more nodes, each with 16 cores and a GPU. More details follow.

discuss use of NVCC, which Makefiles to examine

use a C++11 compatible compiler KOKKOS_DEVICES = Cuda, OpenMP KOKKOS_ARCH = Kepler35 make yes-kokkos make machine Make.py -p kokkos -kokkos cuda arch=31 -o kokkos_cuda -a file kokkos_cuda

```
mpirun -np 1 lmp_cuda -k on t 6 -sf kk -in in.lj          # one MPI task, 6 threads on CPU
mpirun -np 4 -ppn 1 lmp_cuda -k on t 6 -sf kk -in in.lj   # ditto on 4 nodes

mpirun -np 2 lmp_cuda -k on t 8 g 2 -sf kk -in in.lj           # two MPI tasks, 8 threads per CPU
mpirun -np 32 -ppn 2 lmp_cuda -k on t 8 g 2 -sf kk -in in.lj   # ditto on 16 nodes
```

Here is a quick overview of how to use the KOKKOS package for the Intel Phi:

```
use a C++11 compatible compiler
KOKKOS_DEVICES = OpenMP
KOKKOS_ARCH = KNC
make yes-kokkos
make machine
Make.py -p kokkos -kokkos phi -o kokkos_phi -a file mpi
```

host=MIC, Intel Phi with 61 cores (240 threads/phi via 4x hardware threading): mpirun -np 1 lmp_g++ -k on t 240 -sf kk -in in.lj # 1 MPI task on 1 Phi, 1*240 = 240 mpirun -np 30 lmp_g++ -k on t 8 -sf kk -in in.lj # 30 MPI tasks on 1 Phi, 30*8 = 240 mpirun -np 12 lmp_g++ -k on t 20 -sf kk -in in.lj # 12 MPI tasks on 1 Phi, 12*20 = 240 mpirun -np 96 -ppn 12 lmp_g++ -k on t 20 -sf kk -in in.lj # ditto on 8 Phis

Required hardware/software:

Kokkos support within LAMMPS must be built with a C++11 compatible compiler. If using gcc, version 4.8.1 or later is required.

To build with Kokkos support for CPUs, your compiler must support the OpenMP interface. You should have one or more multi-core CPUs so that multiple threads can be launched by each MPI task running on a CPU.

To build with Kokkos support for NVIDIA GPUs, NVIDIA Cuda software version 6.5 or later must be installed on your system. See the discussion for the USER-CUDA and GPU packages for details of how to check and do this.

NOTE: For good performance of the KOKKOS package on GPUs, you must have Kepler generation GPUs (or later). The Kokkos library exploits texture cache options not supported by Telsa generation GPUs (or older).

To build with Kokkos support for Intel Xeon Phi coprocessors, your sysmte must be configured to use them in "native" mode, not "offload" mode like the USER-INTEL package supports.

Building LAMMPS with the KOKKOS package:

You must choose at build time whether to build for CPUs (OpenMP), GPUs, or Phi.

You can do any of these in one line, using the src/Make.py script, described in Section 2.4 of the manual. Type "Make.py -h" for help. If run from the src directory, these commands will create src/lmp_kokkos_omp, lmp_kokkos_cuda, and lmp_kokkos_phi. Note that the OMP and PHI options use src/MAKE/Makefile.mpi as the starting Makefile.machine. The CUDA option uses src/MAKE/OPTIONS/Makefile.kokkos_cuda.

The latter two steps can be done using the "-k on", "-pk kokkos" and "-sf kk" command-line switches respectively. Or the effect of the "-pk" or "-sf" switches can be duplicated by adding the package kokkos or suffix

kk commands respectively to your input script.

Or you can follow these steps:

CPU-only (run all-MPI or with OpenMP threading):

```
cd lammps/src
make yes-kokkos
make g++ KOKKOS_DEVICES=OpenMP
```

Intel Xeon Phi:

```
cd lammps/src
make yes-kokkos
make g++ KOKKOS_DEVICES=OpenMP KOKKOS_ARCH=KNC
```

CPUs and GPUs:

```
cd lammps/src
make yes-kokkos
make cuda KOKKOS_DEVICES=Cuda
```

These examples set the KOKKOS-specific OMP, MIC, CUDA variables on the make command line which requires a GNU-compatible make command. Try "gmake" if your system's standard make complains.

NOTE: If you build using make line variables and re-build LAMMPS twice with different KOKKOS options and the *same* target, e.g. g++ in the first two examples above, then you *must* perform a "make clean-all" or "make clean-machine" before each build. This is to force all the KOKKOS-dependent files to be re-compiled with the new options.

You can also hardwire these make variables in the specified machine makefile, e.g. src/MAKE/Makefile.g++ in the first two examples above, with a line like:

```
KOKKOS_ARCH = KNC
```

Note that if you build LAMMPS multiple times in this manner, using different KOKKOS options (defined in different machine makefiles), you do not have to worry about doing a "clean" in between. This is because the targets will be different.

NOTE: The 3rd example above for a GPU, uses a different machine makefile, in this case src/MAKE/Makefile.cuda, which is included in the LAMMPS distribution. To build the KOKKOS package for a GPU, this makefile must use the NVIDA "nvcc" compiler. And it must have a KOKKOS_ARCH setting that is appropriate for your NVIDIA hardware and installed software. Typical values for KOKKOS_ARCH are given below, as well as other settings that must be included in the machine makefile, if you create your own.

NOTE: Currently, there are no precision options with the KOKKOS package. All compilation and computation is performed in double precision.

There are other allowed options when building with the KOKKOS package. As above, they can be set either as variables on the make command line or in Makefile.machine. This is the full list of options, including those discussed above, Each takes a value shown below. The default value is listed, which is set in the lib/kokkos/Makefile.kokkos file.

#Default settings specific options #Options: force_uvm,use_ldg,rdc

- KOKKOS_DEVICES, values = *OpenMP*, *Serial*, *Pthreads*, *Cuda*, default = *OpenMP*
- KOKKOS_ARCH, values = *KNC*, *SNB*, *HSW*, *Kepler*, *Kepler30*, *Kepler32*, *Kepler35*, *Kepler37*, *Maxwell*, *Maxwell50*, *Maxwell52*, *Maxwell53*, *ARMv8*, *BGQ*, *Power7*, *Power8*, default = *none*
- KOKKOS_DEBUG, values = *yes*, *no*, default = *no*
- KOKKOS_USE_TPLS, values = *hwloc*, *librt*, default = *none*
- KOKKOS_CUDA_OPTIONS, values = *force_uvm*, *use_ldg*, *rdc*

KOKKOS_DEVICE sets the parallelization method used for Kokkos code (within LAMMPS). KOKKOS_DEVICES=OpenMP means that OpenMP will be used. KOKKOS_DEVICES=Pthreads means that pthreads will be used. KOKKOS_DEVICES=Cuda means an NVIDIA GPU running CUDA will be used.

If KOKKOS_DEVICES=Cuda, then the lo-level Makefile in the src/MAKE directory must use "nvcc" as its compiler, via its CC setting. For best performance its CCFLAGS setting should use -O3 and have a KOKKOS_ARCH setting that matches the compute capability of your NVIDIA hardware and software installation, e.g. KOKKOS_ARCH=Kepler30. Note the minimal required compute capability is 2.0, but this will give signicantly reduced performance compared to Kepler generation GPUs with compute capability 3.x. For the LINK setting, "nvcc" should not be used; instead use g++ or another compiler suitable for linking C++ applications. Often you will want to use your MPI compiler wrapper for this setting (i.e. mpicxx). Finally, the lo-level Makefile must also have a "Compilation rule" for creating *.o files from *.cu files. See src/Makefile.cuda for an example of a lo-level Makefile with all of these settings.

KOKKOS_USE_TPLS=hwloc binds threads to hardware cores, so they do not migrate during a simulation. KOKKOS_USE_TPLS=hwloc should always be used if running with KOKKOS_DEVICES=Pthreads for pthreads. It is not necessary for KOKKOS_DEVICES=OpenMP for OpenMP, because OpenMP provides alternative methods via environment variables for binding threads to hardware cores. More info on binding threads to cores is given in this section.

KOKKOS_ARCH=KNC enables compiler switches needed when compling for an Intel Phi processor.

KOKKOS_USE_TPLS=librt enables use of a more accurate timer mechanism on most Unix platforms. This library is not available on all platforms.

KOKKOS_DEBUG is only useful when developing a Kokkos-enabled style within LAMMPS. KOKKOS_DEBUG=yes enables printing of run-time debugging information that can be useful. It also enables runtime bounds checking on Kokkos data structures.

KOKKOS_CUDA_OPTIONS are additional options for CUDA.

For more information on Kokkos see the Kokkos programmers' guide here: /lib/kokkos/doc/Kokkos_PG.pdf.

Run with the KOKKOS package from the command line:

The mpirun or mpiexec command sets the total number of MPI tasks used by LAMMPS (one or multiple per compute node) and the number of MPI tasks used per node. E.g. the mpirun command in MPICH does this via its -np and -ppn switches. Ditto for OpenMPI via -np and -npernode.

When using KOKKOS built with host=OMP, you need to choose how many OpenMP threads per MPI task will be used (via the "-k" command-line switch discussed below). Note that the product of MPI tasks * OpenMP threads/task should not exceed the physical number of cores (on a node), otherwise performance will suffer.

When using the KOKKOS package built with device=CUDA, you must use exactly one MPI task per physical GPU.

When using the KOKKOS package built with host=MIC for Intel Xeon Phi coprocessor support you need to insure there are one or more MPI tasks per coprocessor, and choose the number of coprocessor threads to use per MPI task (via the "-k" command-line switch discussed below). The product of MPI tasks * coprocessor threads/task should not exceed the maximum number of threads the coproprocessor is designed to run, otherwise performance will suffer. This value is 240 for current generation Xeon Phi(TM) chips, which is 60 physical cores * 4 threads/core. Note that with the KOKKOS package you do not need to specify how many Phi coprocessors there are per node; each coprocessors is simply treated as running some number of MPI tasks.

You must use the "-k on" command-line switch to enable the KOKKOS package. It takes additional arguments for hardware settings appropriate to your system. Those arguments are documented here. The two most commonly used options are:

```
-k on t Nt g Ng
```

The "t Nt" option applies to host=OMP (even if device=CUDA) and host=MIC. For host=OMP, it specifies how many OpenMP threads per MPI task to use with a node. For host=MIC, it specifies how many Xeon Phi threads per MPI task to use within a node. The default is Nt = 1. Note that for host=OMP this is effectively MPI-only mode which may be fine. But for host=MIC you will typically end up using far less than all the 240 available threads, which could give very poor performance.

The "g Ng" option applies to device=CUDA. It specifies how many GPUs per compute node to use. The default is 1, so this only needs to be specified is you have 2 or more GPUs per compute node.

The "-k on" switch also issues a "package kokkos" command (with no additional arguments) which sets various KOKKOS options to default values, as discussed on the package command doc page.

Use the "-sf kk" command-line switch, which will automatically append "kk" to styles that support it. Use the "-pk kokkos" command-line switch if you wish to change any of the default package kokkos optionns set by the "-k on" command-line switch.

Note that the default for the package kokkos command is to use "full" neighbor lists and set the Newton flag to "off" for both pairwise and bonded interactions. This typically gives fastest performance. If the newton command is used in the input script, it can override the Newton flag defaults.

However, when running in MPI-only mode with 1 thread per MPI task, it will typically be faster to use "half" neighbor lists and set the Newton flag to "on", just as is the case for non-accelerated pair styles. You can do this with the "-pk" command-line switch.

Or run with the KOKKOS package by editing an input script:

The discussion above for the mpirun/mpiexec command and setting appropriate thread and GPU values for host=OMP or host=MIC or device=CUDA are the same.

You must still use the "-k on" command-line switch to enable the KOKKOS package, and specify its additional arguments for hardware options appopriate to your system, as documented above.

Use the suffix kk command, or you can explicitly add a "kk" suffix to individual styles in your input script, e.g.

```
pair_style lj/cut/kk 2.5
```

You only need to use the package kokkos command if you wish to change any of its option defaults, as set by the "-k on" command-line switch.

Speed-ups to expect:

The performance of KOKKOS running in different modes is a function of your hardware, which KOKKOS-enable styles are used, and the problem size.

Generally speaking, the following rules of thumb apply:

- When running on CPUs only, with a single thread per MPI task, performance of a KOKKOS style is somewhere between the standard (un-accelerated) styles (MPI-only mode), and those provided by the USER-OMP package. However the difference between all 3 is small (less than 20%).
- When running on CPUs only, with multiple threads per MPI task, performance of a KOKKOS style is a bit slower than the USER-OMP package.
- When running on GPUs, KOKKOS is typically faster than the USER-CUDA and GPU packages.
- When running on Intel Xeon Phi, KOKKOS is not as fast as the USER-INTEL package, which is optimized for that hardware.

See the Benchmark page of the LAMMPS web site for performance of the KOKKOS package on different hardware.

Guidelines for best performance:

Here are guidline for using the KOKKOS package on the different hardware configurations listed above.

Many of the guidelines use the package kokkos command See its doc page for details and default settings. Experimenting with its options can provide a speed-up for specific calculations.

Running on a multi-core CPU:

If N is the number of physical cores/node, then the number of MPI tasks/node * number of threads/task should not exceed N, and should typically equal N. Note that the default threads/task is 1, as set by the "t" keyword of the "-k" command-line switch. If you do not change this, no additional parallelism (beyond MPI) will be invoked on the host CPU(s).

You can compare the performance running in different modes:

- run with 1 MPI task/node and N threads/task
- run with N MPI tasks/node and 1 thread/task
- run with settings in between these extremes

Examples of mpirun commands in these modes are shown above.

When using KOKKOS to perform multi-threading, it is important for performance to bind both MPI tasks to physical cores, and threads to physical cores, so they do not migrate during a simulation.

If you are not certain MPI tasks are being bound (check the defaults for your MPI installation), binding can be forced with these flags:

```
OpenMPI 1.8: mpirun -np 2 -bind-to socket -map-by socket ./lmp_openmpi ...
Mvapich2 2.0: mpiexec -np 2 -bind-to socket -map-by socket ./lmp_mvapich ...
```

For binding threads with the KOKKOS OMP option, use thread affinity environment variables to force binding. With OpenMP 3.1 (gcc 4.7 or later, intel 12 or later) setting the environment variable OMP_PROC_BIND=true should be sufficient. For binding threads with the KOKKOS pthreads option, compile LAMMPS the KOKKOS

HWLOC=yes option, as discussed in Section 2.3.4 of the manual.

Running on GPUs:

Insure the -arch setting in the machine makefile you are using, e.g. src/MAKE/Makefile.cuda, is correct for your GPU hardware/software (see this section of the manual for details).

The -np setting of the mpirun command should set the number of MPI tasks/node to be equal to the # of physical GPUs on the node.

Use the "-k" command-line switch to specify the number of GPUs per node, and the number of threads per MPI task. As above for multi-core CPUs (and no GPU), if N is the number of physical cores/node, then the number of MPI tasks/node * number of threads/task should not exceed N. With one GPU (and one MPI task) it may be faster to use less than all the available cores, by setting threads/task to a smaller value. This is because using all the cores on a dual-socket node will incur extra cost to copy memory from the 2nd socket to the GPU.

Examples of mpirun commands that follow these rules are shown above.

NOTE: When using a GPU, you will achieve the best performance if your input script does not use any fix or compute styles which are not yet Kokkos-enabled. This allows data to stay on the GPU for multiple timesteps, without being copied back to the host CPU. Invoking a non-Kokkos fix or compute, or performing I/O for thermo or dump output will cause data to be copied back to the CPU.

You cannot yet assign multiple MPI tasks to the same GPU with the KOKKOS package. We plan to support this in the future, similar to the GPU package in LAMMPS.

You cannot yet use both the host (multi-threaded) and device (GPU) together to compute pairwise interactions with the KOKKOS package. We hope to support this in the future, similar to the GPU package in LAMMPS.

Running on an Intel Phi:

Kokkos only uses Intel Phi processors in their "native" mode, i.e. not hosted by a CPU.

As illustrated above, build LAMMPS with OMP=yes (the default) and MIC=yes. The latter insures code is correctly compiled for the Intel Phi. The OMP setting means OpenMP will be used for parallelization on the Phi, which is currently the best option within Kokkos. In the future, other options may be added.

Current-generation Intel Phi chips have either 61 or 57 cores. One core should be excluded for running the OS, leaving 60 or 56 cores. Each core is hyperthreaded, so there are effectively N = 240 (4*60) or N = 224 (4*56) cores to run on.

The -np setting of the mpirun command sets the number of MPI tasks/node. The "-k on t Nt" command-line switch sets the number of threads/task as Nt. The product of these 2 values should be N, i.e. 240 or 224. Also, the number of threads/task should be a multiple of 4 so that logical threads from more than one MPI task do not run on the same physical core.

Examples of mpirun commands that follow these rules are shown above.

Restrictions:

As noted above, if using GPUs, the number of MPI tasks per compute node should equal to the number of GPUs per compute node. In the future Kokkos will support assigning multiple MPI tasks to a single GPU.

Currently Kokkos does not support AMD GPUs due to limits in the available backend programming models. Specifically, Kokkos requires extensive C++ support from the Kernel language. This is expected to change in the future.

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5.3.5 USER-OMP package

The USER-OMP package was developed by Axel Kohlmeyer at Temple University. It provides multi-threaded versions of most pair styles, nearly all bonded styles (bond, angle, dihedral, improper), several Kspace styles, and a few fix styles. The package currently uses the OpenMP interface for multi-threading.

Here is a quick overview of how to use the USER-OMP package, assuming one or more 16-core nodes. More details follow.

```
use -fopenmp with CCFLAGS and LINKFLAGS in Makefile.machine
make yes-user-omp
make mpi                                    # build with USER-OMP package, if settings added to Makef
make omp                                    # or Makefile.omp already has settings
Make.py -v -p omp -o mpi -a file mpi        # or one-line build via Make.py

lmp_mpi -sf omp -pk omp 16 <in.script                          # 1 MPI task, 16 threads
mpirun -np 4 lmp_mpi -sf omp -pk omp 4 -in in.script            # 4 MPI tasks, 4 threads/task
mpirun -np 32 -ppn 4 lmp_mpi -sf omp -pk omp 4 -in in.script    # 8 nodes, 4 MPI tasks/node, 4 thread
```

Required hardware/software:

Your compiler must support the OpenMP interface. You should have one or more multi-core CPUs so that multiple threads can be launched by each MPI task running on a CPU.

Building LAMMPS with the USER-OMP package:

The lines above illustrate how to include/build with the USER-OMP package in two steps, using the "make" command. Or how to do it with one command via the src/Make.py script, described in Section 2.4 of the manual. Type "Make.py -h" for help.

Note that the CCFLAGS and LINKFLAGS settings in Makefile.machine must include "-fopenmp". Likewise, if you use an Intel compiler, the CCFLAGS setting must include "-restrict". The Make.py command will add these automatically.

Run with the USER-OMP package from the command line:

The mpirun or mpiexec command sets the total number of MPI tasks used by LAMMPS (one or multiple per compute node) and the number of MPI tasks used per node. E.g. the mpirun command in MPICH does this via its -np and -ppn switches. Ditto for OpenMPI via -np and -npernode.

You need to choose how many OpenMP threads per MPI task will be used by the USER-OMP package. Note that the product of MPI tasks * threads/task should not exceed the physical number of cores (on a node), otherwise performance will suffer.

As in the lines above, use the "-sf omp" command-line switch, which will automatically append "omp" to styles that support it. The "-sf omp" switch also issues a default package omp 0 command, which will set the number of threads per MPI task via the OMP_NUM_THREADS environment variable.

You can also use the "-pk omp Nt" command-line switch, to explicitly set Nt = # of OpenMP threads per MPI task to use, as well as additional options. Its syntax is the same as the package omp command whose doc page

gives details, including the default values used if it is not specified. It also gives more details on how to set the number of threads via the OMP_NUM_THREADS environment variable.

Or run with the USER-OMP package by editing an input script:

The discussion above for the mpirun/mpiexec command, MPI tasks/node, and threads/MPI task is the same.

Use the suffix omp command, or you can explicitly add an "omp" suffix to individual styles in your input script, e.g.

```
pair_style lj/cut/omp 2.5
```

You must also use the package omp command to enable the USER-OMP package. When you do this you also specify how many threads per MPI task to use. The command doc page explains other options and how to set the number of threads via the OMP_NUM_THREADS environment variable.

Speed-ups to expect:

Depending on which styles are accelerated, you should look for a reduction in the "Pair time", "Bond time", "KSpace time", and "Loop time" values printed at the end of a run.

You may see a small performance advantage (5 to 20%) when running a USER-OMP style (in serial or parallel) with a single thread per MPI task, versus running standard LAMMPS with its standard un-accelerated styles (in serial or all-MPI parallelization with 1 task/core). This is because many of the USER-OMP styles contain similar optimizations to those used in the OPT package, described in Section accelerate 5.3.6.

With multiple threads/task, the optimal choice of number of MPI tasks/node and OpenMP threads/task can vary a lot and should always be tested via benchmark runs for a specific simulation running on a specific machine, paying attention to guidelines discussed in the next sub-section.

A description of the multi-threading strategy used in the USER-OMP package and some performance examples are presented here

Guidelines for best performance:

For many problems on current generation CPUs, running the USER-OMP package with a single thread/task is faster than running with multiple threads/task. This is because the MPI parallelization in LAMMPS is often more efficient than multi-threading as implemented in the USER-OMP package. The parallel efficiency (in a threaded sense) also varies for different USER-OMP styles.

Using multiple threads/task can be more effective under the following circumstances:

- Individual compute nodes have a significant number of CPU cores but the CPU itself has limited memory bandwidth, e.g. for Intel Xeon 53xx (Clovertown) and 54xx (Harpertown) quad-core processors. Running one MPI task per CPU core will result in significant performance degradation, so that running with 4 or even only 2 MPI tasks per node is faster. Running in hybrid MPI+OpenMP mode will reduce the inter-node communication bandwidth contention in the same way, but offers an additional speedup by utilizing the otherwise idle CPU cores.
- The interconnect used for MPI communication does not provide sufficient bandwidth for a large number of MPI tasks per node. For example, this applies to running over gigabit ethernet or on Cray XT4 or XT5 series supercomputers. As in the aforementioned case, this effect worsens when using an increasing number of nodes.

- The system has a spatially inhomogeneous particle density which does not map well to the domain decomposition scheme or load-balancing options that LAMMPS provides. This is because multi-threading achives parallelism over the number of particles, not via their distribution in space.
- A machine is being used in "capability mode", i.e. near the point where MPI parallelism is maxed out. For example, this can happen when using the PPPM solver for long-range electrostatics on large numbers of nodes. The scaling of the KSpace calculation (see the kspace_style command) becomes the performance-limiting factor. Using multi-threading allows less MPI tasks to be invoked and can speed-up the long-range solver, while increasing overall performance by parallelizing the pairwise and bonded calculations via OpenMP. Likewise additional speedup can be sometimes be achived by increasing the length of the Coulombic cutoff and thus reducing the work done by the long-range solver. Using the run_style verlet/split command, which is compatible with the USER-OMP package, is an alternative way to reduce the number of MPI tasks assigned to the KSpace calculation.

Additional performance tips are as follows:

- The best parallel efficiency from *omp* styles is typically achieved when there is at least one MPI task per physical CPU chip, i.e. socket or die.
- It is usually most efficient to restrict threading to a single socket, i.e. use one or more MPI task per socket.
- NOTE: By default, several current MPI implementations use a processor affinity setting that restricts each MPI task to a single CPU core. Using multi-threading in this mode will force all threads to share the one core and thus is likely to be counterproductive. Instead, binding MPI tasks to a (multi-core) socket, should solve this issue.

Restrictions:

None.

Return to Section accelerate overview

5.3.6 OPT package

The OPT package was developed by James Fischer (High Performance Technologies), David Richie, and Vincent Natoli (Stone Ridge Technologies). It contains a handful of pair styles whose compute() methods were rewritten in C++ templated form to reduce the overhead due to if tests and other conditional code.

Here is a quick overview of how to use the OPT package. More details follow.

```
make yes-opt
make mpi                                # build with the OPT pacakge
Make.py -v -p opt -o mpi -a file mpi    # or one-line build via Make.py

lmp_mpi -sf opt -in in.script                 # run in serial
mpirun -np 4 lmp_mpi -sf opt -in in.script    # run in parallel
```

Required hardware/software:

None.

Building LAMMPS with the OPT package:

The lines above illustrate how to build LAMMPS with the OPT package in two steps, using the "make" command. Or how to do it with one command via the src/Make.py script, described in Section 2.4 of the manual. Type "Make.py -h" for help.

Note that if you use an Intel compiler to build with the OPT package, the CCFLAGS setting in your Makefile.machine must include "-restrict". The Make.py command will add this automatically.

Run with the OPT package from the command line:

As in the lines above, use the "-sf opt" command-line switch, which will automatically append "opt" to styles that support it.

Or run with the OPT package by editing an input script:

Use the suffix opt command, or you can explicitly add an "opt" suffix to individual styles in your input script, e.g.

```
pair_style lj/cut/opt 2.5
```

Speed-ups to expect:

You should see a reduction in the "Pair time" value printed at the end of a run. On most machines for reasonable problem sizes, it will be a 5 to 20% savings.

Guidelines for best performance:

Just try out an OPT pair style to see how it performs.

Restrictions:

None.

angle_style charmm command

angle_style charmm/intel command

angle_style charmm/kk command

angle_style charmm/omp command

Syntax:

```
angle_style charmm
```

Examples:

```
angle_style charmm
angle_coeff 1 300.0 107.0 50.0 3.0
```

Description:

The *charmm* angle style uses the potential

$$E = K(\theta - \theta_0)^2 + K_{UB}(r - r_{UB})^2$$

with an additional Urey_Bradley term based on the distance *r* between the 1st and 3rd atoms in the angle. K, theta0, Kub, and Rub are coefficients defined for each angle type.

See (MacKerell) for a description of the CHARMM force field.

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/radian^2)
- theta0 (degrees)
- K_ub (energy/distance^2)
- r_ub (distance)

Theta0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K are in energy/radian^2.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making

LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff

Default: none

(MacKerell) MacKerell, Bashford, Bellott, Dunbrack, Evanseck, Field, Fischer, Gao, Guo, Ha, et al, J Phys Chem, 102, 3586 (1998).

angle_style class2 command

angle_style class2/omp command

Syntax:

```
angle_style class2
```

Examples:

```
angle_style class2
angle_coeff * 75.0
angle_coeff 1 bb 10.5872 1.0119 1.5228
angle_coeff * ba 3.6551 24.895 1.0119 1.5228
```

Description:

The *class2* angle style uses the potential

$$
\begin{aligned}
E &= E_a + E_{bb} + E_{ba} \\
E_a &= K_2(\theta - \theta_0)^2 + K_3(\theta - \theta_0)^3 + K_4(\theta - \theta_0)^4 \\
E_{bb} &= M(r_{ij} - r_1)(r_{jk} - r_2) \\
E_{ba} &= N_1(r_{ij} - r_1)(\theta - \theta_0) + N_2(r_{jk} - r_2)(\theta - \theta_0)
\end{aligned}
$$

where Ea is the angle term, Ebb is a bond-bond term, and Eba is a bond-angle term. Theta0 is the equilibrium angle and r1 and r2 are the equilibrium bond lengths.

See (Sun) for a description of the COMPASS class2 force field.

Coefficients for the Ea, Ebb, and Eba formulas must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands.

These are the 4 coefficients for the Ea formula:

- theta0 (degrees)
- K2 (energy/radian^2)
- K3 (energy/radian^3)
- K4 (energy/radian^4)

Theta0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of the various K are in per-radian.

For the Ebb formula, each line in a angle_coeff command in the input script lists 4 coefficients, the first of which is "bb" to indicate they are BondBond coefficients. In a data file, these coefficients should be listed under a "BondBond Coeffs" heading and you must leave out the "bb", i.e. only list 3 coefficients after the angle type.

- bb
- M (energy/distance^2)
- r1 (distance)
- r2 (distance)

For the Eba formula, each line in a angle_coeff command in the input script lists 5 coefficients, the first of which is "ba" to indicate they are BondAngle coefficients. In a data file, these coefficients should be listed under a "BondAngle Coeffs" heading and you must leave out the "ba", i.e. only list 4 coefficients after the angle type.

- ba
- N1 (energy/distance^2)
- N2 (energy/distance^2)
- r1 (distance)
- r2 (distance)

The theta0 value in the Eba formula is not specified, since it is the same value from the Ea formula.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the CLASS2 package. See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff

Default: none

(Sun) Sun, J Phys Chem B 102, 7338-7364 (1998).

angle_coeff command

Syntax:

```
angle_coeff N args
```

- N = angle type (see asterisk form below)
- args = coefficients for one or more angle types

Examples:

```
angle_coeff 1 300.0 107.0
angle_coeff * 5.0
angle_coeff 2*10 5.0
```

Description:

Specify the angle force field coefficients for one or more angle types. The number and meaning of the coefficients depends on the angle style. Angle coefficients can also be set in the data file read by the read_data command or in a restart file.

N can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to set the coefficients for multiple angle types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of angle types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

Note that using an angle_coeff command can override a previous setting for the same angle type. For example, these commands set the coeffs for all angle types, then overwrite the coeffs for just angle type 2:

```
angle_coeff * 200.0 107.0 1.2
angle_coeff 2 50.0 107.0
```

A line in a data file that specifies angle coefficients uses the exact same format as the arguments of the angle_coeff command in an input script, except that wild-card asterisks should not be used since coefficients for all N types must be listed in the file. For example, under the "Angle Coeffs" section of a data file, the line that corresponds to the 1st example above would be listed as

```
1 300.0 107.0
```

The angle_style class2 is an exception to this rule, in that an additional argument is used in the input script to allow specification of the cross-term coefficients. See its doc page for details.

Here is an alphabetic list of angle styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated angle_coeff command.

Note that there are also additional angle styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the angle section of this page.

- angle_style none - turn off angle interactions
- angle_style hybrid - define multiple styles of angle interactions

- angle_style charmm - CHARMM angle
- angle_style class2 - COMPASS (class 2) angle
- angle_style cosine - cosine angle potential
- angle_style cosine/delta - difference of cosines angle potential
- angle_style cosine/periodic - DREIDING angle
- angle_style cosine/squared - cosine squared angle potential
- angle_style harmonic - harmonic angle
- angle_style table - tabulated by angle

Restrictions:

This command must come after the simulation box is defined by a read_data, read_restart, or create_box command.

An angle style must be defined before any angle coefficients are set, either in the input script or in a data file.

Related commands:

angle_style

Default: none

angle_style cosine command

angle_style cosine/omp command

Syntax:

```
angle_style cosine
```

Examples:

```
angle_style cosine
angle_coeff * 75.0
```

Description:

The *cosine* angle style uses the potential

$$E = K[1 + \cos(\theta)]$$

where K is defined for each angle type.

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff

Default: none

angle_style cosine/delta command

angle_style cosine/delta/omp command

Syntax:

```
angle_style cosine/delta
```

Examples:

```
angle_style cosine/delta
angle_coeff 2*4 75.0 100.0
```

Description:

The *cosine/delta* angle style uses the potential

$$E = K[1 - \cos(\theta - \theta_0)]$$

where theta0 is the equilibrium value of the angle, and K is a prefactor. Note that the usual 1/2 factor is included in K.

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy)
- theta0 (degrees)

Theta0 is specified in degrees, but LAMMPS converts it to radians internally.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff, angle_style cosine/squared

Default: none

angle_style cosine/periodic command

angle_style cosine/periodic/omp command

Syntax:

```
angle_style cosine/periodic
```

Examples:

```
angle_style cosine/periodic
angle_coeff * 75.0 1 6
```

Description:

The *cosine/periodic* angle style uses the following potential, which is commonly used in the DREIDING force field, particularly for organometallic systems where $n = 4$ might be used for an octahedral complex and $n = 3$ might be used for a trigonal center:

$$E = C\left[1 - B(-1)^n cos\left(n\theta\right)\right]$$

where C, B and n are coefficients defined for each angle type.

See (Mayo) for a description of the DREIDING force field

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- C (energy)
- B = 1 or -1
- n = 1, 2, 3, 4, 5 or 6 for periodicity

Note that the prefactor C is specified and not the overall force constant K = C / n^2. When B = 1, it leads to a minimum for the linear geometry. When B = -1, it leads to a maximum for the linear geometry.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff

Default: none

(Mayo) Mayo, Olfason, Goddard III, J Phys Chem, 94, 8897-8909 (1990).

angle_style cosine/shift command

angle_style cosine/shift/omp command

Syntax:

```
angle_style cosine/shift
```

Examples:

```
angle_style cosine/shift
angle_coeff * 10.0 45.0
```

Description:

The *cosine/shift* angle style uses the potential

$$E = -\frac{Umin}{2}\left[1 + Cos(\theta - \theta_0)\right]$$

where theta0 is the equilibrium angle. The potential is bounded between -Umin and zero. In the neighborhood of the minimum E=- Umin + Umin/4(theta-theta0)^2 hence the spring constant is umin/2.

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- umin (energy)
- theta (angle)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff, angle_cosineshiftexp

Default: none

angle_style cosine/shift/exp command

angle_style cosine/shift/exp/omp command

Syntax:

```
angle_style cosine/shift/exp
```

Examples:

```
angle_style cosine/shift/exp
angle_coeff * 10.0 45.0 2.0
```

Description:

The *cosine/shift/exp* angle style uses the potential

$$E = -U_{min}\frac{e^{-aU(\theta,\theta_0)}-1}{e^{a}-1} \quad \text{with} \quad U(\theta,\theta_0) = -0.5\left(1+\cos(\theta-\theta_0)\right)$$

where Umin, theta, and a are defined for each angle type.

The potential is bounded between [-Umin:0] and the minimum is located at the angle theta0. The a parameter can be both positive or negative and is used to control the spring constant at the equilibrium.

The spring constant is given by k = A exp(A) Umin / [2 (Exp(a)-1)]. For a > 3, k/Umin = a/2 to better than 5% relative error. For negative values of the a parameter, the spring constant is essentially zero, and anharmonic terms takes over. The potential is furthermore well behaved in the limit a -> 0, where it has been implemented to linear order in a for a < 0.001. In this limit the potential reduces to the cosineshifted potential.

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- umin (energy)
- theta (angle)
- A (real number)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff, angle_cosineshift, dihedral_cosineshift

Default: none

angle_style cosine/squared command

angle_style cosine/squared/omp command

Syntax:

```
angle_style cosine/squared
```

Examples:

```
angle_style cosine/squared
angle_coeff 2*4 75.0 100.0
```

Description:

The *cosine/squared* angle style uses the potential

$$E = K[\cos(\theta) - \cos(\theta_0)]^2$$

where theta0 is the equilibrium value of the angle, and K is a prefactor. Note that the usual 1/2 factor is included in K.

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy)
- theta0 (degrees)

Theta0 is specified in degrees, but LAMMPS converts it to radians internally.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff

Default: none

angle_style dipole command

angle_style dipole/omp command

Syntax:

```
angle_style dipole
```

Examples:

```
angle_style dipole
angle_coeff 6 2.1 180.0
```

Description:

The *dipole* angle style is used to control the orientation of a dipolar atom within a molecule (Orsi). Specifically, the *dipole* angle style restrains the orientation of a point dipole mu_j (embedded in atom 'j') with respect to a reference (bond) vector r_ij = r_i - r_j, where 'i' is another atom of the same molecule (typically, 'i' and 'j' are also covalently bonded).

It is convenient to define an angle gamma between the 'free' vector mu_j and the reference (bond) vector r_ij:

$$\cos\gamma = \frac{\vec{\mu_j} \bullet \vec{r_{ij}}}{\mu_j r_{ij}}$$

The *dipole* angle style uses the potential:

$$E = K(\cos\gamma - \cos\gamma_0)^2$$

where K is a rigidity constant and gamma0 is an equilibrium (reference) angle.

The torque on the dipole can be obtained by differentiating the potential using the 'chain rule' as in appendix C.3 of (Allen):

$$\vec{T_j} = \frac{2K(\cos\gamma - \cos\gamma_0)}{\mu_j r_{ij}} \vec{r_{ij}} \times \vec{\mu_j}$$

Example: if gamma0 is set to 0 degrees, the torque generated by the potential will tend to align the dipole along the reference direction defined by the (bond) vector r_ij (in other words, mu_j is restrained to point towards atom 'i').

The dipolar torque T_j must be counterbalanced in order to conserve the local angular momentum. This is achieved via an additional force couple generating a torque equivalent to the opposite of T_j:

$$\begin{aligned} -\vec{T}_j &= \vec{r_{ij}} \times \vec{F}_i \\ \vec{F}_j &= -\vec{F}_i \end{aligned}$$

where F_i and F_j are applied on atoms i and j, respectively.

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy)
- gamma0 (degrees)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

NOTE: In the "Angles" section of the data file, the atom ID 'j' corresponding to the dipole to restrain must come before the atom ID of the reference atom 'i'. A third atom ID 'k' must also be provided, although 'k' is just a 'dummy' atom which can be any atom; it may be useful to choose a convention (e.g., 'k'='i') and adhere to it. For example, if ID=1 for the dipolar atom to restrain, and ID=2 for the reference atom, the corresponding line in the "Angles" section of the data file would read: X X 1 2 2

The "newton" command for intramolecular interactions must be "on" (which is the default).

This angle style should not be used with SHAKE.

Related commands:

angle_coeff, angle_hybrid

Default: none

(Orsi) Orsi & Essex, The ELBA force field for coarse-grain modeling of lipid membranes, PloS ONE 6(12): e28637, 2011.

(Allen) Allen & Tildesley, Computer Simulation of Liquids, Clarendon Press, Oxford, 1987.

angle_style fourier command

angle_style fourier/omp command

Syntax:

```
angle_style fourier
```

Examples:

angle_style fourier angle_coeff 75.0 1.0 1.0 1.0

Description:

The *fourier* angle style uses the potential

$$E = K[C_0 + C_1 \cos(\theta) + C_2 \cos(2\theta)]$$

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy)
- C0 (real)
- C1 (real)
- C2 (real)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the USER_MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff

Default: none

angle_style fourier/simple command

angle_style fourier/simple/omp command

Syntax:

```
angle_style fourier/simple
```

Examples:

angle_style fourier/simple angle_coeff 100.0 -1.0 1.0

Description:

The *fourier/simple* angle style uses the potential

$$E = K[1.0 + c\cos(n\theta)]$$

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy)
- c (real)
- n (real)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the USER_MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff

Default: none

angle_style harmonic command

angle_style harmonic/intel command

angle_style harmonic/kk command

angle_style harmonic/omp command

Syntax:

```
angle_style harmonic
```

Examples:

```
angle_style harmonic
angle_coeff 1 300.0 107.0
```

Description:

The *harmonic* angle style uses the potential

$$E = K(\theta - \theta_0)^2$$

where theta0 is the equilibrium value of the angle, and K is a prefactor. Note that the usual 1/2 factor is included in K.

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/radian^2)
- theta0 (degrees)

Theta0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K are in energy/radian^2.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions: none

This angle style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff

Default: none

angle_style hybrid command

Syntax:

```
angle_style hybrid style1 style2 ...
```

- style1,style2 = list of one or more angle styles

Examples:

```
angle_style hybrid harmonic cosine
angle_coeff 1 harmonic 80.0 30.0
angle_coeff 2* cosine 50.0
```

Description:

The *hybrid* style enables the use of multiple angle styles in one simulation. An angle style is assigned to each angle type. For example, angles in a polymer flow (of angle type 1) could be computed with a *harmonic* potential and angles in the wall boundary (of angle type 2) could be computed with a *cosine* potential. The assignment of angle type to style is made via the angle_coeff command or in the data file.

In the angle_coeff commands, the name of an angle style must be added after the angle type, with the remaining coefficients being those appropriate to that style. In the example above, the 2 angle_coeff commands set angles of angle type 1 to be computed with a *harmonic* potential with coefficients 80.0, 30.0 for K, theta0. All other angle types (2-N) are computed with a *cosine* potential with coefficient 50.0 for K.

If angle coefficients are specified in the data file read via the read_data command, then the same rule applies. E.g. "harmonic" or "cosine", must be added after the angle type, for each line in the "Angle Coeffs" section, e.g.

```
Angle Coeffs

1 harmonic 80.0 30.0
2 cosine 50.0
...
```

If *class2* is one of the angle hybrid styles, the same rule holds for specifying additional BondBond (and BondAngle) coefficients either via the input script or in the data file. I.e. *class2* must be added to each line after the angle type. For lines in the BondBond (or BondAngle) section of the data file for angle types that are not *class2*, you must use an angle style of *skip* as a placeholder, e.g.

```
BondBond Coeffs

1 skip
2 class2 3.6512 1.0119 1.0119
...
```

Note that it is not necessary to use the angle style *skip* in the input script, since BondBond (or BondAngle) coefficients need not be specified at all for angle types that are not *class2*.

An angle style of *none* with no additional coefficients can be used in place of an angle style, either in a input script angle_coeff command or in the data file, if you desire to turn off interactions for specific angle types.

Restrictions:

This angle style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Unlike other angle styles, the hybrid angle style does not store angle coefficient info for individual sub-styles in a binary restart files. Thus when retarting a simulation from a restart file, you need to re-specify angle_coeff commands.

Related commands:

angle_coeff

Default: none

angle_style none command

Syntax:

```
angle_style none
```

Examples:

```
angle_style none
```

Description:

Using an angle style of none means angle forces are not computed, even if triplets of angle atoms were listed in the data file read by the read_data command.

Restrictions: none

Related commands: none

Default: none

angle_style quartic command

angle_style quartic/omp command

Syntax:

```
angle_style quartic
```

Examples:

```
angle_style quartic
angle_coeff 1 129.1948 56.8726 -25.9442 -14.2221
```

Description:

The *quartic* angle style uses the potential

$$E = K_2(\theta - \theta_0)^2 + K_3(\theta - \theta_0)^3 + K_4(\theta - \theta_0)^4$$

where theta0 is the equilibrium value of the angle, and K is a prefactor. Note that the usual 1/2 factor is included in K.

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- theta0 (degrees)
- K2 (energy/radian^2)
- K3 (energy/radian^3)
- K4 (energy/radian^4)

Theta0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K are in energy/radian^2.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the USER_MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff

Default: none

angle_style sdk command

Syntax:

```
angle_style sdk

angle_style sdk/omp
```

Examples:

```
angle_style sdk
angle_coeff 1 300.0 107.0
```

Description:

The *sdk* angle style is a combination of the harmonic angle potential,

$$E = K(\theta - \theta_0)^2$$

where theta0 is the equilibrium value of the angle and K a prefactor, with the *repulsive* part of the non-bonded *lj/sdk* pair style between the atoms 1 and 3. This angle potential is intended for coarse grained MD simulations with the CMM parametrization using the pair_style lj/sdk. Relative to the pair_style *lj/sdk*, however, the energy is shifted by *epsilon*, to avoid sudden jumps. Note that the usual 1/2 factor is included in K.

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above:

- K (energy/radian^2)
- theta0 (degrees)

Theta0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K are in energy/radian^2. The also required *lj/sdk* parameters will be extracted automatically from the pair_style.

Restrictions:

This angle style can only be used if LAMMPS was built with the USER-CG-CMM package. See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff, angle_style harmonic, pair_style lj/sdk, pair_style lj/sdk/coul/long

Default: none

angle_style command

Syntax:

```
angle_style style
```

- style = *none* or *hybrid* or *charmm* or *class2* or *cosine* or *cosine/squared* or *harmonic*

Examples:

```
angle_style harmonic
angle_style charmm
angle_style hybrid harmonic cosine
```

Description:

Set the formula(s) LAMMPS uses to compute angle interactions between triplets of atoms, which remain in force for the duration of the simulation. The list of angle triplets is read in by a read_data or read_restart command from a data or restart file.

Hybrid models where angles are computed using different angle potentials can be setup using the *hybrid* angle style.

The coefficients associated with a angle style can be specified in a data or restart file or via the angle_coeff command.

All angle potentials store their coefficient data in binary restart files which means angle_style and angle_coeff commands do not need to be re-specified in an input script that restarts a simulation. See the read_restart command for details on how to do this. The one exception is that angle_style *hybrid* only stores the list of sub-styles in the restart file; angle coefficients need to be re-specified.

NOTE: When both an angle and pair style is defined, the special_bonds command often needs to be used to turn off (or weight) the pairwise interaction that would otherwise exist between 3 bonded atoms.

In the formulas listed for each angle style, *theta* is the angle between the 3 atoms in the angle.

Here is an alphabetic list of angle styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated angle_coeff command.

Note that there are also additional angle styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the angle section of this page.

- angle_style none - turn off angle interactions
- angle_style hybrid - define multiple styles of angle interactions

- angle_style charmm - CHARMM angle
- angle_style class2 - COMPASS (class 2) angle
- angle_style cosine - cosine angle potential
- angle_style cosine/delta - difference of cosines angle potential
- angle_style cosine/periodic - DREIDING angle
- angle_style cosine/squared - cosine squared angle potential

- angle_style harmonic - harmonic angle
- angle_style table - tabulated by angle

Restrictions:

Angle styles can only be set for atom_styles that allow angles to be defined.

Most angle styles are part of the MOLECULE package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info on packages. The doc pages for individual bond potentials tell if it is part of a package.

Related commands:

angle_coeff

Default:

```
angle_style none
```

angle_style table command

angle_style table/omp command

Syntax:

```
angle_style table style N
```

- style = *linear* or *spline* = method of interpolation
- N = use N values in table

Examples:

```
angle_style table linear 1000
angle_coeff 3 file.table ENTRY1
```

Description:

Style *table* creates interpolation tables of length *N* from angle potential and derivative values listed in a file(s) as a function of angle The files are read by the angle_coeff command.

The interpolation tables are created by fitting cubic splines to the file values and interpolating energy and derivative values at each of *N* angles. During a simulation, these tables are used to interpolate energy and force values on individual atoms as needed. The interpolation is done in one of 2 styles: *linear* or *spline*.

For the *linear* style, the angle is used to find 2 surrounding table values from which an energy or its derivative is computed by linear interpolation.

For the *spline* style, a cubic spline coefficients are computed and stored at each of the *N* values in the table. The angle is used to find the appropriate set of coefficients which are used to evaluate a cubic polynomial which computes the energy or derivative.

The following coefficients must be defined for each angle type via the angle_coeff command as in the example above.

- filename
- keyword

The filename specifies a file containing tabulated energy and derivative values. The keyword specifies a section of the file. The format of this file is described below.

The format of a tabulated file is as follows (without the parenthesized comments):

```
# Angle potential for harmonic (one or more comment or blank lines)

HAM                          (keyword is the first text on line)
N 181 FP 0 0 EQ 90.0         (N, FP, EQ parameters)
                             (blank line)
N 181 FP 0 0                 (N, FP parameters)
1 0.0 200.5 2.5              (index, angle, energy, derivative)
2 1.0 198.0 2.5
...
```

```
181 180.0 0.0 0.0
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the angle_coeff command. The next line lists (in any order) one or more parameters for the table. Each parameter is a keyword followed by one or more numeric values.

The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the *N* specified in the angle_style table command. Let Ntable = *N* in the angle_style command, and Nfile = "N" in the tabulated file. What LAMMPS does is a preliminary interpolation by creating splines using the Nfile tabulated values as nodal points. It uses these to interpolate as needed to generate energy and derivative values at Ntable different points. The resulting tables of length Ntable are then used as described above, when computing energy and force for individual angles and their atoms. This means that if you want the interpolation tables of length Ntable to match exactly what is in the tabulated file (with effectively no preliminary interpolation), you should set Ntable = Nfile.

The "FP" parameter is optional. If used, it is followed by two values fplo and fphi, which are the 2nd derivatives at the innermost and outermost angle settings. These values are needed by the spline construction routines. If not specified by the "FP" parameter, they are estimated (less accurately) by the first two and last two derivative values in the table.

The "EQ" parameter is also optional. If used, it is followed by a the equilibrium angle value, which is used, for example, by the fix shake command. If not used, the equilibrium angle is set to 180.0.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is the angle value (in degrees), the 3rd value is the energy (in energy units), and the 4th is -dE/d(theta) (also in energy units). The 3rd term is the energy of the 3-atom configuration for the specified angle. The last term is the derivative of the energy with respect to the angle (in degrees, not radians). Thus the units of the last term are still energy, not force. The angle values must increase from one line to the next. The angle values must also begin with 0.0 and end with 180.0, i.e. span the full range of possible angles.

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

angle_coeff

Default: none

atom_modify command

Syntax:

```
atom_modify keyword values ...
```

- one or more keyword/value pairs may be appended
- keyword = *id* or *map* or *first* or *sort*

```
id value = yes or no
   map value = array or hash
   first value = group-ID = group whose atoms will appear first in internal atom lists
   sort values = Nfreq binsize
     Nfreq = sort atoms spatially every this many time steps
     binsize = bin size for spatial sorting (distance units)
```

Examples:

```
atom_modify map hash
atom_modify map array sort 10000 2.0
atom_modify first colloid
```

Description:

Modify certain attributes of atoms defined and stored within LAMMPS, in addition to what is specified by the atom_style command. The *id* and *map* keywords must be specified before a simulation box is defined; other keywords can be specified any time.

The *id* keyword determines whether non-zero atom IDs can be assigned to each atom. If the value is *yes*, which is the default, IDs are assigned, whether you use the create atoms or read_data or read_restart commands to initialize atoms. If the value is *no* the IDs for all atoms are assumed to be 0.

If atom IDs are used, they must all be positive integers. They should also be unique, though LAMMPS does not check for this. Typically they should also be consecutively numbered (from 1 to Natoms), though this is not required. Molecular atom styles are those that store bond topology information (styles bond, angle, molecular, full). These styles require atom IDs since the IDs are used to encode the topology. Some other LAMMPS commands also require the use of atom IDs. E.g. some many-body pair styles use them to avoid double computation of the I-J interaction between two atoms.

The only reason not to use atom IDs is if you are running an atomic simulation so large that IDs cannot be uniquely assigned. For a default LAMMPS build this limit is 2^31 or about 2 billion atoms. However, even in this case, you can use 64-bit atom IDs, allowing 2^63 or about 9e18 atoms, if you build LAMMPS with the -DLAMMPS_BIGBIG switch. This is described in Section 2.2 of the manual. If atom IDs are not used, they must be specified as 0 for all atoms, e.g. in a data or restart file.

The *map* keyword determines how atom ID lookup is done for molecular atom styles. Lookups are performed by bond (angle, etc) routines in LAMMPS to find the local atom index associated with a global atom ID.

When the *array* value is used, each processor stores a lookup table of length N, where N is the largest atom ID in the system. This is a fast, simple method for many simulations, but requires too much memory for large simulations. The *hash* value uses a hash table to perform the lookups. This can be slightly slower than the *array* method, but its memory cost is proportional to the number of atoms owned by a processor, i.e. N/P when N is the

total number of atoms in the system and P is the number of processors.

When this setting is not specified in your input script, LAMMPS creates a map, if one is needed, as an array or hash. See the discussion of default values below for how LAMMPS chooses which kind of map to build. Note that atomic systems do not normally need to create a map. However, even in this case some LAMMPS commands will create a map to find atoms (and then destroy it), or require a permanent map. An example of the former is the velocity loop all command, which uses a map when looping over all atoms and insuring the same velocity values are assigned to an atom ID, no matter which processor owns it.

The *first* keyword allows a group to be specified whose atoms will be maintained as the first atoms in each processor's list of owned atoms. This in only useful when the specified group is a small fraction of all the atoms, and there are other operations LAMMPS is performing that will be sped-up significantly by being able to loop over the smaller set of atoms. Otherwise the reordering required by this option will be a net slow-down. The neigh_modify include and comm_modify group commands are two examples of commands that require this setting to work efficiently. Several fixes, most notably time integration fixes like fix nve, also take advantage of this setting if the group they operate on is the group specified by this command. Note that specifying "all" as the group-ID effectively turns off the *first* option.

It is OK to use the *first* keyword with a group that has not yet been defined, e.g. to use the atom_modify first command at the beginning of your input script. LAMMPS does not use the group until a simullation is run.

The *sort* keyword turns on a spatial sorting or reordering of atoms within each processor's sub-domain every *Nfreq* timesteps. If *Nfreq* is set to 0, then sorting is turned off. Sorting can improve cache performance and thus speed-up a LAMMPS simulation, as discussed in a paper by (Meloni). Its efficacy depends on the problem size (atoms/processor), how quickly the system becomes disordered, and various other factors. As a general rule, sorting is typically more effective at speeding up simulations of liquids as opposed to solids. In tests we have done, the speed-up can range from zero to 3-4x.

Reordering is peformed every *Nfreq* timesteps during a dynamics run or iterations during a minimization. More precisely, reordering occurs at the first reneighboring that occurs after the target timestep. The reordering is performed locally by each processor, using bins of the specified *binsize*. If *binsize* is set to 0.0, then a binsize equal to half the neighbor cutoff distance (force cutoff plus skin distance) is used, which is a reasonable value. After the atoms have been binned, they are reordered so that atoms in the same bin are adjacent to each other in the processor's 1d list of atoms.

The goal of this procedure is for atoms to put atoms close to each other in the processor's one-dimensional list of atoms that are also near to each other spatially. This can improve cache performance when pairwise intereractions and neighbor lists are computed. Note that if bins are too small, there will be few atoms/bin. Likewise if bins are too large, there will be many atoms/bin. In both cases, the goal of cache locality will be undermined.

NOTE: Running a simulation with sorting on versus off should not change the simulation results in a statistical sense. However, a different ordering will induce round-off differences, which will lead to diverging trajectories over time when comparing two simluations. Various commands, particularly those which use random numbers (e.g. velocity create, and fix langevin), may generate (statistically identical) results which depend on the order in which atoms are processed. The order of atoms in a dump file will also typically change if sorting is enabled.

Restrictions:

The *first* and *sort* options cannot be used together. Since sorting is on by default, it will be turned off if the *first* keyword is used with a group-ID that is not "all".

Related commands: none

Default:

By default, *id* is yes. By default, atomic systems (no bond topology info) do not use a map. For molecular systems (with bond topology info), a map is used. The default map style is array if no atom ID is larger than 1 million, otherwise the default is hash. By default, a "first" group is not defined. By default, sorting is enabled with a frequency of 1000 and a binsize of 0.0, which means the neighbor cutoff will be used to set the bin size.

(Meloni) Meloni, Rosati and Colombo, J Chem Phys, 126, 121102 (2007).

atom_style command

Syntax:

```
atom_style style args
```

- style = *angle* or *atomic* or *body* or *bond* or *charge* or *dipole* or *dpd* or *electron* or *ellipsoid* or *full* or *line* or *meso* or *molecular* or *peri* or *smd* or *sphere* or *tri* or *template* or *hybrid*

```
args = none for any style except the following
body args = bstyle bstyle-args
  bstyle = style of body particles
  bstyle-args = additional arguments specific to the bstyle
                see the body doc page for details
template args = template-ID
  template-ID = ID of molecule template specified in a separate molecule command
hybrid args = list of one or more sub-styles, each with their args
```

- accelerated styles (with same args) = *angle/cuda* or *angle/kk* or *atomic/cuda* or *atomic/kk* or *bond/kk* or *charge/cuda* or *charge/kk* or *full/cuda* or *full/kk* or *molecular/kk*

Examples:

```
atom_style atomic
atom_style bond
atom_style full
atom_style full/cuda
atom_style body nparticle 2 10
atom_style hybrid charge bond
atom_style hybrid charge body nparticle 2 5
atom_style template myMols
```

Description:

Define what style of atoms to use in a simulation. This determines what attributes are associated with the atoms. This command must be used before a simulation is setup via a read_data, read_restart, or create_box command.

NOTE: Many of the atom styles discussed here are only enabled if LAMMPS was built with a specific package, as listed below in the Restrictions section.

Once a style is assigned, it cannot be changed, so use a style general enough to encompass all attributes. E.g. with style *bond*, angular terms cannot be used or added later to the model. It is OK to use a style more general than needed, though it may be slightly inefficient.

The choice of style affects what quantities are stored by each atom, what quantities are communicated between processors to enable forces to be computed, and what quantities are listed in the data file read by the read_data command.

These are the additional attributes of each style and the typical kinds of physical systems they are used to model. All styles store coordinates, velocities, atom IDs and types. See the read_data, create_atoms, and set commands for info on how to set these various quantities.

angle	bonds and angles	bead-spring polymers with stiffness
atomic	only the default values	coarse-grain liquids, solids, metals

body	mass, inertia moments, quaternion, angular momentum	arbitrary bodies
bond	bonds	bead-spring polymers
charge	charge	atomic system with charges
dipole	charge and dipole moment	system with dipolar particles
dpd	internal temperature and internal energies	DPD particles
electron	charge and spin and eradius	electronic force field
ellipsoid	shape, quaternion, angular momentum	aspherical particles
full	molecular + charge	bio-molecules
line	end points, angular velocity	rigid bodies
meso	rho, e, cv	SPH particles
molecular	bonds, angles, dihedrals, impropers	uncharged molecules
peri	mass, volume	mesocopic Peridynamic models
smd	volume, kernel diameter, contact radius, mass	solid and fluid SPH particles
sphere	diameter, mass, angular velocity	granular models
template	template index, template atom	small molecules with fixed topology
tri	corner points, angular momentum	rigid bodies
wavepacket	charge, spin, eradius, etag, cs_re, cs_im	AWPMD

NOTE: It is possible to add some attributes, such as a molecule ID, to atom styles that do not have them via the fix property/atom command. This command also allows new custom attributes consisting of extra integer or floating-point values to be added to atoms. See the fix property/atom doc page for examples of cases where this is useful and details on how to initialize, access, and output the custom values.

All of the above styles define point particles, except the *sphere*, *ellipsoid*, *electron*, *peri*, *wavepacket*, *line*, *tri*, and *body* styles, which define finite-size particles. See Section_howto 14 for an overview of using finite-size particle models with LAMMPS.

All of the point-particle styles assign mass to particles on a per-type basis, using the mass command, The finite-size particle styles assign mass to individual particles on a per-particle basis.

For the *sphere* style, the particles are spheres and each stores a per-particle diameter and mass. If the diameter > 0.0, the particle is a finite-size sphere. If the diameter = 0.0, it is a point particle.

For the *ellipsoid* style, the particles are ellipsoids and each stores a flag which indicates whether it is a finite-size ellipsoid or a point particle. If it is an ellipsoid, it also stores a shape vector with the 3 diamters of the ellipsoid and a quaternion 4-vector with its orientation.

For the *dipole* style, a point dipole is defined for each point particle. Note that if you wish the particles to be finite-size spheres as in a Stockmayer potential for a dipolar fluid, so that the particles can rotate due to dipole-dipole interactions, then you need to use atom_style hybrid sphere dipole, which will assign both a diameter and dipole moment to each particle.

For the *electron* style, the particles representing electrons are 3d Gaussians with a specified position and bandwidth or uncertainty in position, which is represented by the eradius = electron size.

For the *peri* style, the particles are spherical and each stores a per-particle mass and volume.

The *dpd* style is for dissipative particle dynamics (DPD) particles which store the particle internal temperature (dpdTheta), internal conductive energy (uCond) and internal mechanical energy (uMech).

The *meso* style is for smoothed particle hydrodynamics (SPH) particles which store a density (rho), energy (e), and heat capacity (cv).

The *smd* style is for a general formulation of Smooth Particle Hydrodynamics. Both fluids and solids can be modeled. Particles store the mass and volume of an integration point, a kernel diameter used for calculating the field variables (e.g. stress and deformation) and a contact radius for calculating repulsive forces which prevent individual physical bodies from penetretating each other.

The *wavepacket* style is similar to *electron*, but the electrons may consist of several Gaussian wave packets, summed up with coefficients cs= (cs_re,cs_im). Each of the wave packets is treated as a separate particle in LAMMPS, wave packets belonging to the same electron must have identical *etag* values.

For the *line* style, the particles are idealized line segments and each stores a per-particle mass and length and orientation (i.e. the end points of the line segment).

For the *tri* style, the particles are planar triangles and each stores a per-particle mass and size and orientation (i.e. the corner points of the triangle).

The *template* style allows molecular topolgy (bonds,angles,etc) to be defined via a molecule template using the molecule command. The template stores one or more molecules with a single copy of the topology info (bonds,angles,etc) of each. Individual atoms only store a template index and template atom to identify which molecule and which atom-within-the-molecule they represent. Using the *template* style instead of the *bond*, *angle*, *molecular* styles can save memory for systems comprised of a large number of small molecules, all of a single type (or small number of types). See the paper by Grime and Voth, in (Grime), for examples of how this can be advantageous for large-scale coarse-grained systems.

NOTE: When using the *template* style with a molecule template that contains multiple molecules, you should insure the atom types, bond types, angle_types, etc in all the molecules are consistent. E.g. if one molecule represents H2O and another CO2, then you probably do not want each molecule file to define 2 atom types and a single bond type, because they will conflict with each other when a mixture system of H2O and CO2 molecules is defined, e.g. by the read_data command. Rather the H2O molecule should define atom types 1 and 2, and bond type 1. And the CO2 molecule should define atom types 3 and 4 (or atom types 3 and 2 if a single oxygen type is desired), and bond type 2.

For the *body* style, the particles are arbitrary bodies with internal attributes defined by the "style" of the bodies, which is specified by the *bstyle* argument. Body particles can represent complex entities, such as surface meshes of discrete points, collections of sub-particles, deformable objects, etc.

The body doc page descibes the body styles LAMMPS currently supports, and provides more details as to the kind of body particles they represent. For all styles, each body particle stores moments of inertia and a quaternion 4-vector, so that its orientation and position can be time integrated due to forces and torques.

Note that there may be additional arguments required along with the *bstyle* specification, in the atom_style body command. These arguments are described in the body doc page.

Typically, simulations require only a single (non-hybrid) atom style. If some atoms in the simulation do not have all the properties defined by a particular style, use the simplest style that defines all the needed properties by any atom. For example, if some atoms in a simulation are charged, but others are not, use the *charge* style. If some atoms have bonds, but others do not, use the *bond* style.

The only scenario where the *hybrid* style is needed is if there is no single style which defines all needed properties of all atoms. For example, as mentioned above, if you want dipolar particles which will rotate due to torque, you

need to use "atom_style hybrid sphere dipole". When a hybrid style is used, atoms store and communicate the union of all quantities implied by the individual styles.

When using the *hybrid* style, you cannot combine the *template* style with another molecular style that stores bond,angle,etc info on a per-atom basis.

LAMMPS can be extended with new atom styles as well as new body styles; see this section.

Styles with a *cuda* or *kk* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

Note that other acceleration packages in LAMMPS, specifically the GPU, USER-INTEL, USER-OMP, and OPT packages do not use accelerated atom styles.

The accelerated styles are part of the USER-CUDA and KOKKOS packages respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This command cannot be used after the simulation box is defined by a read_data or create_box command.

Many of the styles listed above are only enabled if LAMMPS was built with a specific package, as listed below. See the Making LAMMPS section for more info.

The *angle*, *bond*, *full*, *molecular*, and *template* styles are part of the MOLECULE package.

The *line* and *tri* styles are part of the ASPHERE pacakge.

The *body* style is part of the BODY package.

The *dipole* style is part of the DIPOLE package.

The *peri* style is part of the PERI package for Peridynamics.

The *electron* style is part of the USER-EFF package for electronic force fields.

The *dpd* style is part of the USER-DPD package for dissipative particle dynamics (DPD).

The *meso* style is part of the USER-SPH package for smoothed particle hydrodyanmics (SPH). See this PDF guide to using SPH in LAMMPS.

The *wavepacket* style is part of the USER-AWPMD package for the antisymmetrized wave packet MD method.

Related commands:

read_data, pair_style

Default:

atom_style atomic

(Grime) Grime and Voth, to appear in J Chem Theory & Computation (2014).

balance command

Syntax:

```
balance thresh style args ... keyword value ...
```

- thresh = imbalance threshhold that must be exceeded to perform a re-balance
- one style/arg pair can be used (or multiple for *x*,*y*,*z*)
- style = *x* or *y* or *z* or *shift* or *rcb*

```
  x args = uniform or Px-1 numbers between 0 and 1
      uniform = evenly spaced cuts between processors in x dimension
      numbers = Px-1 ascending values between 0 and 1, Px - # of processors in x dimension
      x can be specified together with y or z
    y args = uniform or Py-1 numbers between 0 and 1
      uniform = evenly spaced cuts between processors in y dimension
      numbers = Py-1 ascending values between 0 and 1, Py - # of processors in y dimension
      y can be specified together with x or z
    z args = uniform or Pz-1 numbers between 0 and 1
      uniform = evenly spaced cuts between processors in z dimension
      numbers = Pz-1 ascending values between 0 and 1, Pz - # of processors in z dimension
      z can be specified together with x or y
    shift args = dimstr Niter stopthresh
      dimstr = sequence of letters containing "x" or "y" or "z", each not more than once
      Niter = # of times to iterate within each dimension of dimstr sequence
      stopthresh = stop balancing when this imbalance threshhold is reached
    rcb args = none
```

- zero or more keyword/value pairs may be appended
- keyword = *out*

```
  out value = filename
      filename = write each processor's sub-domain to a file
```

Examples:

```
balance 0.9 x uniform y 0.4 0.5 0.6
balance 1.2 shift xz 5 1.1
balance 1.0 shift xz 5 1.1
balance 1.1 rcb
balance 1.0 shift x 20 1.0 out tmp.balance
```

Description:

This command adjusts the size and shape of processor sub-domains within the simulation box, to attempt to balance the number of particles and thus the computational cost (load) evenly across processors. The load balancing is "static" in the sense that this command performs the balancing once, before or between simulations. The processor sub-domains will then remain static during the subsequent run. To perform "dynamic" balancing, see the fix balance command, which can adjust processor sub-domain sizes and shapes on-the-fly during a run.

Load-balancing is typically only useful if the particles in the simulation box have a spatially-varying density distribution. E.g. a model of a vapor/liquid interface, or a solid with an irregular-shaped geometry containing void regions. In this case, the LAMMPS default of dividing the simulation box volume into a regular-spaced grid of 3d bricks, with one equal-volume sub-domain per procesor, may assign very different numbers of particles per processor. This can lead to poor performance when the simulation is run in parallel.

Note that the processors command allows some control over how the box volume is split across processors. Specifically, for a Px by Py by Pz grid of processors, it allows choice of Px, Py, and Pz, subject to the constraint that Px * Py * Pz = P, the total number of processors. This is sufficient to achieve good load-balance for some problems on some processor counts. However, all the processor sub-domains will still have the same shape and same volume.

The requested load-balancing operation is only performed if the current "imbalance factor" in particles owned by each processor exceeds the specified *thresh* parameter. The imbalance factor is defined as the maximum number of particles owned by any processor, divided by the average number of particles per processor. Thus an imbalance factor of 1.0 is perfect balance.

As an example, for 10000 particles running on 10 processors, if the most heavily loaded processor has 1200 particles, then the factor is 1.2, meaning there is a 20% imbalance. Note that a re-balance can be forced even if the current balance is perfect (1.0) be specifying a *thresh* < 1.0.

NOTE: Balancing is performed even if the imbalance factor does not exceed the *thresh* parameter if a "grid" style is specified when the current partitioning is "tiled". The meaning of "grid" vs "tiled" is explained below. This is to allow forcing of the partitioning to "grid" so that the comm_style brick command can then be used to replace a current comm_style tiled setting.

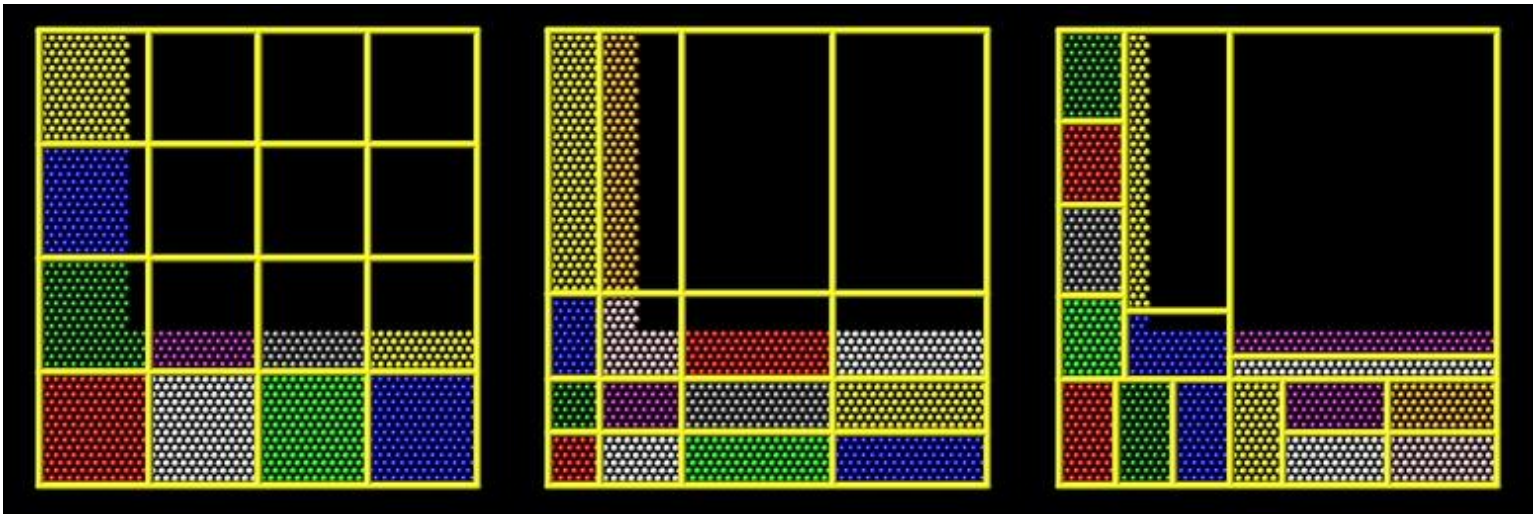
When the balance command completes, it prints statistics about the result, including the change in the imbalance factor and the change in the maximum number of particles on any processor. For "grid" methods (defined below) that create a logical 3d grid of processors, the positions of all cutting planes in each of the 3 dimensions (as fractions of the box length) are also printed.

NOTE: This command attempts to minimize the imbalance factor, as defined above. But depending on the method a perfect balance (1.0) may not be achieved. For example, "grid" methods (defined below) that create a logical 3d grid cannot achieve perfect balance for many irregular distributions of particles. Likewise, if a portion of the system is a perfect lattice, e.g. the intiial system is generated by the create_atoms command, then "grid" methods may be unable to achieve exact balance. This is because entire lattice planes will be owned or not owned by a single processor.

NOTE: The imbalance factor is also an estimate of the maximum speed-up you can hope to achieve by running a perfectly balanced simulation versus an imbalanced one. In the example above, the 10000 particle simulation could run up to 20% faster if it were perfectly balanced, versus when imbalanced. However, computational cost is not strictly proportional to particle count, and changing the relative size and shape of processor sub-domains may lead to additional computational and communication overheads, e.g. in the PPPM solver used via the kspace_style command. Thus you should benchmark the run times of a simulation before and after balancing.

The method used to perform a load balance is specified by one of the listed styles (or more in the case of *x*,*y*,*z*), which are described in detail below. There are 2 kinds of styles.

The *x*, *y*, *z*, and *shift* styles are "grid" methods which produce a logical 3d grid of processors. They operate by changing the cutting planes (or lines) between processors in 3d (or 2d), to adjust the volume (area in 2d) assigned to each processor, as in the following 2d diagram where processor sub-domains are shown and atoms are colored by the processor that owns them. The leftmost diagram is the default partitioning of the simulation box across processors (one sub-box for each of 16 processors); the middle diagram is after a "grid" method has been applied.



The *rcb* style is a "tiling" method which does not produce a logical 3d grid of processors. Rather it tiles the simulation domain with rectangular sub-boxes of varying size and shape in an irregular fashion so as to have equal numbers of particles in each sub-box, as in the rightmost diagram above.

The "grid" methods can be used with either of the comm_style command options, *brick* or *tiled*. The "tiling" methods can only be used with comm_style tiled. Note that it can be useful to use a "grid" method with comm_style tiled to return the domain partitioning to a logical 3d grid of processors so that "comm_style brick" can afterwords be specified for subsequent run commands.

When a "grid" method is specified, the current domain partitioning can be either a logical 3d grid or a tiled partitioning. In the former case, the current logical 3d grid is used as a starting point and changes are made to improve the imbalance factor. In the latter case, the tiled partitioning is discarded and a logical 3d grid is created with uniform spacing in all dimensions. This becomes the starting point for the balancing operation.

When a "tiling" method is specified, the current domain partitioning ("grid" or "tiled") is ignored, and a new partitioning is computed from scratch.

The *x*, *y*, and *z* styles invoke a "grid" method for balancing, as described above. Note that any or all of these 3 styles can be specified together, one after the other, but they cannot be used with any other style. This style adjusts the position of cutting planes between processor sub-domains in specific dimensions. Only the specified dimensions are altered.

The *uniform* argument spaces the planes evenly, as in the left diagrams above. The *numeric* argument requires listing Ps-1 numbers that specify the position of the cutting planes. This requires knowing Ps = Px or Py or Pz = the number of processors assigned by LAMMPS to the relevant dimension. This assignment is made (and the Px, Py, Pz values printed out) when the simulation box is created by the "create_box" or "read_data" or "read_restart" command and is influenced by the settings of the processors command.

Each of the numeric values must be between 0 and 1, and they must be listed in ascending order. They represent the fractional position of the cutting place. The left (or lower) edge of the box is 0.0, and the right (or upper) edge is 1.0. Neither of these values is specified. Only the interior Ps-1 positions are specified. Thus is there are 2 procesors in the x dimension, you specify a single value such as 0.75, which would make the left processor's sub-domain 3x larger than the right processor's sub-domain.

The *shift* style invokes a "grid" method for balancing, as described above. It changes the positions of cutting planes between processors in an iterative fashion, seeking to reduce the imbalance factor, similar to how the fix balance shift command operates.

The *dimstr* argument is a string of characters, each of which must be an "x" or "y" or "z". Eacn character can appear zero or one time, since there is no advantage to balancing on a dimension more than once. You should normally only list dimensions where you expect there to be a density variation in the particles.

Balancing proceeds by adjusting the cutting planes in each of the dimensions listed in *dimstr*, one dimension at a time. For a single dimension, the balancing operation (described below) is iterated on up to *Niter* times. After each dimension finishes, the imbalance factor is re-computed, and the balancing operation halts if the *stopthresh* criterion is met.

A rebalance operation in a single dimension is performed using a recursive multisectioning algorithm, where the position of each cutting plane (line in 2d) in the dimension is adjusted independently. This is similar to a recursive bisectioning for a single value, except that the bounds used for each bisectioning take advantage of information from neighboring cuts if possible. At each iteration, the count of particles on either side of each plane is tallied. If the counts do not match the target value for the plane, the position of the cut is adjusted to be halfway between a low and high bound. The low and high bounds are adjusted on each iteration, using new count information, so that they become closer together over time. Thus as the recustion progresses, the count of particles on either side of the plane gets closer to the target value.

Once the rebalancing is complete and final processor sub-domains assigned, particles are migrated to their new owning processor, and the balance procedure ends.

NOTE: At each rebalance operation, the bisectioning for each cutting plane (line in 2d) typcially starts with low and high bounds separated by the extent of a processor's sub-domain in one dimension. The size of this bracketing region shrinks by 1/2 every iteration. Thus if *Niter* is specified as 10, the cutting plane will typically be positioned to 1 part in 1000 accuracy (relative to the perfect target position). For *Niter* = 20, it will be accurate to 1 part in a million. Thus there is no need ot set *Niter* to a large value. LAMMPS will check if the threshold accuracy is reached (in a dimension) is less iterations than *Niter* and exit early. However, *Niter* should also not be set too small, since it will take roughly the same number of iterations to converge even if the cutting plane is initially close to the target value.

The *rcb* style invokes a "tiled" method for balancing, as described above. It performs a recursive coordinate bisectioning (RCB) of the simulation domain. The basic idea is as follows.

The simulation domain is cut into 2 boxes by an axis-aligned cut in the longest dimension, leaving one new box on either side of the cut. All the processors are also partitioned into 2 groups, half assigned to the box on the lower side of the cut, and half to the box on the upper side. (If the processor count is odd, one side gets an extra processor.) The cut is positioned so that the number of atoms in the lower box is exactly the number that the processors assigned to that box should own for load balance to be perfect. This also makes load balance for the upper box perfect. The positioning is done iteratively, by a bisectioning method. Note that counting atoms on either side of the cut requires communication between all processors at each iteration.

That is the procedure for the first cut. Subsequent cuts are made recursively, in exactly the same manner. The subset of processors assigned to each box make a new cut in the longest dimension of that box, splitting the box, the subset of processsors, and the atoms in the box in two. The recursion continues until every processor is assigned a sub-box of the entire simulation domain, and owns the atoms in that sub-box.

The *out* keyword writes a text file to the specified *filename* with the results of the balancing operation. The file contains the bounds of the sub-domain for each processor after the balancing operation completes. The format of the file is compatible with the Pizza.py *mdump* tool which has support for manipulating and visualizing mesh files. An example is shown here for a balancing by 4 processors for a 2d problem:

```
ITEM: TIMESTEP
0
```

```
ITEM: NUMBER OF NODES
16
ITEM: BOX BOUNDS
0 10
0 10
0 10
ITEM: NODES
1 1 0 0 0
2 1 5 0 0
3 1 5 5 0
4 1 0 5 0
5 1 5 0 0
6 1 10 0 0
7 1 10 5 0
8 1 5 5 0
9 1 0 5 0
10 1 5 5 0
11 1 5 10 0
12 1 10 5 0
13 1 5 5 0
14 1 10 5 0
15 1 10 10 0
16 1 5 10 0
ITEM: TIMESTEP
0
ITEM: NUMBER OF SQUARES
4
ITEM: SQUARES
1 1 1 2 3 4
2 1 5 6 7 8
3 1 9 10 11 12
4 1 13 14 15 16
```

The coordinates of all the vertices are listed in the NODES section, 5 per processor. Note that the 4 sub-domains share vertices, so there will be duplicate nodes in the list.

The "SQUARES" section lists the node IDs of the 4 vertices in a rectangle for each processor (1 to 4).

For a 3d problem, the syntax is similar with 8 vertices listed for each processor, instead of 4, and "SQUARES" replaced by "CUBES".

Restrictions:

For 2d simulations, the *z* style cannot be used. Nor can a "z" appear in *dimstr* for the *shift* style.

Related commands:

processors, fix balance

Default: none

Body particles

Overview:

This doc page is not about a LAMMPS input script command, but about body particles, which are generalized finite-size particles. Individual body particles can represent complex entities, such as surface meshes of discrete points, collections of sub-particles, deformable objects, etc. Note that other kinds of finite-size spherical and aspherical particles are also supported by LAMMPS, such as spheres, ellipsoids, line segments, and triangles, but they are simpler entities that body particles. See Section_howto 14 for a general overview of all these particle types.

Body particles are used via the atom_style body command. It takes a body style as an argument. The current body styles supported by LAMMPS are as follows. The name in the first column is used as the *bstyle* argument for the atom_style body command.

nparticle	rigid body with N sub-particles
rounded/polygon	2d convex polygon with N vertices

The body style determines what attributes are stored for each body and thus how they can be used to compute pairwise body/body or bond/non-body (point particle) interactions. More details of each style are described below.

NOTE: The rounded/polygon style listed in the table above and described below has not yet been relesed in LAMMPS. It will be soon.

We hope to add more styles in the future. See Section_modify 12 for details on how to add a new body style to the code.

When to use body particles:

You should not use body particles to model a rigid body made of simpler particles (e.g. point, sphere, ellipsoid, line segment, triangular particles), if the interaction between pairs of rigid bodies is just the summation of pairwise interactions between the simpler particles. LAMMPS already supports this kind of model via the fix rigid command. Any of the numerous pair styles that compute interactions between simpler particles can be used. The fix rigid command time integrates the motion of the rigid bodies. All of the standard LAMMPS commands for thermostatting, adding constraints, performing output, etc will operate as expected on the simple particles.

By contrast, when body particles are used, LAMMPS treats an entire body as a single particle for purposes of computing pairwise interactions, building neighbor lists, migrating particles between processors, outputting particles to a dump file, etc. This means that interactions between pairs of bodies or between a body and non-body (point) particle need to be encoded in an appropriate pair style. If such a pair style were to mimic the fix rigid model, it would need to loop over the entire collection of interactions between pairs of simple particles within the two bodies, each time a single body/body interaction was computed.

Thus it only makes sense to use body particles and develop such a pair style, when particle/particle interactions are more complex than what the fix rigid command can already calculate. For example, if particles have one or more of the following attributes:

- represented by a surface mesh
- represented by a collection of geometric entities (e.g. planes + spheres)

- deformable
- internal stress that induces fragmentation

then the interaction between pairs of particles is likely to be more complex than the summation of simple sub-particle interactions. An example is contact or frictional forces between particles with planar sufaces that inter-penetrate.

These are additional LAMMPS commands that can be used with body particles of different styles

fix nve/body	integrate motion of a body particle in NVE ensemble
fix nvt/body	ditto for NVT ensemble
fix npt/body	ditto for NPT ensemble
fix nph/body	ditto for NPH ensemble
compute body/local	store sub-particle attributes of a body particle
compute temp/body	compute temperature of body particles
dump local	output sub-particle attributes of a body particle
dump image	output body particle attributes as an image

The pair styles defined for use with specific body styles are listed in the sections below.

Specifics of body style nparticle:

The *nparticle* body style represents body particles as a rigid body with a variable number N of sub-particles. It is provided as a vanillia, prototypical example of a body particle, although as mentioned above, the fix rigid command already duplicates its functionality.

The atom_style body command for this body style takes two additional arguments:

```
atom_style body nparticle Nmin Nmax
Nmin = minimum # of sub-particles in any body in the system
Nmax = maximum # of sub-particles in any body in the system
```

The Nmin and Nmax arguments are used to bound the size of data structures used internally by each particle.

When the read_data command reads a data file for this body style, the following information must be provided for each entry in the *Bodies* section of the data file:

```
atom-ID 1 M
N
ixx iyy izz ixy ixz iyz
x1 y1 z1
...
xN yN zN
```

N is the number of sub-particles in the body particle. M = 6 + 3*N. The integer line has a single value N. The floating point line(s) list 6 moments of inertia followed by the coordinates of the N sub-particles (x1 to zN) as 3N values. These values can be listed on as many lines as you wish; see the read_data command for more details.

The 6 moments of inertia (ixx,iyy,izz,ixy,ixz,iyz) should be the values consistent with the current orientation of the rigid body around its center of mass. The values are with respect to the simulation box XYZ axes, not with respect to the prinicpal axes of the rigid body itself. LAMMPS performs the latter calculation internally. The coordinates of each sub-particle are specified as its x,y,z displacement from the center-of-mass of the body particle. The center-of-mass position of the particle is specified by the x,y,z values in the *Atoms* section of the

data file, as is the total mass of the body particle.

The pair_style body command can be used with this body style to compute body/body and body/non-body interactions.

For output purposes via the compute body/local and dump local commands, this body style produces one datum for each of the N sub-particles in a body particle. The datum has 3 values:

```
1 = x position of sub-particle
2 = y position of sub-particle
3 = z position of sub-particle
```

These values are the current position of the sub-particle within the simulation domain, not a displacement from the center-of-mass (COM) of the body particle itself. These values are calculated using the current COM and orientation of the body particle.

For images created by the dump image command, if the *body* keyword is set, then each body particle is drawn as a collection of spheres, one for each sub-particle. The size of each sphere is determined by the *bflag1* parameter for the *body* keyword. The *bflag2* argument is ignored.

Specifics of body style rounded/polygon:

The *rounded/polygon* body style represents body particles as a convex polygon with a variable number N > 2 of vertices, which can only be used for 2d models. One example use of this body style is for 2d discrete element models, as described in Fraige. Similar to body style *nparticle*, the atom_style body command for this body style takes two additional arguments:

```
atom_style body rounded/polygon Nmin Nmax
Nmin = minimum # of vertices in any body in the system
Nmax = maximum # of vertices in any body in the system
```

The Nmin and Nmax arguments are used to bound the size of data structures used internally by each particle.

When the read_data command reads a data file for this body style, the following information must be provided for each entry in the *Bodies* section of the data file:

```
atom-ID 1 M
N
ixx iyy izz ixy ixz iyz
x1 y1 z1
...
xN yN zN
i j j k k ...
radius
```

N is the number of vertices in the body particle. M = 6 + 3*N + 2*N + 1. The integer line has a single value N. The floating point line(s) list 6 moments of inertia followed by the coordinates of the N vertices (x1 to zN) as 3N values, followed by 2N vertex indices corresponding to the end points of the N edges, followed by a single radius value = the smallest circle encompassing the polygon. That last value is used to facilitate the body/body contact detection. These floating-point values can be listed on as many lines as you wish; see the read_data command for more details.

The 6 moments of inertia (ixx,iyy,izz,ixy,ixz,iyz) should be the values consistent with the current orientation of the rigid body around its center of mass. The values are with respect to the simulation box XYZ axes, not with respect to the prinicpal axes of the rigid body itself. LAMMPS performs the latter calculation internally. The

coordinates of each vertex are specified as its x,y,z displacement from the center-of-mass of the body particle. The center-of-mass position of the particle is specified by the x,y,z values in the *Atoms* section of the data file.

For example, the following information would specify a square particles whose edge length is sqrt(2):

```
3 1 27
4
1 1 4 0 0 0
-0.7071 -0.7071 0
-0.7071 0.7071 0
0.7071 0.7071 0
0.7071 -0.7071 0
0 1 1 2 2 3 3 0
1.0
```

The pair_style body/rounded/polygon command can be used with this body style to compute body/body interactions.

For output purposes via the compute body/local and dump local commands, this body style produces one datum for each of the N sub-particles in a body particle. The datum has 3 values:

```
1 = x position of vertex
2 = y position of vertex
3 = z position of vertex
```

These values are the current position of the vertex within the simulation domain, not a displacement from the center-of-mass (COM) of the body particle itself. These values are calculated using the current COM and orientation of the body particle.

For images created by the dump image command, if the *body* keyword is set, then each body particle is drawn as a convex polygon consisting of N line segments. Note that the line segments are drawn between the N vertices, which does not correspond exactly to the physical extent of the body (because the pair_style rounded/polygon defines finite-size spheres at those point and the line segments between the spheres are tangent to the spheres). The drawn diameter of each line segment is determined by the *bflag1* parameter for the *body* keyword. The *bflag2* argument is ignored.

(Fraige) F. Y. Fraige, P. A. Langston, A. J. Matchett, J. Dodds, Particuology, 6, 455 (2008).

bond_style class2 command

bond_style class2/omp command

Syntax:

```
bond_style class2
```

Examples:

```
bond_style class2
bond_coeff 1 1.0 100.0 80.0 80.0
```

Description:

The *class2* bond style uses the potential

$$E = K_2(r - r_0)^2 + K_3(r - r_0)^3 + K_4(r - r_0)^4$$

where r0 is the equilibrium bond distance.

See (Sun) for a description of the COMPASS class2 force field.

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- R0 (distance)
- K2 (energy/distance^2)
- K3 (energy/distance^3)
- K4 (energy/distance^4)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This bond style can only be used if LAMMPS was built with the CLASS2 package. See the Making LAMMPS section for more info on packages.

Related commands:

bond_coeff, delete_bonds

Default: none

(Sun) Sun, J Phys Chem B 102, 7338-7364 (1998).

bond_coeff command

Syntax:

```
bond_coeff N args
```

- N = bond type (see asterisk form below)
- args = coefficients for one or more bond types

Examples:

```
bond_coeff 5 80.0 1.2
bond_coeff * 30.0 1.5 1.0 1.0
bond_coeff 1*4 30.0 1.5 1.0 1.0
bond_coeff 1 harmonic 200.0 1.0
```

Description:

Specify the bond force field coefficients for one or more bond types. The number and meaning of the coefficients depends on the bond style. Bond coefficients can also be set in the data file read by the read_data command or in a restart file.

N can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to set the coefficients for multiple bond types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of bond types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

Note that using a bond_coeff command can override a previous setting for the same bond type. For example, these commands set the coeffs for all bond types, then overwrite the coeffs for just bond type 2:

```
bond_coeff * 100.0 1.2
bond_coeff 2 200.0 1.2
```

A line in a data file that specifies bond coefficients uses the exact same format as the arguments of the bond_coeff command in an input script, except that wild-card asterisks should not be used since coefficients for all N types must be listed in the file. For example, under the "Bond Coeffs" section of a data file, the line that corresponds to the 1st example above would be listed as

```
5 80.0 1.2
```

Here is an alphabetic list of bond styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated bond_coeff command.

Note that here are also additional bond styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the bond section of this page.

- bond_style none - turn off bonded interactions
- bond_style hybrid - define multiple styles of bond interactions

- bond_style class2 - COMPASS (class 2) bond

- bond_style fene - FENE (finite-extensible non-linear elastic) bond
- bond_style fene/expand - FENE bonds with variable size particles
- bond_style harmonic - harmonic bond
- bond_style morse - Morse bond
- bond_style nonlinear - nonlinear bond
- bond_style quartic - breakable quartic bond
- bond_style table - tabulated by bond length

Restrictions:

This command must come after the simulation box is defined by a read_data, read_restart, or create_box command.

A bond style must be defined before any bond coefficients are set, either in the input script or in a data file.

Related commands:

bond_style

Default: none

bond_style fene command

bond_style fene/kk command

bond_style fene/omp command

Syntax:

```
bond_style fene
```

Examples:

```
bond_style fene
bond_coeff 1 30.0 1.5 1.0 1.0
```

Description:

The *fene* bond style uses the potential

$$E = -0.5 K R_0^2 \ln \left[1 - \left(\frac{r}{R_0} \right)^2 \right] + 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] + \epsilon$$

to define a finite extensible nonlinear elastic (FENE) potential (Kremer), used for bead-spring polymer models. The first term is attractive, the 2nd Lennard-Jones term is repulsive. The first term extends to R0, the maximum extent of the bond. The 2nd term is cutoff at 2^(1/6) sigma, the minimum of the LJ potential.

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/distance^2)
- R0 (distance)
- epsilon (energy)
- sigma (distance)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This bond style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

You typically should specify special_bonds fene or special_bonds lj/coul 0 1 1 to use this bond style. LAMMPS will issue a warning it that's not the case.

Related commands:

bond_coeff, delete_bonds

Default: none

(Kremer) Kremer, Grest, J Chem Phys, 92, 5057 (1990).

bond_style fene/expand command

bond_style fene/expand/omp command

Syntax:

```
bond_style fene/expand
```

Examples:

```
bond_style fene/expand
bond_coeff 1 30.0 1.5 1.0 1.0 0.5
```

Description:

The *fene/expand* bond style uses the potential

$$E = -0.5KR_0^2 \ln\left[1 - \left(\frac{(r-\Delta)}{R_0}\right)^2\right] + 4\epsilon\left[\left(\frac{\sigma}{(r-\Delta)}\right)^{12} - \left(\frac{\sigma}{(r-\Delta)}\right)^{6}\right] +$$

to define a finite extensible nonlinear elastic (FENE) potential (Kremer), used for bead-spring polymer models. The first term is attractive, the 2nd Lennard-Jones term is repulsive.

The *fene/expand* bond style is similar to *fene* except that an extra shift factor of delta (positive or negative) is added to *r* to effectively change the bead size of the bonded atoms. The first term now extends to R0 + delta and the 2nd term is cutoff at 2^(1/6) sigma + delta.

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/distance^2)
- R0 (distance)
- epsilon (energy)
- sigma (distance)
- delta (distance)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This bond style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

You typically should specify special_bonds fene or special_bonds lj/coul 0 1 1 to use this bond style. LAMMPS will issue a warning it that's not the case.

Related commands:

bond_coeff, delete_bonds

Default: none

(Kremer) Kremer, Grest, J Chem Phys, 92, 5057 (1990).

bond_style harmonic command

bond_style harmonic/intel command

bond_style harmonic/kk command

bond_style harmonic/omp command

Syntax:

```
bond_style harmonic
```

Examples:

```
bond_style harmonic
bond_coeff 5 80.0 1.2
```

Description:

The *harmonic* bond style uses the potential

$$E = K(r - r_0)^2$$

where r0 is the equilibrium bond distance. Note that the usual 1/2 factor is included in K.

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/distance^2)
- r0 (distance)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This bond style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

bond_coeff, delete_bonds

Default: none

bond_style harmonic/shift command

bond_style harmonic/shift/omp command

Syntax:

```
bond_style harmonic/shift
```

Examples:

```
bond_style harmonic/shift
bond_coeff 5 10.0 0.5 1.0
```

Description:

The *harmonic/shift* bond style is a shifted harmonic bond that uses the potential

$$E = \frac{Umin}{(r_0 - r_c)^2} \left[(r - r_0)^2 - (r_c - r_0)^2 \right]$$

where r0 is the equilibrium bond distance, and rc the critical distance. The potential is -Umin at r0 and zero at rc. The spring constant is k = Umin / [2 (r0-rc)^2].

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- Umin (energy)
- r0 (distance)
- rc (distance)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This bond style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

bond_coeff, delete_bonds, bond_harmonic

Default: none

bond_style harmonic/shift/cut command

bond_style harmonic/shift/cut/omp command

Syntax:

```
bond_style harmonic/shift/cut
```

Examples:

```
bond_style harmonic/shift/cut
bond_coeff 5 10.0 0.5 1.0
```

Description:

The *harmonic/shift/cut* bond style is a shifted harmonic bond that uses the potential

$$E = \frac{Umin}{(r_0 - r_c)^2} \left[(r - r_0)^2 - (r_c - r_0)^2 \right]$$

where r0 is the equilibrium bond distance, and rc the critical distance. The bond potential is zero for distances r > rc. The potential is -Umin at r0 and zero at rc. The spring constant is k = Umin / [2 (r0-rc)^2].

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- Umin (energy)
- r0 (distance)
- rc (distance)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This bond style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

bond_coeff, delete_bonds, bond_harmonic, bond_harmonicshift

Default: none

bond_style hybrid command

Syntax:

```
bond_style hybrid style1 style2 ...
```

- style1,style2 = list of one or more bond styles

Examples:

```
bond_style hybrid harmonic fene
bond_coeff 1 harmonic 80.0 1.2
bond_coeff 2* fene 30.0 1.5 1.0 1.0
```

Description:

The *hybrid* style enables the use of multiple bond styles in one simulation. A bond style is assigned to each bond type. For example, bonds in a polymer flow (of bond type 1) could be computed with a *fene* potential and bonds in the wall boundary (of bond type 2) could be computed with a *harmonic* potential. The assignment of bond type to style is made via the bond_coeff command or in the data file.

In the bond_coeff commands, the name of a bond style must be added after the bond type, with the remaining coefficients being those appropriate to that style. In the example above, the 2 bond_coeff commands set bonds of bond type 1 to be computed with a *harmonic* potential with coefficients 80.0, 1.2 for K, r0. All other bond types (2-N) are computed with a *fene* potential with coefficients 30.0, 1.5, 1.0, 1.0 for K, R0, epsilon, sigma.

If bond coefficients are specified in the data file read via the read_data command, then the same rule applies. E.g. "harmonic" or "fene" must be added after the bond type, for each line in the "Bond Coeffs" section, e.g.

```
Bond Coeffs

1 harmonic 80.0 1.2
2 fene 30.0 1.5 1.0 1.0
...
```

A bond style of *none* with no additional coefficients can be used in place of a bond style, either in a input script bond_coeff command or in the data file, if you desire to turn off interactions for specific bond types.

Restrictions:

This bond style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Unlike other bond styles, the hybrid bond style does not store bond coefficient info for individual sub-styles in a binary restart files. Thus when retarting a simulation from a restart file, you need to re-specify bond_coeff commands.

Related commands:

bond_coeff, delete_bonds

Default: none

bond_style morse command

bond_style morse/omp command

Syntax:

```
bond_style morse
```

Examples:

```
bond_style morse
bond_coeff 5 1.0 2.0 1.2
```

Description:

The *morse* bond style uses the potential

$$E = D\left[1 - e^{-\alpha(r-r_0)}\right]^2$$

where r0 is the equilibrium bond distance, alpha is a stiffness parameter, and D determines the depth of the potential well.

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- D (energy)
- alpha (inverse distance)
- r0 (distance)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This bond style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

bond_coeff, delete_bonds

Default: none

bond_style none command

Syntax:

```
bond_style none
```

Examples:

```
bond_style none
```

Description:

Using a bond style of none means bond forces are not computed, even if pairs of bonded atoms were listed in the data file read by the read_data command.

Restrictions: none

Related commands: none

Default: none

bond_style nonlinear command

bond_style nonlinear/omp command

Syntax:

```
bond_style nonlinear
```

Examples:

```
bond_style nonlinear
bond_coeff 2 100.0 1.1 1.4
```

Description:

The *nonlinear* bond style uses the potential

$$E = \frac{\epsilon(r - r_0)^2}{[\lambda^2 - (r - r_0)^2]}$$

to define an anharmonic spring (Rector) of equilibrium length r0 and maximum extension lamda.

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- epsilon (energy)
- r0 (distance)
- lamda (distance)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This bond style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

bond_coeff, delete_bonds

Default: none

(Rector) Rector, Van Swol, Henderson, Molecular Physics, 82, 1009 (1994).

bond_style quartic command

bond_style quartic/omp command

Syntax:

```
bond_style quartic
```

Examples:

```
bond_style quartic
bond_coeff 2 1200 -0.55 0.25 1.3 34.6878
```

Description:

The *quartic* bond style uses the potential

$$E = K(r - R_c)^2(r - R_c - B_1)(r - R_c - B_2) + U_0 + 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] +$$

to define a bond that can be broken as the simulation proceeds (e.g. due to a polymer being stretched). The sigma and epsilon used in the LJ portion of the formula are both set equal to 1.0 by LAMMPS.

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/distance^4)
- B1 (distance)
- B2 (distance)
- Rc (distance)
- U0 (energy)

This potential was constructed to mimic the FENE bond potential for coarse-grained polymer chains. When monomers with sigma = epsilon = 1.0 are used, the following choice of parameters gives a quartic potential that looks nearly like the FENE potential: K = 1200, B1 = -0.55, B2 = 0.25, Rc = 1.3, and U0 = 34.6878. Different parameters can be specified using the bond_coeff command, but you will need to choose them carefully so they form a suitable bond potential.

Rc is the cutoff length at which the bond potential goes smoothly to a local maximum. If a bond length ever becomes > Rc, LAMMPS "breaks" the bond, which means two things. First, the bond potential is turned off by setting its type to 0, and is no longer computed. Second, a pairwise interaction between the two atoms is turned on, since they are no longer bonded.

LAMMPS does the second task via a computational sleight-of-hand. It subtracts the pairwise interaction as part of the bond computation. When the bond breaks, the subtraction stops. For this to work, the pairwise interaction must always be computed by the pair_style command, whether the bond is broken or not. This means that special_bonds must be set to 1,1,1, as indicated as a restriction below.

Note that when bonds are dumped to a file via the dump local command, bonds with type 0 are not included. The delete_bonds command can also be used to query the status of broken bonds or permanently delete them, e.g.:

```
delete_bonds all stats
delete_bonds all bond 0 remove
```

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This bond style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

The *quartic* style requires that special_bonds parameters be set to 1,1,1. Three- and four-body interactions (angle, dihedral, etc) cannot be used with *quartic* bonds.

Related commands:

bond_coeff, delete_bonds

Default: none

bond_style command

Syntax:

```
bond_style style args
```

- style = *none* or *hybrid* or *class2* or *fene* or *fene/expand* or *harmonic* or *morse* or *nonlinear* or *quartic*

```
  args = none for any style except hybrid
  hybrid args = list of one or more styles
```

Examples:

```
bond_style harmonic
bond_style fene
bond_style hybrid harmonic fene
```

Description:

Set the formula(s) LAMMPS uses to compute bond interactions between pairs of atoms. In LAMMPS, a bond differs from a pairwise interaction, which are set via the pair_style command. Bonds are defined between specified pairs of atoms and remain in force for the duration of the simulation (unless the bond breaks which is possible in some bond potentials). The list of bonded atoms is read in by a read_data or read_restart command from a data or restart file. By contrast, pair potentials are typically defined between all pairs of atoms within a cutoff distance and the set of active interactions changes over time.

Hybrid models where bonds are computed using different bond potentials can be setup using the *hybrid* bond style.

The coefficients associated with a bond style can be specified in a data or restart file or via the bond_coeff command.

All bond potentials store their coefficient data in binary restart files which means bond_style and bond_coeff commands do not need to be re-specified in an input script that restarts a simulation. See the read_restart command for details on how to do this. The one exception is that bond_style *hybrid* only stores the list of sub-styles in the restart file; bond coefficients need to be re-specified.

NOTE: When both a bond and pair style is defined, the special_bonds command often needs to be used to turn off (or weight) the pairwise interaction that would otherwise exist between 2 bonded atoms.

In the formulas listed for each bond style, r is the distance between the 2 atoms in the bond.

Here is an alphabetic list of bond styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated bond_coeff command.

Note that there are also additional bond styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the bond section of this page.

- bond_style none - turn off bonded interactions
- bond_style hybrid - define multiple styles of bond interactions

- bond_style class2 - COMPASS (class 2) bond
- bond_style fene - FENE (finite-extensible non-linear elastic) bond
- bond_style fene/expand - FENE bonds with variable size particles
- bond_style harmonic - harmonic bond
- bond_style morse - Morse bond
- bond_style nonlinear - nonlinear bond
- bond_style quartic - breakable quartic bond
- bond_style table - tabulated by bond length

Restrictions:

Bond styles can only be set for atom styles that allow bonds to be defined.

Most bond styles are part of the MOLECULE package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info on packages. The doc pages for individual bond potentials tell if it is part of a package.

Related commands:

bond_coeff, delete_bonds

Default:

bond_style none

bond_style table command

bond_style table/omp command

Syntax:

```
bond_style table style N
```

- style = *linear* or *spline* = method of interpolation
- N = use N values in table

Examples:

```
bond_style table linear 1000
bond_coeff 1 file.table ENTRY1
```

Description:

Style *table* creates interpolation tables of length *N* from bond potential and force values listed in a file(s) as a function of bond length. The files are read by the bond_coeff command.

The interpolation tables are created by fitting cubic splines to the file values and interpolating energy and force values at each of *N* distances. During a simulation, these tables are used to interpolate energy and force values as needed. The interpolation is done in one of 2 styles: *linear* or *spline*.

For the *linear* style, the bond length is used to find 2 surrounding table values from which an energy or force is computed by linear interpolation.

For the *spline* style, a cubic spline coefficients are computed and stored at each of the *N* values in the table. The bond length is used to find the appropriate set of coefficients which are used to evaluate a cubic polynomial which computes the energy or force.

The following coefficients must be defined for each bond type via the bond_coeff command as in the example above.

- filename
- keyword

The filename specifies a file containing tabulated energy and force values. The keyword specifies a section of the file. The format of this file is described below.

The format of a tabulated file is as follows (without the parenthesized comments):

```
# Bond potential for harmonic (one or more comment or blank lines)

HAM                           (keyword is the first text on line)
N 101 FP 0 0 EQ 0.5           (N, FP, EQ  parameters)
                              (blank line)
1 0.00 338.0000 1352.0000     (index, bond-length, energy, force)
2 0.01 324.6152 1324.9600
...
101 1.00 338.0000 -1352.0000
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the bond_coeff command. The next line lists (in any order) one or more parameters for the table. Each parameter is a keyword followed by one or more numeric values.

The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the *N* specified in the bond_style table command. Let Ntable = *N* in the bond_style command, and Nfile = "N" in the tabulated file. What LAMMPS does is a preliminary interpolation by creating splines using the Nfile tabulated values as nodal points. It uses these to interpolate as needed to generate energy and force values at Ntable different points. The resulting tables of length Ntable are then used as described above, when computing energy and force for individual bond lengths. This means that if you want the interpolation tables of length Ntable to match exactly what is in the tabulated file (with effectively no preliminary interpolation), you should set Ntable = Nfile.

The "FP" parameter is optional. If used, it is followed by two values fplo and fphi, which are the derivatives of the force at the innermost and outermost bond lengths. These values are needed by the spline construction routines. If not specified by the "FP" parameter, they are estimated (less accurately) by the first two and last two force values in the table.

The "EQ" parameter is also optional. If used, it is followed by a the equilibrium bond length, which is used, for example, by the fix shake command. If not used, the equilibrium bond length is set to 0.0.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is the bond length r (in distance units), the 3rd value is the energy (in energy units), and the 4th is the force (in force units). The bond lengths must range from a LO value to a HI value, and increase from one line to the next. If the actual bond length is ever smaller than the LO value or larger than the HI value, then the bond energy and force is evaluated as if the bond were the LO or HI length.

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This bond style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

bond_coeff, delete_bonds

Default: none

boundary command

Syntax:

```
boundary x y z
```

- x,y,z = *p* or *s* or *f* or *m*, one or two letters

```
  p is periodic
    f is non-periodic and fixed
    s is non-periodic and shrink-wrapped
    m is non-periodic and shrink-wrapped with a minimum value
```

Examples:

```
boundary p p f
boundary p fs p
boundary s f fm
```

Description:

Set the style of boundaries for the global simulation box in each dimension. A single letter assigns the same style to both the lower and upper face of the box. Two letters assigns the first style to the lower face and the second style to the upper face. The initial size of the simulation box is set by the read_data, read_restart, or create_box commands.

The style *p* means the box is periodic, so that particles interact across the boundary, and they can exit one end of the box and re-enter the other end. A periodic dimension can change in size due to constant pressure boundary conditions or box deformation (see the fix npt and fix deform commands). The *p* style must be applied to both faces of a dimension.

The styles *f*, *s*, and *m* mean the box is non-periodic, so that particles do not interact across the boundary and do not move from one side of the box to the other.

For style *f*, the position of the face is fixed. If an atom moves outside the face it will be deleted on the next timestep that reneighboring occurs. This will typically generate an error unless you have set the thermo_modify lost option to allow for lost atoms.

For style *s*, the position of the face is set so as to encompass the atoms in that dimension (shrink-wrapping), no matter how far they move.

For style *m*, shrink-wrapping occurs, but is bounded by the value specified in the data or restart file or set by the create_box command. For example, if the upper z face has a value of 50.0 in the data file, the face will always be positioned at 50.0 or above, even if the maximum z-extent of all the atoms becomes less than 50.0. This can be useful if you start a simulation with an empty box or if you wish to leave room on one side of the box, e.g. for atoms to evaporate from a surface.

For triclinic (non-orthogonal) simulation boxes, if the 2nd dimension of a tilt factor (e.g. y for xy) is periodic, then the periodicity is enforced with the tilt factor offset. If the 1st dimension is shrink-wrapped, then the shrink wrapping is applied to the tilted box face, to encompass the atoms. E.g. for a positive xy tilt, the xlo and xhi faces of the box are planes tilting in the +y direction as y increases. These tilted planes are shrink-wrapped around the

atoms to determine the x extent of the box.

See Section_howto 12 of the doc pages for a geometric description of triclinic boxes, as defined by LAMMPS, and how to transform these parameters to and from other commonly used triclinic representations.

Restrictions:

This command cannot be used after the simulation box is defined by a read_data or create_box command or read_restart command. See the change_box command for how to change the simulation box boundaries after it has been defined.

For 2d simulations, the z dimension must be periodic.

Related commands:

See the thermo_modify command for a discussion of lost atoms.

Default:

```
boundary p p p
```

box command

Syntax:

```
box keyword value ...
```

- one or more keyword/value pairs may be appended
- keyword = *tilt*

```
  tilt value = small or large
```

Examples:

```
box tilt large
box tilt small
```

Description:

Set attributes of the simulation box.

For triclinic (non-orthogonal) simulation boxes, the *tilt* keyword allows simulation domains to be created with arbitrary tilt factors, e.g. via the create_box or read_data commands. Tilt factors determine how skewed the triclinic box is; see this section of the manual for a discussion of triclinic boxes in LAMMPS.

LAMMPS normally requires that no tilt factor can skew the box more than half the distance of the parallel box length, which is the 1st dimension in the tilt factor (x for xz). If *tilt* is set to *small*, which is the default, then an error will be generated if a box is created which exceeds this limit. If *tilt* is set to *large*, then no limit is enforced. You can create a box with any tilt factors you wish.

Note that if a simulation box has a large tilt factor, LAMMPS will run less efficiently, due to the large volume of communication needed to acquire ghost atoms around a processor's irregular-shaped sub-domain. For extreme values of tilt, LAMMPS may also lose atoms and generate an error.

Restrictions:

This command cannot be used after the simulation box is defined by a read_data or create_box command or read_restart command.

Related commands: none

Default:

The default value is tilt = small.

change_box command

Syntax:

```
change_box group-ID parameter args ... keyword args ...
```

- group-ID = ID of group of atoms to (optionally) displace
- one or more parameter/arg pairs may be appended

```
parameter = x or y or z or xy or xz or yz or boundary or ortho or triclinic or set or remap
  x, y, z args = style value(s)
    style = final or delta or scale or volume
      final values = lo hi
        lo hi = box boundaries after displacement (distance units)
      delta values = dlo dhi
        dlo dhi = change in box boundaries after displacement (distance units)
      scale values = factor
        factor = multiplicative factor for change in box length after displacement
      volume value = none = adjust this dim to preserve volume of system
  xy, xz, yz args = style value
    style = final or delta
      final value = tilt
        tilt = tilt factor after displacement (distance units)
      delta value = dtilt
        dtilt = change in tilt factor after displacement (distance units)
  boundary args = x y z
    x,y,z = p or s or f or m, one or two letters
    p is periodic
    f is non-periodic and fixed
    s is non-periodic and shrink-wrapped
    m is non-periodic and shrink-wrapped with a minimum value
  ortho args = none = change box to orthogonal
  triclinic args = none = change box to triclinic
  set args = none = store state of current box
  remap args = none = remap atom coords from last saved state to current box
```

- zero or more keyword/value pairs may be appended
- keyword = *units*

```
units value = lattice or box
    lattice = distances are defined in lattice units
    box = distances are defined in simulation box units
```

Examples:

```
change_box all xy final -2.0 z final 0.0 5.0 boundary p p f remap units box
change_box all x scale 1.1 y volume z volume remap
```

Description:

Change the volume and/or shape and/or boundary conditions for the simulation box. Orthogonal simulation boxes have 3 adjustable size parameters (x,y,z). Triclinic (non-orthogonal) simulation boxes have 6 adjustable size/shape parameters (x,y,z,xy,xz,yz). Any or all of them can be adjusted independently by this command. Thus it can be used to expand or contract a box, or to apply a shear strain to a non-orthogonal box. It can also be used to change the boundary conditions for the simulation box, similar to the boundary command.

The size and shape of the initial simulation box are specified by the create_box or read_data or read_restart command used to setup the simulation. The size and shape may be altered by subsequent runs, e.g. by use of the fix npt or fix deform commands. The create_box, read data, and read_restart commands also determine whether the simulation box is orthogonal or triclinic and their doc pages explain the meaning of the xy,xz,yz tilt factors.

See Section_howto 12 of the doc pages for a geometric description of triclinic boxes, as defined by LAMMPS, and how to transform these parameters to and from other commonly used triclinic representations.

The keywords used in this command are applied sequentially to the simulation box and the atoms in it, in the order specified.

Before the sequence of keywords are invoked, the current box size/shape is stored, in case a *remap* keyword is used to map the atom coordinates from a previously stored box size/shape to the current one.

After all the keywords have been processed, any shrink-wrap boundary conditions are invoked (see the boundary command) which may change simulation box boundaries, and atoms are migrated to new owning processors.

NOTE: This means that you cannot use the change_box command to enlarge a shrink-wrapped box, e.g. to make room to insert more atoms via the create_atoms command, because the simulation box will be re-shrink-wrapped before the change_box command completes. Instead you could do something like this, assuming the simulation box is non-periodic and atoms extend from 0 to 20 in all dimensions:

```
change_box all x final -10 20
create_atoms 1 single -5 5 5   # this will fail to insert an atom

change_box all x final -10 20 boundary f s s
create_atoms 1 single -5 5 5
change_box boundary s s s      # this will work
```

NOTE: Unlike the earlier "displace_box" version of this command, atom remapping is NOT performed by default. This command allows remapping to be done in a more general way, exactly when you specify it (zero or more times) in the sequence of transformations. Thus if you do not use the *remap* keyword, atom coordinates will not be changed even if the box size/shape changes. If a uniformly strained state is desired, the *remap* keyword should be specified.

NOTE: It is possible to lose atoms with this command. E.g. by changing the box without remapping the atoms, and having atoms end up outside of non-periodic boundaries. It is also possible to alter bonds between atoms straddling a boundary in bad ways. E.g. by converting a boundary from periodic to non-periodic. It is also possible when remapping atoms to put them (nearly) on top of each other. E.g. by converting a boundary from non-periodic to periodic. All of these will typically lead to bad dynamics and/or generate error messages.

NOTE: The simulation box size/shape can be changed by arbitrarily large amounts by this command. This is not a problem, except that the mapping of processors to the simulation box is not changed from its initial 3d configuration; see the processors command. Thus, if the box size/shape changes dramatically, the mapping of processors to the simulation box may not end up as optimal as the initial mapping attempted to be.

NOTE: Because the keywords used in this command are applied one at a time to the simulation box and the atoms in it, care must be taken with triclinic cells to avoid exceeding the limits on skew after each transformation in the sequence. If skew is exceeded before the final transformation this can be avoided by changing the order of the sequence, or breaking the transformation into two or more smaller transformations. For more information on the allowed limits for box skew see the discussion on triclinic boxes on this page.

For the *x*, *y*, and *z* parameters, this is the meaning of their styles and values.

For style *final*, the final lo and hi box boundaries of a dimension are specified. The values can be in lattice or box distance units. See the discussion of the units keyword below.

For style *delta*, plus or minus changes in the lo/hi box boundaries of a dimension are specified. The values can be in lattice or box distance units. See the discussion of the units keyword below.

For style *scale*, a multiplicative factor to apply to the box length of a dimension is specified. For example, if the initial box length is 10, and the factor is 1.1, then the final box length will be 11. A factor less than 1.0 means compression.

The *volume* style changes the specified dimension in such a way that the overall box volume remains constant with respect to the operation performed by the preceding keyword. The *volume* style can only be used following a keyword that changed the volume, which is any of the *x*, *y*, *z* keywords. If the preceding keyword "key" had a *volume* style, then both it and the current keyword apply to the keyword preceding "key". I.e. this sequence of keywords is allowed:

```
change_box all x scale 1.1 y volume z volume
```

The *volume* style changes the associated dimension so that the overall box volume is unchanged relative to its value before the preceding keyword was invoked.

If the following command is used, then the z box length will shrink by the same 1.1 factor the x box length was increased by:

```
change_box all x scale 1.1 z volume
```

If the following command is used, then the y,z box lengths will each shrink by sqrt(1.1) to keep the volume constant. In this case, the y,z box lengths shrink so as to keep their relative aspect ratio constant:

```
change_box all"x scale 1.1 y volume z volume
```

If the following command is used, then the final box will be a factor of 10% larger in x and y, and a factor of 21% smaller in z, so as to keep the volume constant:

```
change_box all x scale 1.1 z volume y scale 1.1 z volume
```

NOTE: For solids or liquids, when one dimension of the box is expanded, it may be physically undesirable to hold the other 2 box lengths constant since that implies a density change. For solids, adjusting the other dimensions via the *volume* style may make physical sense (just as for a liquid), but may not be correct for materials and potentials whose Poisson ratio is not 0.5.

For the *scale* and *volume* styles, the box length is expanded or compressed around its mid point.

For the *xy*, *xz*, and *yz* parameters, this is the meaning of their styles and values. Note that changing the tilt factors of a triclinic box does not change its volume.

For style *final*, the final tilt factor is specified. The value can be in lattice or box distance units. See the discussion of the units keyword below.

For style *delta*, a plus or minus change in the tilt factor is specified. The value can be in lattice or box distance units. See the discussion of the units keyword below.

All of these styles change the xy, xz, yz tilt factors. In LAMMPS, tilt factors (xy,xz,yz) for triclinic boxes are required to be no more than half the distance of the parallel box length. For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = ..., -15, -5, 5, 15, 25, ... are all equivalent. Any tilt factor specified by this command must be within these limits.

The *boundary* keyword takes arguments that have exactly the same meaning as they do for the boundary command. In each dimension, a single letter assigns the same style to both the lower and upper face of the box. Two letters assigns the first style to the lower face and the second style to the upper face.

The style *p* means the box is periodic; the other styles mean non-periodic. For style *f*, the position of the face is fixed. For style *s*, the position of the face is set so as to encompass the atoms in that dimension (shrink-wrapping), no matter how far they move. For style *m*, shrink-wrapping occurs, but is bounded by the current box edge in that dimension, so that the box will become no smaller. See the boundary command for more explanation of these style options.

Note that the "boundary" command itself can only be used before the simulation box is defined via a read_data or create_box or read_restart command. This command allows the boundary conditions to be changed later in your input script. Also note that the read_restart will change boundary conditions to match what is stored in the restart file. So if you wish to change them, you should use the change_box command after the read_restart command.

The *ortho* and *triclinic* keywords convert the simulation box to be orthogonal or triclinic (non-orthongonal). See this section for a discussion of how non-orthongal boxes are represented in LAMMPS.

The simulation box is defined as either orthogonal or triclinic when it is created via the create_box, read_data, or read_restart commands.

These keywords allow you to toggle the existing simulation box from orthogonal to triclinic and vice versa. For example, an initial equilibration simulation can be run in an orthogonal box, the box can be toggled to triclinic, and then a non-equilibrium MD (NEMD) simulation can be run with deformation via the fix deform command.

If the simulation box is currently triclinic and has non-zero tilt in xy, yz, or xz, then it cannot be converted to an orthogonal box.

The *set* keyword saves the current box size/shape. This can be useful if you wish to use the *remap* keyword more than once or if you wish it to be applied to an intermediate box size/shape in a sequence of keyword operations. Note that the box size/shape is saved before any of the keywords are processed, i.e. the box size/shape at the time the create_box command is encountered in the input script.

The *remap* keyword remaps atom coordinates from the last saved box size/shape to the current box state. For example, if you stretch the box in the x dimension or tilt it in the xy plane via the *x* and *xy* keywords, then the *remap* commmand will dilate or tilt the atoms to conform to the new box size/shape, as if the atoms moved with the box as it deformed.

Note that this operation is performed without regard to periodic boundaries. Also, any shrink-wrapping of non-periodic boundaries (see the boundary command) occurs after all keywords, including this one, have been processed.

Only atoms in the specified group are remapped.

The *units* keyword determines the meaning of the distance units used to define various arguments. A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacing.

Restrictions:

If you use the *ortho* or *triclinic* keywords, then at the point in the input script when this command is issued, no dumps can be active, nor can a fix ave/spatial or fix deform be active. This is because these commands test whether the simulation box is orthogonal when they are first issued. Note that these commands can be used in your script before a change_box command is issued, so long as an undump or unfix command is also used to turn them off.

Related commands:

fix deform, boundary

Default:

The option default is units = lattice.

clear command

Syntax:

```
clear
```

Examples:

```
(commands for 1st simulation)
clear
(commands for 2nd simulation)
```

Description:

This command deletes all atoms, restores all settings to their default values, and frees all memory allocated by LAMMPS. Once a clear command has been executed, it is almost as if LAMMPS were starting over, with only the exceptions noted below. This command enables multiple jobs to be run sequentially from one input script.

These settings are not affected by a clear command: the working directory (shell command), log file status (log command), echo status (echo command), and input script variables (variable command).

Restrictions: none

Related commands: none

Default: none

comm_modify command

Syntax:

```
comm_modify keyword value ...
```

- zero or more keyword/value pairs may be appended
- keyword = *mode* or *cutoff* or *cutoff/multi* or *group* or *vel*

```
  mode value = single or multi = communicate atoms within a single or multiple distances
    cutoff value = Rcut (distance units) = communicate atoms from this far away
    cutoff/multi type value
       type = atom type or type range (supports asterisk notation)
       value = Rcut (distance units) = communicate atoms for selected types from this far away
    group value = group-ID = only communicate atoms in the group
    vel value = yes or no = do or do not communicate velocity info with ghost atoms
```

Examples:

```
comm_modify mode multi
comm_modify mode multi group solvent
comm_modift mode multi cutoff/multi 1 10.0 cutoff/multi 2*4 15.0
comm_modify vel yes
comm_modify mode single cutoff 5.0 vel yes
comm_modify cutoff/multi * 0.0
```

Description:

This command sets parameters that affect the inter-processor communication of atom information that occurs each timestep as coordinates and other properties are exchanged between neighboring processors and stored as properties of ghost atoms.

NOTE: These options apply to the currently defined comm style. When you specify a comm_style command, all communication settings are restored to their default values, including those previously reset by a comm_modify command. Thus if your input script specifies a comm_style command, you should use the comm_modify command after it.

The *mode* keyword determines whether a single or multiple cutoff distances are used to determine which atoms to communicate.

The default mode is *single* which means each processor acquires information for ghost atoms that are within a single distance from its sub-domain. The distance is by default the maximum of the neighbor cutoff across all atom type pairs.

For many systems this is an efficient algorithm, but for systems with widely varying cutoffs for different type pairs, the *multi* mode can be faster. In this case, each atom type is assigned its own distance cutoff for communication purposes, and fewer atoms will be communicated. See the neighbor multi command for a neighbor list construction option that may also be beneficial for simulations of this kind.

The *cutoff* keyword allows you to extend the ghost cutoff distance for communication mode *single*, which is the distance from the borders of a processor's sub-domain at which ghost atoms are acquired from other processors. By default the ghost cutoff = neighbor cutoff = pairwise force cutoff + neighbor skin. See the neighbor command

for more information about the skin distance. If the specified Rcut is greater than the neighbor cutoff, then extra ghost atoms will be acquired. If the provided cutoff is smaller, the provided value will be ignored and the ghost cutoff is set to the neighbor cutoff. Specifying a cutoff value of 0.0 will reset any previous value to the default.

The *cutoff/multi* option is equivalent to *cutoff*, but applies to communication mode *multi* instead. Since in this case the communication cutoffs are determined per atom type, a type specifier is needed and cutoff for one or multiple types can be extended. Also ranges of types using the usual asterisk notation can be given.

These are simulation scenarios in which it may be useful or even necessary to set a ghost cutoff > neighbor cutoff:

- a single polymer chain with bond interactions, but no pairwise interactions
- bonded interactions (e.g. dihedrals) extend further than the pairwise cutoff
- ghost atoms beyond the pairwise cutoff are needed for some computation

In the first scenario, a pairwise potential is not defined. Thus the pairwise neighbor cutoff will be 0.0. But ghost atoms are still needed for computing bond, angle, etc interactions between atoms on different processors, or when the interaction straddles a periodic boundary.

The appropriate ghost cutoff depends on the newton bond setting. For newton bond *off*, the distance needs to be the furthest distance between any two atoms in the bond, angle, etc. E.g. the distance between 1-4 atoms in a dihedral. For newton bond *on*, the distance between the central atom in the bond, angle, etc and any other atom is sufficient. E.g. the distance between 2-4 atoms in a dihedral.

In the second scenario, a pairwise potential is defined, but its neighbor cutoff is not sufficiently long enough to enable bond, angle, etc terms to be computed. As in the previous scenario, an appropriate ghost cutoff should be set.

In the last scenario, a fix or compute or pairwise potential needs to calculate with ghost atoms beyond the normal pairwise cutoff for some computation it performs (e.g. locate neighbors of ghost atoms in a multibody pair potential). Setting the ghost cutoff appropriately can insure it will find the needed atoms.

NOTE: In these scenarios, if you do not set the ghost cutoff long enough, and if there is only one processor in a periodic dimension (e.g. you are running in serial), then LAMMPS may "find" the atom it is looking for (e.g. the partner atom in a bond), that is on the far side of the simulation box, across a periodic boundary. This will typically lead to bad dynamics (i.e. the bond length is now the simulation box length). To detect if this is happening, see the neigh_modify cluster command.

The *group* keyword will limit communication to atoms in the specified group. This can be useful for models where no ghost atoms are needed for some kinds of particles. All atoms (not just those in the specified group) will still migrate to new processors as they move. The group specified with this option must also be specified via the atom_modify first command.

The *vel* keyword enables velocity information to be communicated with ghost particles. Depending on the atom_style, velocity info includes the translational velocity, angular velocity, and angular momentum of a particle. If the *vel* option is set to *yes*, then ghost atoms store these quantities; if *no* then they do not. The *yes* setting is needed by some pair styles which require the velocity state of both the I and J particles to compute a pairwise I,J interaction.

Note that if the fix deform command is being used with its "remap v" option enabled, then the velocities for ghost atoms (in the fix deform group) mirrored across a periodic boundary will also include components due to any velocity shift that occurs across that boundary (e.g. due to dilation or shear).

Restrictions:

Communication mode *multi* is currently only available for comm_style *brick*.

Related commands:

comm_style, neighbor

Default:

The option defauls are mode = single, group = all, cutoff = 0.0, vel = no. The cutoff default of 0.0 means that ghost cutoff = neighbor cutoff = pairwise force cutoff + neighbor skin.

comm_style command

Syntax:

```
comm_style style
```

- style = *brick* or *tiled*

Examples:

```
comm_style brick
comm_style tiled
```

Description:

This command sets the style of inter-processor communication of atom information that occurs each timestep as coordinates and other properties are exchanged between neighboring processors and stored as properties of ghost atoms.

For the default *brick* style, the domain decomposition used by LAMMPS to partition the simulation box must be a regular 3d grid of bricks, one per processor. Each processor communicates with its 6 Cartesian neighbors in the grid to acquire information for nearby atoms.

For the *tiled* style, a more general domain decomposition can be used, as triggered by the balance or fix balance commands. The simulation box can be partitioned into non-overlapping rectangular-shaped "tiles" or varying sizes and shapes. Again there is one tile per processor. To acquire information for nearby atoms, communication must now be done with a more complex pattern of neighboring processors.

Note that this command does not actually define a partitoining of the simulation box (a domain decomposition), rather it determines what kinds of decompositions are allowed and the pattern of communication used to enable the decomposition. A decomposition is created when the simulation box is first created, via the create_box or read_data or read_restart commands. For both the *brick* and *tiled* styles, the initial decomposition will be the same, as described by create_box and processors commands. The decomposition can be changed via the balance or fix_balance commands.

Restrictions: none

Related commands:

comm_modify, processors, balance, fix balance

Default:

The default style is brick.

compute command

Syntax:

```
compute ID group-ID style args
```

- ID = user-assigned name for the computation
- group-ID = ID of the group of atoms to perform the computation on
- style = one of a list of possible style names (see below)
- args = arguments used by a particular style

Examples:

```
compute 1 all temp
compute newtemp flow temp/partial 1 1 0
compute 3 all ke/atom
```

Description:

Define a computation that will be performed on a group of atoms. Quantities calculated by a compute are instantaneous values, meaning they are calculated from information about atoms on the current timestep or iteration, though a compute may internally store some information about a previous state of the system. Defining a compute does not perform a computation. Instead computes are invoked by other LAMMPS commands as needed, e.g. to calculate a temperature needed for a thermostat fix or to generate thermodynamic or dump file output. See this howto section for a summary of various LAMMPS output options, many of which involve computes.

The ID of a compute can only contain alphanumeric characters and underscores.

Computes calculate one of three styles of quantities: global, per-atom, or local. A global quantity is one or more system-wide values, e.g. the temperature of the system. A per-atom quantity is one or more values per atom, e.g. the kinetic energy of each atom. Per-atom values are set to 0.0 for atoms not in the specified compute group. Local quantities are calculated by each processor based on the atoms it owns, but there may be zero or more per atom, e.g. a list of bond distances. Computes that produce per-atom quantities have the word "atom" in their style, e.g. *ke/atom*. Computes that produce local quantities have the word "local" in their style, e.g. *bond/local*. Styles with neither "atom" or "local" in their style produce global quantities.

Note that a single compute produces either global or per-atom or local quantities, but never more than one of these (with only a few exceptions, as documented by individual compute commands).

Global, per-atom, and local quantities each come in three kinds: a single scalar value, a vector of values, or a 2d array of values. The doc page for each compute describes the style and kind of values it produces, e.g. a per-atom vector. Some computes produce more than one kind of a single style, e.g. a global scalar and a global vector.

When a compute quantity is accessed, as in many of the output commands discussed below, it can be referenced via the following bracket notation, where ID is the ID of the compute:

c_ID	entire scalar, vector, or array
c_ID[I]	one element of vector, one column of array
c_ID[I][J]	one element of array

In other words, using one bracket reduces the dimension of the quantity once (vector -> scalar, array -> vector). Using two brackets reduces the dimension twice (array -> scalar). Thus a command that uses scalar compute values as input can also process elements of a vector or array.

Note that commands and variables which use compute quantities typically do not allow for all kinds, e.g. a command may require a vector of values, not a scalar. This means there is no ambiguity about referring to a compute quantity as c_ID even if it produces, for example, both a scalar and vector. The doc pages for various commands explain the details.

In LAMMPS, the values generated by a compute can be used in several ways:

- The results of computes that calculate a global temperature or pressure can be used by fixes that do thermostatting or barostatting or when atom velocities are created.
- Global values can be output via the thermo_style custom or fix ave/time command. Or the values can be referenced in a variable equal or variable atom command.
- Per-atom values can be output via the dump custom command or the fix ave/spatial command. Or they can be time-averaged via the fix ave/atom command or reduced by the compute reduce command. Or the per-atom values can be referenced in an atom-style variable.
- Local values can be reduced by the compute reduce command, or histogrammed by the fix ave/histo command, or output by the dump local command.

The results of computes that calculate global quantities can be either "intensive" or "extensive" values. Intensive means the value is independent of the number of atoms in the simulation, e.g. temperature. Extensive means the value scales with the number of atoms in the simulation, e.g. total rotational kinetic energy. Thermodynamic output will normalize extensive values by the number of atoms in the system, depending on the "thermo_modify norm" setting. It will not normalize intensive values. If a compute value is accessed in another way, e.g. by a variable, you may want to know whether it is an intensive or extensive value. See the doc page for individual computes for further info.

LAMMPS creates its own computes internally for thermodynamic output. Three computes are always created, named "thermo_temp", "thermo_press", and "thermo_pe", as if these commands had been invoked in the input script:

```
compute thermo_temp all temp
compute thermo_press all pressure thermo_temp
compute thermo_pe all pe
```

Additional computes for other quantities are created if the thermo style requires it. See the documentation for the thermo_style command.

Fixes that calculate temperature or pressure, i.e. for thermostatting or barostatting, may also create computes. These are discussed in the documentation for specific fix commands.

In all these cases, the default computes LAMMPS creates can be replaced by computes defined by the user in the input script, as described by the thermo_modify and fix modify commands.

Properties of either a default or user-defined compute can be modified via the compute_modify command.

Computes can be deleted with the uncompute command.

Code for new computes can be added to LAMMPS (see this section of the manual) and the results of their calculations accessed in the various ways described above.

Each compute style has its own doc page which describes its arguments and what it does. Here is an alphabetic list of compute styles available in LAMMPS. They are also given in more compact form in the Compute section of this page.

There are also additional compute styles (not listed here) submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the compute section of this page.

- angle/local - theta and energy of each angle
- angmom/chunk - angular momentum for each chunk
- body/local - attributes of body sub-particles
- bond/local - distance and energy of each bond
- centro/atom - centro-symmetry parameter for each atom
- chunk/atom - assign chunk IDs to each atom
- cluster/atom - cluster ID for each atom
- cna/atom - common neighbor analysis (CNA) for each atom
- com - center-of-mass of group of atoms
- com/chunk - center-of-mass for each chunk
- contact/atom - contact count for each spherical particle
- coord/atom - coordination number for each atom
- damage/atom - Peridynamic damage for each atom
- dihedral/local - angle of each dihedral
- dilatation/atom - Peridynamic dilatation for each atom
- displace/atom - displacement of each atom
- erotate/asphere - rotational energy of aspherical particles
- erotate/rigid - rotational energy of rigid bodies
- erotate/sphere - rotational energy of spherical particles
- erotate/sphere/atom - rotational energy for each spherical particle
- event/displace - detect event on atom displacement
- group/group - energy/force between two groups of atoms
- gyration - radius of gyration of group of atoms
- gyration/chunk - radius of gyration for each chunk
- heat/flux - heat flux through a group of atoms
- hexorder/atom - bond orientational order parameter q6
- improper/local - angle of each improper
- inertia/chunk - inertia tensor for each chunk
- ke - translational kinetic energy
- ke/atom - kinetic energy for each atom
- ke/rigid - translational kinetic energy of rigid bodies
- msd - mean-squared displacement of group of atoms
- msd/chunk - mean-squared displacement for each chunk
- msd/nongauss - MSD and non-Gaussian parameter of group of atoms
- omega/chunk - angular velocity for each chunk
- orientorder/atom - Steinhardt bond orientational order parameters Ql
- pair - values computed by a pair style
- pair/local - distance/energy/force of each pairwise interaction
- pe - potential energy
- pe/atom - potential energy for each atom
- plasticity/atom - Peridynamic plasticity for each atom
- pressure - total pressure and pressure tensor
- property/atom - convert atom attributes to per-atom vectors/arrays
- property/local - convert local attributes to localvectors/arrays

- property/chunk - extract various per-chunk attributes
- rdf - radial distribution function g(r) histogram of group of atoms
- reduce - combine per-atom quantities into a single global value
- reduce/region - same as compute reduce, within a region
- slice - extract values from global vector or array
- sna/atom - calculate bispectrum coefficients for each atom
- snad/atom - derivative of bispectrum coefficients for each atom
- snav/atom - virial contribution from bispectrum coefficients for each atom
- stress/atom - stress tensor for each atom
- temp - temperature of group of atoms
- temp/asphere - temperature of aspherical particles
- temp/chunk - temperature of each chunk
- temp/com - temperature after subtracting center-of-mass velocity
- temp/deform - temperature excluding box deformation velocity
- temp/partial - temperature excluding one or more dimensions of velocity
- temp/profile - temperature excluding a binned velocity profile
- temp/ramp - temperature excluding ramped velocity component
- temp/region - temperature of a region of atoms
- temp/sphere - temperature of spherical particles
- ti - thermodyanmic integration free energy values
- torque/chunk - torque applied on each chunk
- vacf - velocity-autocorrelation function of group of atoms
- vcm/chunk - velocity of center-of-mass for each chunk
- voronoi/atom - Voronoi volume and neighbors for each atom

There are also additional compute styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the compute section of this page.

There are also additional accelerated compute styles included in the LAMMPS distribution for faster performance on CPUs and GPUs. The list of these with links to the individual styles are given in the pair section of this page.

Restrictions: none

Related commands:

uncompute, compute_modify, fix ave/atom, fix ave/spatial, fix ave/time, fix ave/histo

Default: none

compute ackland/atom command

Syntax:

```
compute ID group-ID ackland/atom
```

- ID, group-ID are documented in compute command
- ackland/atom = style name of this compute command

Examples:

```
compute 1 all ackland/atom
```

Description:

Defines a computation that calculates the local lattice structure according to the formulation given in (Ackland).

In contrast to the centro-symmetry parameter this method is stable against temperature boost, because it is based not on the distance between particles but the angles. Therefore statistical fluctuations are averaged out a little more. A comparison with the Common Neighbor Analysis metric is made in the paper.

The result is a number which is mapped to the following different lattice structures:

- 0 = UNKNOWN
- 1 = BCC
- 2 = FCC
- 3 = HCP
- 4 = ICO

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently or to have multiple compute/dump commands, each of which computes this quantity.-

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

Restrictions:

This compute is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The per-atom vector values will be unitless since they are the integers defined above.

Related commands:

compute centro/atom

Default: none

(Ackland) Ackland, Jones, Phys Rev B, 73, 054104 (2006).

compute angle/local command

Syntax:

```
compute ID group-ID angle/local input1 input2 ...
```

- ID, group-ID are documented in compute command
- angle/local = style name of this compute command
- one or more keywords may be appended
- keyword = *theta* or *eng*

```
  theta = tabulate angles
    eng = tabulate angle energies
```

Examples:

```
compute 1 all angle/local theta
compute 1 all angle/local eng theta
```

Description:

Define a computation that calculates properties of individual angle interactions. The number of datums generated, aggregated across all processors, equals the number of angles in the system, modified by the group parameter as explained below.

The local data stored by this command is generated by looping over all the atoms owned on a processor and their angles. An angle will only be included if all 3 atoms in the angle are in the specified compute group. Any angles that have been broken (see the angle_style command) by setting their angle type to 0 are not included. Angles that have been turned off (see the fix shake or delete_bonds commands) by setting their angle type negative are written into the file, but their energy will be 0.0.

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For example, angle output from the compute property/local command can be combined with data from this command and output by the dump local command in a consistent way.

Output info:

This compute calculates a local vector or local array depending on the number of keywords. The length of the vector or number of rows in the array is the number of angles. If a single keyword is specified, a local vector is produced. If two or more keywords are specified, a local array is produced where the number of columns = the number of keywords. The vector or array can be accessed by any command that uses local values from a compute as input. See this section for an overview of LAMMPS output options.

The output for *theta* will be in degrees. The output for *eng* will be in energy units.

Restrictions: none

Related commands:

dump local, compute property/local

Default: none

compute angmom/chunk command

Syntax:

```
compute ID group-ID angmom/chunk chunkID
```

- ID, group-ID are documented in compute command
- angmom/chunk = style name of this compute command
- chunkID = ID of compute chunk/atom command

Examples:

```
compute 1 fluid angmom/chunk molchunk
```

Description:

Define a computation that calculates the angular momemtum of multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a compute chunk/atom command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the compute chunk/atom doc page and "Section_howto 23 for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates the 3 components of the angular momentum vector for each chunk, due to the velocity/momentum of the individual atoms in the chunk around the center-of-mass of the chunk. The calculation includes all effects due to atoms passing thru periodic boundaries.

Note that only atoms in the specified group contribute to the calculation. The compute chunk/atom command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

NOTE: The coordinates of an atom contribute to the chunk's angular momentum in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

The simplest way to output the results of the compute angmom/chunk calculation to a file is to use the fix ave/time command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all angmom/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk file tmp.out mode vector
```

Output info:

This compute calculates a global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified compute chunk/atom command. The number of columns = 3 for the 3 xyz components of the angular momentum for each chunk. These values can be accessed by any command that uses global array values

from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in mass-velocity-distance units.

Restrictions: none

Related commands:

variable angmom() function

Default: none

compute basal/atom command

Syntax:

```
compute ID group-ID basal/atom
```

- ID, group-ID are documented in compute command
- basal/atom = style name of this compute command

Examples:

```
compute 1 all basal/atom
```

Description:

Defines a computation that calculates the hexagonal close-packed "c" lattice vector for each atom in the group. It does this by calculating the normal unit vector to the basal plane for each atom. The results enable efficient identification and characterization of twins and grains in hexagonal close-packed structures.

The output of the compute is thus the 3 components of a unit vector associdate with each atom. The components are set to 0.0 for atoms not in the group.

Details of the calculation are given in (Barrett).

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently or to have multiple compute/dump commands, each of which computes this quantity.

An example input script that uses this compute is provided in examples/USER/misc/basal.

Output info:

This compute calculates a per-atom array with 3 columns, which can be accessed by indices 1-3 by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values are unitless since the 3 columns represent components of a unit vector.

Restrictions:

This compute is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The output of this compute will be meaningless unless the atoms are on (or near) hcp lattice sites, since the calculation assumes a well-defined basal plane.

Related commands:

compute centro/atom, compute ackland/atom

Default: none

(Barrett) Barrett, Tschopp, El Kadiri, Scripta Mat. 66, p.666 (2012).

compute body/local command

Syntax:

```
compute ID group-ID body/local input1 input2 ...
```

- ID, group-ID are documented in compute command
- body/local = style name of this compute command
- one or more keywords may be appended
- keyword = *id* or *type* or *integer*

```
  id = atom ID of the body particle
    type = atom type of the body particle
    integer = 1,2,3,etc = index of fields defined by body style
```

Examples:

```
compute 1 all body/local type 1 2 3
compute 1 all body/local 3 6
```

Description:

Define a computation that calculates properties of individual body sub-particles. The number of datums generated, aggregated across all processors, equals the number of body sub-particles plus the number of non-body particles in the system, modified by the group parameter as explained below. See Section_howto 14 of the manual and the body doc page for more details on using body particles.

The local data stored by this command is generated by looping over all the atoms. An atom will only be included if it is in the group. If the atom is a body particle, then its N sub-particles will be looped over, and it will contribute N datums to the count of datums. If it is not a body particle, it will contribute 1 datum.

For both body particles and non-body particles, the *id* keyword will store the ID of the particle.

For both body particles and non-body particles, the *type* keyword will store the type of the particle.

The *integer* keywords mean different things for body and non-body particles. If the atom is not a body particle, only its *x*, *y*, *z* coordinates can be referenced, using the *integer* keywords 1,2,3. Note that this means that if you want to access more fields than this for body particles, then you cannot include non-body particles in the group.

For a body particle, the *integer* keywords refer to fields calculated by the body style for each sub-particle. The body style, as specified by the atom_style body, determines how many fields exist and what they are. See the body doc page for details of the different styles.

Here is an example of how to output body information using the dump local command with this compute. If fields 1,2,3 for the body sub-particles are x,y,z coordinates, then the dump file will be formatted similar to the output of a dump atom or custom command.

```
compute 1 all body/local type 1 2 3
dump 1 all local 1000 tmp.dump index c_1[1] c_1[2] c_1[3] c_1[4]
```

Output info:

This compute calculates a local vector or local array depending on the number of keywords. The length of the vector or number of rows in the array is the number of datums as described above. If a single keyword is specified, a local vector is produced. If two or more keywords are specified, a local array is produced where the number of columns = the number of keywords. The vector or array can be accessed by any command that uses local values from a compute as input. See this section for an overview of LAMMPS output options.

The units for output values depend on the body style.

Restrictions: none

Related commands:

dump local

Default: none

compute bond/local command

Syntax:

```
compute ID group-ID bond/local input1 input2 ...
```

- ID, group-ID are documented in compute command
- bond/local = style name of this compute command
- one or more keywords may be appended
- keyword = *dist* or *eng*

```
  dist = bond distance
    eng = bond energy
    force = bond force
```

Examples:

```
compute 1 all bond/local eng
compute 1 all bond/local dist eng force
```

Description:

Define a computation that calculates properties of individual bond interactions. The number of datums generated, aggregated across all processors, equals the number of bonds in the system, modified by the group parameter as explained below.

The local data stored by this command is generated by looping over all the atoms owned on a processor and their bonds. A bond will only be included if both atoms in the bond are in the specified compute group. Any bonds that have been broken (see the bond_style command) by setting their bond type to 0 are not included. Bonds that have been turned off (see the fix shake or delete_bonds commands) by setting their bond type negative are written into the file, but their energy will be 0.0.

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For example, bond output from the compute property/local command can be combined with data from this command and output by the dump local command in a consistent way.

Here is an example of how to do this:

```
compute 1 all property/local batom1 batom2 btype
compute 2 all bond/local dist eng
dump 1 all local 1000 tmp.dump index c_1[1] c_1[2] c_1[3] c_2[1] c_2[2]
```

Output info:

This compute calculates a local vector or local array depending on the number of keywords. The length of the vector or number of rows in the array is the number of bonds. If a single keyword is specified, a local vector is produced. If two or more keywords are specified, a local array is produced where the number of columns = the number of keywords. The vector or array can be accessed by any command that uses local values from a compute as input. See this section for an overview of LAMMPS output options.

The output for *dist* will be in distance units. The output for *eng* will be in energy units. The output for *force* will be in force units.

Restrictions: none

Related commands:

dump local, compute property/local

Default: none

compute centro/atom command

Syntax:

```
compute ID group-ID centro/atom lattice
```

- ID, group-ID are documented in compute command
- centro/atom = style name of this compute command
- lattice = *fcc* or *bcc* or N = # of neighbors per atom to include

Examples:

```
compute 1 all centro/atom fcc

compute 1 all centro/atom 8
```

Description:

Define a computation that calculates the centro-symmetry parameter for each atom in the group. In solid-state systems the centro-symmetry parameter is a useful measure of the local lattice disorder around an atom and can be used to characterize whether the atom is part of a perfect lattice, a local defect (e.g. a dislocation or stacking fault), or at a surface.

The value of the centro-symmetry parameter will be 0.0 for atoms not in the specified compute group.

This parameter is computed using the following formula from (Kelchner)

$$CS = \sum_{i=1}^{N/2} |\vec{R}_i + \vec{R}_{i+N/2}|^2$$

where the *N* nearest neighbors or each atom are identified and Ri and Ri+N/2 are vectors from the central atom to a particular pair of nearest neighbors. There are N*(N-1)/2 possible neighbor pairs that can contribute to this formula. The quantity in the sum is computed for each, and the N/2 smallest are used. This will typically be for pairs of atoms in symmetrically opposite positions with respect to the central atom; hence the i+N/2 notation.

N is an input parameter, which should be set to correspond to the number of nearest neighbors in the underlying lattice of atoms. If the keyword *fcc* or *bcc* is used, *N* is set to 12 and 8 respectively. More generally, *N* can be set to a positive, even integer.

For an atom on a lattice site, surrounded by atoms on a perfect lattice, the centro-symmetry parameter will be 0. It will be near 0 for small thermal perturbations of a perfect lattice. If a point defect exists, the symmetry is broken, and the parameter will be a larger positive value. An atom at a surface will have a large positive parameter. If the atom does not have *N* neighbors (within the potential cutoff), then its centro-symmetry parameter is set to 0.0.

Only atoms within the cutoff of the pairwise neighbor list are considered as possible neighbors. Atoms not in the compute group are included in the *N* neighbors used in this calculation.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (e.g. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently or to have multiple compute/dump commands, each with a *centro/atom* style.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values are unitless values >= 0.0. Their magnitude depends on the lattice style due to the number of contibuting neighbor pairs in the summation in the formula above. And it depends on the local defects surrounding the central atom, as described above.

Here are typical centro-symmetry values, from a a nanoindentation simulation into gold (FCC). These were provided by Jon Zimmerman (Sandia):

```
Bulk lattice = 0
Dislocation core ~ 1.0 (0.5 to 1.25)
Stacking faults ~ 5.0 (4.0 to 6.0)
Free surface ~ 23.0
```

These values are *not* normalized by the square of the lattice parameter. If they were, normalized values would be:

```
Bulk lattice = 0
Dislocation core ~ 0.06 (0.03 to 0.075)
Stacking faults ~ 0.3 (0.24 to 0.36)
Free surface ~ 1.38
```

For BCC materials, the values for dislocation cores and free surfaces would be somewhat different, due to their being only 8 neighbors instead of 12.

Restrictions: none

Related commands:

compute cna/atom

Default: none

(Kelchner) Kelchner, Plimpton, Hamilton, Phys Rev B, 58, 11085 (1998).

compute chunk/atom command

Syntax:

```
compute ID group-ID chunk/atom style args keyword values ...
```

- ID, group-ID are documented in compute command
- chunk/atom = style name of this compute command

```
style = bin/1d or bin/2d or bin/3d or bin/sphere or type or molecule or compute/fix/variable
  bin/1d args = dim origin delta
    dim = x or y or z
    origin = lower or center or upper or coordinate value (distance units)
    delta = thickness of spatial bins in dim (distance units)
  bin/2d args = dim origin delta dim origin delta
    dim = x or y or z
    origin = lower or center or upper or coordinate value (distance units)
    delta = thickness of spatial bins in dim (distance units)
  bin/3d args = dim origin delta dim origin delta dim origin delta
    dim = x or y or z
    origin = lower or center or upper or coordinate value (distance units)
    delta = thickness of spatial bins in dim (distance units)
  bin/sphere args = xorig yorig zorig rmin rmax nsbin
    xorig,yorig,zorig = center point of sphere
    srmin,srmax = bin from sphere radius rmin to rmax
    nsbin = # of spherical shell bins between rmin and rmax
  bin/cylinder args = dim origin delta c1 c2 rmin rmax ncbin
    dim = x or y or z = axis of cylinder axis
    origin = lower or center or upper or coordinate value (distance units)
    delta = thickness of spatial bins in dim (distance units)
    c1,c2 = coords of cylinder axis in other 2 dimensions (distance units)
    crmin,crmax = bin from cylinder radius rmin to rmax (distance units)
    ncbin = # of concentric circle bins between rmin and rmax
  type args = none
  molecule args = none
  compute/fix/variable = c_ID, c_ID[I], f_ID, f_ID[I], v_name with no args
    c_ID = per-atom vector calculated by a compute with ID
    c_ID[I] = Ith column of per-atom array calculated by a compute with ID
    f_ID = per-atom vector calculated by a fix with ID
    f_ID[I] = Ith column of per-atom array calculated by a fix with ID
    v_name = per-atom vector calculated by an atom-style variable with name
```

- zero or more keyword/values pairs may be appended
- keyword = *region* or *nchunk* or *static* or *compress* or *bound* or *discard* or *pbc* or *units*

```
region value = region-ID
    region-ID = ID of region atoms must be in to be part of a chunk
  nchunk value = once or every
    once = only compute the number of chunks once
    every = re-compute the number of chunks whenever invoked
  limit values = 0 or Nc max or Nc exact
    0 = no limit on the number of chunks
    Nc max = limit number of chunks to be <= Nc
    Nc exact = set number of chunks to exactly Nc
  ids value = once or nfreq or every
    once = assign chunk IDs to atoms only once, they persist thereafter
    nfreq = assign chunk IDs to atoms only once every Nfreq steps (if invoked by fix ave/chunk
    every = assign chunk IDs to atoms whenever invoked
  compress value = yes or no
    yes = compress chunk IDs to eliminate IDs with no atoms
```

```
    no = do not compress chunk IDs even if some IDs have no atoms
  discard value = yes or no or mixed
    yes = discard atoms with out-of-range chunk IDs by assigning a chunk ID = 0
    no = keep atoms with out-of-range chunk IDs by assigning a valid chunk ID
    mixed = keep or discard such atoms according to spatial binning rule
  bound values = x/y/z lo hi
    x/y/z = x or y or z to bound sptial bins in this dimension
    lo = lower or coordinate value (distance units)
    hi = upper or coordinate value (distance units)
  pbc value = no or yes
    yes = use periodic distance for bin/sphere and bin/cylinder styles
  units value = box or lattice or reduced
```

Examples:

```
compute 1 all chunk/atom type
compute 1 all chunk/atom bin/1d z lower 0.02 units reduced
compute 1 all chunk/atom bin/2d z lower 1.0 y 0.0 2.5
compute 1 all chunk/atom molecule region sphere nchunk once ids once compress yes
compute 1 all chunk/atom bin/sphere 5 5 5 2.0 5.0 5 discard yes
compute 1 all chunk/atom bin/cylinder z lower 2 10 10 2.0 5.0 3 discard yes
```

Description:

Define a computation that calculates an integer chunk ID from 1 to Nchunk for each atom in the group. Values of chunk IDs are determined by the *style* of chunk, which can be based on atom type or molecule ID or spatial binning or a per-atom property or value calculated by another compute, fix, or atom-style variable. Per-atom chunk IDs can be used by other computes with "chunk" in their style name, such as compute com/chunk or compute msd/chunk. Or they can be used by the fix ave/chunk command to sum and time average a variety of per-atom properties over the atoms in each chunk. Or they can simply be accessed by any command that uses per-atom values from a compute as input, as discussed in Section_howto 15.

See Section_howto 23 for an overview of how this compute can be used with a variety of other commands to tabulate properties of a simulation. The howto section gives several examples of input script commands that can be used to calculate interesting properties.

Conceptually it is important to realize that this compute does two simple things. First, it sets the value of *Nchunk* = the number of chunks, which can be a constant value or change over time. Second, it assigns each atom to a chunk via a chunk ID. Chunk IDs range from 1 to *Nchunk* inclusive; some chunks may have no atoms assigned to them. Atoms that do not belong to any chunk are assigned a value of 0. Note that the two operations are not always performed together. For example, spatial bins can be setup once (which sets *Nchunk*), and atoms assigned to those bins many times thereafter (setting their chunk IDs).

All other commands in LAMMPS that use chunk IDs assume there are *Nchunk* number of chunks, and that every atom is assigned to one of those chunks, or not assigned to any chunk.

There are many options for specifying for how and when *Nchunk* is calculated, and how and when chunk IDs are assigned to atoms. The details depend on the chunk *style* and its *args*, as well as optional keyword settings. They can also depend on whether a fix ave/chunk command is using this compute, since that command requires *Nchunk* to remain static across windows of timesteps it specifies, while it accumulates per-chunk averages.

The details are described below.

The different chunk styles operate as follows. For each style, how it calculates *Nchunk* and assigns chunk IDs to

atoms is explained. Note that using the optional keywords can change both of those actions, as described further below where the keywords are discussed.

The *binning* styles perform a spatial binning of atoms, and assign an atom the chunk ID corresponding to the bin number it is in. *Nchunk* is set to the number of bins, which can change if the simulation box size changes.

The *bin/1d*, *bin/2d*, and *bin/3d* styles define bins as 1d layers (slabs), 2d pencils, or 3d boxes. The *dim*, *origin*, and *delta* settings are specified 1, 2, or 3 times. For 2d or 3d bins, there is no restriction on specifying dim = x before dim = y or z, or dim = y before dim = z. Bins in a particular *dim* have a bin size in that dimension given by *delta*. In each dimension, bins are defined relative to a specified *origin*, which may be the lower/upper edge of the simulation box (in that dimension), or its center point, or a specified coordinate value. Starting at the origin, sufficient bins are created in both directions to completely span the simulation box or the bounds specified by the optional *bounds* keyword.

For orthogonal simulation boxes, the bins are layers, pencils, or boxes aligned with the xyz coordinate axes. For triclinic (non-orthogonal) simulation boxes, the bin faces are parallel to the tilted faces of the simulation box. See this section of the manual for a discussion of the geometry of triclinic boxes in LAMMPS. As described there, a tilted simulation box has edge vectors a,b,c. In that nomenclature, bins in the x dimension have faces with normals in the "b" cross "c" direction. Bins in y have faces normal to the "a" cross "c" direction. And bins in z have faces normal to the "a" cross "b" direction. Note that in order to define the size and position of these bins in an unambiguous fashion, the *units* option must be set to *reduced* when using a triclinic simulation box, as noted below.

The meaning of *origin* and *delta* for triclinic boxes is as follows. Consider a triclinic box with bins that are 1d layers or slabs in the x dimension. No matter how the box is tilted, an *origin* of 0.0 means start layers at the lower "b" cross "c" plane of the simulation box and an *origin* of 1.0 means to start layers at the upper "b" cross "c" face of the box. A *delta* value of 0.1 in *reduced* units means there will be 10 layers from 0.0 to 1.0, regardless of the current size or shape of the simulation box.

The *bin/sphere* style defines a set of spherical shell bins around the origin (*xorig*,*yorig*,*zorig*), using *nsbin* bins with radii equally spaced between *srmin* and *srmax*. This is effectively a 1d vector of bins. For example, if *srmin* = 1.0 and *srmax* = 10.0 and *nsbin* = 9, then the first bin spans 1.0 < r < 2.0, and the last bin spans 9.0 < r 10.0. The geometry of the bins is the same whether the simulation box is orthogonal or triclinic; i.e. the spherical shells are not tilted or scaled differently in different dimensions to transform them into ellipsoidal shells.

The *bin/cylinder* style defines bins for a cylinder oriented along the axis *dim* with the axis coordinates in the other two radial dimensions at (*c1*,*c2*). For dim = x, c1/c2 = y/z; for dim = y, c1/c2 = x/z; for dim = z, c1/c2 = x/y. This is effectively a 2d array of bins. The first dimension is along the cylinder axis, the second dimension is radially outward from the cylinder axis. The bin size and positions along the cylinder axis are specified by the *origin* and *delta* values, the same as for the *bin/1d*, *bin/2d*, and *bin/3d* styles. There are *ncbin* concentric circle bins in the radial direction from the cylinder axis with radii equally spaced between *crmin* and *crmax*. For example, if *crmin* = 1.0 and *crmax* = 10.0 and *ncbin* = 9, then the first bin spans 1.0 < r < 2.0, and the last bin spans 9.0 < r 10.0. The geometry of the bins in the radial dimensions is the same whether the simulation box is orthogonal or triclinic; i.e. the concetric circles are not tilted or scaled differently in the two different dimensions to transform them into ellipses.

The created bins (and hence the chunk IDs) are numbered consecutively from 1 to the number of bins = *Nchunk*. For *bin2d* and *bin3d*, the numbering varies most rapidly in the first dimension (which could be x, y, or z), next rapidly in the 2nd dimension, and most slowly in the 3rd dimension. For *bin/sphere*, the bin with smallest radii is chunk 1 and the bni with largest radii is chunk Nchunk = *ncbin*. For *bin/cylinder*, the numbering varies most rapidly in the dimension along the cylinder axis and most slowly in the radial direction.

Each time this compute is invoked, each atom is mapped to a bin based on its current position. Note that between reneighboring timesteps, atoms can move outside the current simulation box. If the box is periodic (in that dimension) the atom is remapping into the periodic box for purposes of binning. If the box in not periodic, the atom may have moved outside the bounds of all bins. If an atom is not inside any bin, the *discard* keyword is used to determine how a chunk ID is assigned to the atom.

The *type* style uses the atom type as the chunk ID. *Nchunk* is set to the number of atom types defined for the simulation, e.g. via the create_box or read_data commands.

The *molecule* style uses the molecule ID of each atom as its chunk ID. *Nchunk* is set to the largest chunk ID. Note that this excludes molecule IDs for atoms which are not in the specified group or optional region.

There is no requirement that all atoms in a particular molecule are assigned the same chunk ID (zero or non-zero), though you probably want that to be the case, if you wish to compute a per-molecule property. LAMMPS will issue a warning if that is not the case, but only the first time that *Nchunk* is calculated.

Note that atoms with a molecule ID = 0, which may be non-molecular solvent atoms, have an out-of-range chunk ID. These atoms are discarded (not assigned to any chunk) or assigned to *Nchunk*, depending on the value of the *discard* keyword.

The *compute/fix/variable* styles set the chunk ID of each atom based on a quantity calculated and stored by a compute, fix, or variable. In each case, it must be a per-atom quantity. In each case the referenced floating point values are converted to an integer chunk ID as follows. The floating point value is truncated (rounded down) to an integer value. If the integer value is <= 0, then a chunk ID of 0 is assigned to the atom. If the integer value is > 0, it becomes the chunk ID to the atom. *Nchunk* is set to the largest chunk ID. Note that this excludes atoms which are not in the specified group or optional region.

If the style begins with "c_", a compute ID must follow which has been previously defined in the input script. If no bracketed integer is appended, the per-atom vector calculated by the compute is used. If a bracketed integer is appended, the Ith column of the per-atom array calculated by the compute is used. Users can also write code for their own compute styles and add them to LAMMPS.

If the style begins with "f_", a fix ID must follow which has been previously defined in the input script. If no bracketed integer is appended, the per-atom vector calculated by the fix is used. If a bracketed integer is appended, the Ith column of the per-atom array calculated by the fix is used. Note that some fixes only produce their values on certain timesteps, which must be compatible with the timestep on which this compute accesses the fix, else an error results. Users can also write code for their own fix styles and add them to LAMMPS.

If a value begins with "v_", a variable name for an *atom* or *atomfile* style variable must follow which has been previously defined in the input script. Variables of style *atom* can reference thermodynamic keywords and various per-atom attributes, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of generating per-atom quantities to treat as a chunk ID.

Normally, *Nchunk* = the number of chunks, is re-calculated every time this fix is invoked, though the value may or may not change. As explained below, the *nchunk* keyword can be set to *once* which means *Nchunk* will never change.

If a fix ave/chunk command uses this compute, it can also turn off the re-calculation of *Nchunk* for one or more windows of timesteps. The extent of the windows, during which Nchunk is held constant, are determined by the *Nevery*, *Nrepeat*, *Nfreq* values and the *ave* keyword setting that are used by the fix ave/chunk command.

Specifically, if *ave* = *one*, then for each span of *Nfreq* timesteps, *Nchunk* is held constant between the first timestep when averaging is done (within the Nfreq-length window), and the last timestep when averaging is done (multiple of Nfreq). If *ave* = *running* or *window*, then *Nchunk* is held constant forever, starting on the first timestep when the fix ave/chunk command invokes this compute.

Note that multiple fix ave/chunk commands can use the same compute chunk/atom compute. However, the time windows they induce for holding *Nchunk* constant must be identical, else an error will be generated.

The various optional keywords operate as follows. Note that some of them function differently or are ignored by different chunk styles. Some of them also have different default values, depending on the chunk style, as listed below.

The *region* keyword applies to all chunk styles. If used, an atom must be in both the specified group and the specified geometric region to be assigned to a chunk.

The *nchunk* keyword applies to all chunk styles. It specifies how often *Nchunk* is recalculated, which in turn can affect the chunk IDs assigned to individual atoms.

If *nchunk* is set to *once*, then *Nchunk* is only calculated once, the first time this compute is invoked. If *nchunk* is set to *every*, then *Nchunk* is re-calculated every time the compute is invoked. Note that, as described above, the use of this compute by the fix ave/chunk command can override the *every* setting.

The default values for *nchunk* are listed below and depend on the chunk style and other system and keyword settings. They attempt to represent typical use cases for the various chunk styles. The *nchunk* value can always be set explicitly if desired.

The *limit* keyword can be used to limit the calculated value of *Nchunk* = the number of chunks. The limit is applied each time *Nchunk* is calculated, which also limits the chunk IDs assigned to any atom. The *limit* keyword is used by all chunk styles except the *binning* styles, which ignore it. This is because the number of bins can be tailored using the *bound* keyword (described below) which effectively limits the size of *Nchunk*.

If *limit* is set to *Nc* = 0, then no limit is imposed on *Nchunk*, though the *compress* keyword can still be used to reduce *Nchunk*, as described below.

If *Nc* > 0, then the effect of the *limit* keyword depends on whether the *compress* keyword is also used with a setting of *yes*, and whether the *compress* keyword is specified before the *limit* keyword or after.

In all cases, *Nchunk* is first calculated in the usual way for each chunk style, as described above.

First, here is what occurs if *compress yes* is not set. If *limit* is set to *Nc max*, then *Nchunk* is reset to the smaller of *Nchunk* and *Nc*. If *limit* is set to *Nc exact*, then *Nchunk* is reset to *Nc*, whether the original *Nchunk* was larger or smaller than *Nc*. If *Nchunk* shrank due to the *limit* setting, then atom chunk IDs > *Nchunk* will be reset to 0 or *Nchunk*, depending on the setting of the *discard* keyword. If *Nchunk* grew, there will simply be some chunks with no atoms assigned to them.

If *compress yes* is set, and the *compress* keyword comes before the *limit* keyword, the compression operation is performed first, as described below, which resets *Nchunk*. The *limit* keyword is then applied to the new *Nchunk* value, exactly as described in the preceeding paragraph. Note that in this case, all atoms will end up with chunk IDs <= *Nc*, but their original values (e.g. molecule ID or compute/fix/variable value) may have been > *Nc*, because of the compression operation.

If *compress yes* is set, and the *compress* keyword comes after the *limit* keyword, then the *limit* value of *Nc* is applied first to the uncompressed value of *Nchunk*, but only if *Nc* < *Nchunk* (whether *Nc max* or *Nc exact* is used). This effectively means all atoms with chunk IDs > *Nc* have their chunk IDs reset to 0 or *Nc*, depending on the setting of the *discard* keyword. The compression operation is then performed, which may shrink *Nchunk* further. If the new *Nchunk* < *Nc* and *limit* = *Nc exact* is specified, then *Nchunk* is reset to *Nc*, which results in extra chunks with no atoms assigned to them. Note that in this case, all atoms will end up with chunk IDs <= *Nc*, and their original values (e.g. molecule ID or compute/fix/variable value) will also have been <= *Nc*.

The *ids* keyword applies to all chunk styles. If the setting is *once* then the chunk IDs assigned to atoms the first time this compute is invoked will be permanent, and never be re-computed.

If the setting is *nfreq* and if a fix ave/chunk command is using this compute, then in each of the *Nchunk* = constant time windows (discussed above), the chunk ID's assigned to atoms on the first step of the time window will persist until the end of the time window.

If the setting is *every*, which is the default, then chunk IDs are re-calculated on any timestep this compute is invoked.

NOTE: If you want the persistent chunk-IDs calculated by this compute to be continuous when running from a restart file, then you should use the same ID for this compute, as in the original run. This is so that the fix this compute creates to store per-atom quantities will also have the same ID, and thus be initialized correctly with chunk IDs from the restart file.

The *compress* keyword applies to all chunk styles and affects how *Nchunk* is calculated, which in turn affects the chunk IDs assigned to each atom. It is useful for converting a "sparse" set of chunk IDs (with many IDs that have no atoms assigned to them), into a "dense" set of IDs, where every chunk has one or more atoms assigned to it.

Two possible use cases are as follows. If a large simulation box is mostly empty space, then the *binning* style may produce many bins with no atoms. If *compress* is set to *yes*, only bins with atoms will be contribute to *Nchunk*. Likewise, the *molecule* or *compute/fix/variable* styles may produce large *Nchunk* values. For example, the compute cluster/atom command assigns every atom an atom ID for one of the atoms it is clustered with. For a million-atom system with 5 clusters, there would only be 5 unique chunk IDs, but the largest chunk ID might be 1 million, resulting in *Nchunk* = 1 million. If *compress* is set to *yes*, *Nchunk* will be reset to 5.

If *compress* is set to *no*, which is the default, no compression is done. If it is set to *yes*, all chunk IDs with no atoms are removed from the list of chunk IDs, and the list is sorted. The remaining chunk IDs are renumbered from 1 to *Nchunk* where *Nchunk* is the new length of the list. The chunk IDs assigned to each atom reflect the new renumbering from 1 to *Nchunk*.

The original chunk IDs (before renumbering) can be accessed by the compute property/chunk command and its *id* keyword, or by the fix ave/chunk command which outputs the original IDs as one of the columns in its global output array. For example, using the "compute cluster/atom" command discussed above, the original 5 unique chunk IDs might be atom IDs (27,4982,58374,857838,1000000). After compresion, these will be renumbered to (1,2,3,4,5). The original values (27,...,1000000) can be output to a file by the fix ave/chunk command, or by using the fix ave/time command in conjunction with the compute property/chunk command.

NOTE: The compression operation requires global communication across all processors to share their chunk ID values. It can require large memory on every processor to store them, even after they are compressed, if there are are a large number of unique chunk IDs with atoms assigned to them. It uses a STL map to find unique chunk IDs and store them in sorted order. Each time an atom is assigned a compressed chunk ID, it must access the STL map. All of this means that compression can be expensive, both in memory and CPU time. The use of the *limit* keyword in conjunction with the *compress* keyword can affect these costs, depending on which keyword is used

first. So use this option with care.

The *discard* keyword applies to all chunk styles. It affects what chunk IDs are assigned to atoms that do not match one of the valid chunk IDs from 1 to *Nchunk*. Note that it does not apply to atoms that are not in the specified group or optionally specified region. Those atoms are always assigned a chunk ID = 0.

If the calculated chunk ID for an atom is not within the range 1 to *Nchunk* then it is a "discard" atom. Note that *Nchunk* may have been shrunk by the *limit* keyword. Or the *compress* keyword may have eliminated chunk IDs that were valid before the compression took place, and are now not in the compressed list. Also note that for the *molecule* chunk style, if new molecules are added to the system, their chunk IDs may exceed a previously calculated *Nchunk*. Likewise, evaluation of a compute/fix/variable on a later timestep may return chunk IDs that are invalid for the previously calculated *Nchunk*.

All the chunk styles except the *binning* styles, must use *discard* set to either *yes* or *no*. If *discard* is set to *yes*, which is the default, then every "discard" atom has its chunk ID set to 0. If *discard* is set to *no*, every "discard" atom has its chunk ID set to *Nchunk*. I.e. it becomes part of the last chunk.

The *binning* styles use the *discard* keyword to decide whether to discard atoms outside the spatial domain covered by bins, or to assign them to the bin they are nearest to.

For the *bin/1d*, *bin/2d*, *bin/3d* styles the details are as follows. If *discard* is set to *yes*, an out-of-domain atom will have its chunk ID set to 0. If *discard* is set to *no*, the atom will have its chunk ID set to the first or last bin in that dimension. If *discard* is set to *mixed*, which is the default, it will only have its chunk ID set to the first or last bin if bins extend to the simulation box boundary in that dimension. This is the case if the *bound* keyword settings are *lower* and *upper*, which is the default. If the *bound* keyword settings are numeric values, then the atom will have its chunk ID set to 0 if it is outside the bounds of any bin. Note that in this case, it is possible that the first or last bin extends beyond the numeric *bounds* settings, depending on the specified *origin*. If this is the case, the chunk ID of the atom is only set to 0 if it is outside the first or last bin, not if it is simply outside the numeric *bounds* setting.

For the *bin/sphere* style the details are as follows. If *discard* is set to *yes*, an out-of-domain atom will have its chunk ID set to 0. If *discard* is set to *no* or *mixed*, the atom will have its chunk ID set to the first or last bin, i.e. the innermost or outermost spherical shell. If the distance of the atom from the origin is less than *rmin*, it will be assigned to the first bin. If the distance of the atom from the origin is greater than *rmax*, it will be assigned to the last bin.

For the *bin/cylinder* style the details are as follows. If *discard* is set to *yes*, an out-of-domain atom will have its chunk ID set to 0. If *discard* is set to *no*, the atom will have its chunk ID set to the first or last bin in both the radial and axis dimensions. If *discard* is set to *mixed*, which is the default, the the radial dimension is treated the same as for *discard* = no. But for the axis dimensinon, it will only have its chunk ID set to the first or last bin if bins extend to the simulation box boundary in the axis dimension. This is the case if the *bound* keyword settings are *lower* and *upper*, which is the default. If the *bound* keyword settings are numeric values, then the atom will have its chunk ID set to 0 if it is outside the bounds of any bin. Note that in this case, it is possible that the first or last bin extends beyond the numeric *bounds* settings, depending on the specified *origin*. If this is the case, the chunk ID of the atom is only set to 0 if it is outside the first or last bin, not if it is simply outside the numeric *bounds* setting.

If *discard* is set to *no* or *mixed*, the atom will have its chunk ID set to the first or last bin, i.e. the innermost or outermost spherical shell. If the distance of the atom from the origin is less than *rmin*, it will be assigned to the first bin. If the distance of the atom from the origin is greater than *rmax*, it will be assigned to the last bin.

The *bound* keyword only applies to the *bin/1d*, *bin/2d*, *bin/3d* styles and to the axis dimension of the *bin/cylinder* style; otherwise it is ignored. It can be used one or more times to limit the extent of bin coverage in a specified dimension, i.e. to only bin a portion of the box. If the *lo* setting is *lower* or the *hi* setting is *upper*, the bin extent in that direction extends to the box boundary. If a numeric value is used for *lo* and/or *hi*, then the bin extent in the *lo* or *hi* direction extends only to that value, which is assumed to be inside (or at least near) the simulation box boundaries, though LAMMPS does not check for this. Note that using the *bound* keyword typically reduces the total number of bins and thus the number of chunks *Nchunk*.

The *pbc* keyword only applies to the *bin/sphere* and *bin/cylinder* styles. If set to *yes*, the distance an atom is from the sphere origin or cylinder axis is calculated in a minimum image sense with respect to periodic dimensions, when determining which bin the atom is in. I.e. if x is a periodic dimension and the distance between the atom and the sphere center in the x dimension is greater than 0.5 * simulation box length in x, then a box length is subtracted to give a distance < 0.5 * simulation box length. This allosws the sphere or cylinder center to be near a box edge, and atoms on the other side of the periodic box will still be close to the center point/axis. Note that with a setting of *yes*, the outer sphere or cylinder radius must also be <= 0.5 * simulation box length in any periodic dimension except for the cylinder axis dimension, or an error is generated.

The *units* keyword only applies to the *binning* styles; otherwise it is ignored. For the *bin/1d*, *bin/2d*, *bin/3d* styles, it determines the meaning of the distance units used for the bin sizes *delta* and for *origin* and *bounds* values if they are coordinate values. For the *bin/sphere* style it determines the meaning of the distance units used for *xorig*,*yorig*,*zorig* and the radii *srmin* and *srmax*. For the *bin/cylinder* style it determines the meaning of the distance units used for *delta*,*c1*,*c2* and the radii *crmin* and *crmax*.

For orthogonal simulation boxes, any of the 3 options may be used. For non-orthogonal (triclinic) simulation boxes, only the *reduced* option may be used.

A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacing. A *reduced* value means normalized unitless values between 0 and 1, which represent the lower and upper faces of the simulation box respectively. Thus an *origin* value of 0.5 means the center of the box in any dimension. A *delta* value of 0.1 means 10 bins span the box in that dimension.

Note that for the *bin/sphere* style, the radii *srmin* and *srmax* are scaled by the lattice spacing or reduced value of the *x* dimension.

Note that for the *bin/cylinder* style, the radii *crmin* and *crmax* are scaled by the lattice spacing or reduced value of the 1st dimension perpendicular to the cylinder axis. E.g. y for an x-axis cylinder, x for a y-axis cylinder, and x for a z-axis cylinder.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values are unitless chunk IDs, ranging from 1 to *Nchunk* (inclusive) for atoms assigned to chunks, and 0 for atoms not belonging to a chunk.

Restrictions:

Even if the *nchunk* keyword is set to *once*, the chunk IDs assigned to each atom are not stored in a restart files. This means you cannot expect those assignments to persist in a restarted simulation. Instead you must re-specify this command and assign atoms to chunks when the restarted simulation begins.

Related commands:

fix ave/chunk

Default:

The option defaults are as follows:

- region = none
- nchunk = every, if compress is yes, overriding other defaults listed here
- nchunk = once, for type style
- nchunk = once, for mol style if region is none
- nchunk = every, for mol style if region is set
- nchunk = once, for binning style if the simulation box size is static or units = reduced
- nchunk = every, for binning style if the simulation box size is dynamic and units is lattice or box
- nchunk = every, for compute/fix/variable style
- limit = 0
- ids = every
- compress = no
- discard = yes, for all styles except binning
- discard = mixed, for binning styles
- bound = lower and upper in all dimensions
- pbc = no
- units = lattice

compute cluster/atom command

Syntax:

```
compute ID group-ID cluster/atom cutoff
```

- ID, group-ID are documented in compute command
- cluster/atom = style name of this compute command
- cutoff = distance within which to label atoms as part of same cluster (distance units)

Examples:

```
compute 1 all cluster/atom 1.0
```

Description:

Define a computation that assigns each atom a cluster ID.

A cluster is defined as a set of atoms, each of which is within the cutoff distance from one or more other atoms in the cluster. If an atom has no neighbors within the cutoff distance, then it is a 1-atom cluster. The ID of every atom in the cluster will be the smallest atom ID of any atom in the cluster.

Only atoms in the compute group are clustered and assigned cluster IDs. Atoms not in the compute group are assigned a cluster ID = 0.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently or to have multiple compute/dump commands, each of a *clsuter/atom* style.

NOTE: If you have a bonded system, then the settings of special_bonds command can remove pairwise interactions between atoms in the same bond, angle, or dihedral. This is the default setting for the special_bonds command, and means those pairwise interactions do not appear in the neighbor list. Because this fix uses the neighbor list, it also means those pairs will not be included when computing the clusters. This does not apply when using long-range coulomb (*coul/long*, *coul/msm*, *coul/wolf* or similar. One way to get around this would be to set special_bond scaling factors to very tiny numbers that are not exactly zero (e.g. 1.0e-50). Another workaround is to write a dump file, and use the rerun command to compute the clusters for snapshots in the dump file. The rerun script can use a special_bonds command that includes all pairs in the neighbor list.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be an ID > 0, as explained above.

Restrictions: none

Related commands:

compute coord/atom

Default: none

compute cna/atom command

Syntax:

```
compute ID group-ID cna/atom cutoff
```

- ID, group-ID are documented in compute command
- cna/atom = style name of this compute command
- cutoff = cutoff distance for nearest neighbors (distance units)

Examples:

```
compute 1 all cna/atom 3.08
```

Description:

Define a computation that calculates the CNA (Common Neighbor Analysis) pattern for each atom in the group. In solid-state systems the CNA pattern is a useful measure of the local crystal structure around an atom. The CNA methodology is described in (Faken) and (Tsuzuki).

Currently, there are five kinds of CNA patterns LAMMPS recognizes:

- fcc = 1
- hcp = 2
- bcc = 3
- icosohedral = 4
- unknown = 5

The value of the CNA pattern will be 0 for atoms not in the specified compute group. Note that normally a CNA calculation should only be performed on mono-component systems.

The CNA calculation can be sensitive to the specified cutoff value. You should insure the appropriate nearest neighbors of an atom are found within the cutoff distance for the presumed crystal strucure. E.g. 12 nearest neighbor for perfect FCC and HCP crystals, 14 nearest neighbors for perfect BCC crystals. These formulas can be used to obtain a good cutoff distance:

$$
\begin{aligned}
r_c^{fcc} &= \frac{1}{2}\left(\frac{\sqrt{2}}{2}+1\right)\mathrm{a} \simeq 0.8536\,\mathrm{a} \\
r_c^{bcc} &= \frac{1}{2}(\sqrt{2}+1)\mathrm{a} \simeq 1.207\,\mathrm{a} \\
r_c^{hcp} &= \frac{1}{2}\left(1+\sqrt{\frac{4+2x^2}{3}}\right)\mathrm{a}
\end{aligned}
$$

where a is the lattice constant for the crystal structure concerned and in the HCP case, x = (c/a) / 1.633, where 1.633 is the ideal c/a for HCP crystals.

Also note that since the CNA calculation in LAMMPS uses the neighbors of an owned atom to find the nearest neighbors of a ghost atom, the following relation should also be satisfied:

$$Rc + Rs > 2 * \text{cutoff}$$

where Rc is the cutoff distance of the potential, Rs is the skin distance as specified by the neighbor command, and cutoff is the argument used with the compute cna/atom command. LAMMPS will issue a warning if this is not the case.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (e.g. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently or to have multiple compute/dump commands, each with a *cna/atom* style.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be a number from 0 to 5, as explained above.

Restrictions: none

Related commands:

compute centro/atom

Default: none

(Faken) Faken, Jonsson, Comput Mater Sci, 2, 279 (1994).

(Tsuzuki) Tsuzuki, Branicio, Rino, Comput Phys Comm, 177, 518 (2007).

compute com command

Syntax:

```
compute ID group-ID com
```

- ID, group-ID are documented in compute command
- com = style name of this compute command

Examples:

```
compute 1 all com
```

Description:

Define a computation that calculates the center-of-mass of the group of atoms, including all effects due to atoms passing thru periodic boundaries.

A vector of three quantites is calculated by this compute, which are the x,y,z coordinates of the center of mass.

NOTE: The coordinates of an atom contribute to the center-of-mass in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

Output info:

This compute calculates a global vector of length 3, which can be accessed by indices 1-3 by any command that uses global vector values from a compute as input. See this section for an overview of LAMMPS output options.

The vector values are "intensive". The vector values will be in distance units.

Restrictions: none

Related commands:

compute com/chunk

Default: none

compute com/chunk command

Syntax:

```
compute ID group-ID com/chunk chunkID
```

- ID, group-ID are documented in compute command
- com/chunk = style name of this compute command
- chunkID = ID of compute chunk/atom command

Examples:

```
compute 1 fluid com/chunk molchunk
```

Description:

Define a computation that calculates the center-of-mass for multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a compute chunk/atom command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the compute chunk/atom doc page and "Section_howto 23 for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates the x,y,z coordinates of the center-of-mass for each chunk, which includes all effects due to atoms passing thru periodic boundaries.

Note that only atoms in the specified group contribute to the calculation. The compute chunk/atom command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

NOTE: The coordinates of an atom contribute to the chunk's center-of-mass in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

The simplest way to output the results of the compute com/chunk calculation to a file is to use the fix ave/time command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all com/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk file tmp.out mode vector
```

Output info:

This compute calculates a global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified compute chunk/atom command. The number of columns = 3 for the x,y,z center-of-mass coordinates of each chunk. These values can be accessed by any command that uses global array values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in distance units.

Restrictions: none

Related commands:

compute com

Default: none

compute contact/atom command

Syntax:

```
compute ID group-ID contact/atom
```

- ID, group-ID are documented in compute command
- contact/atom = style name of this compute command

Examples:

```
compute 1 all contact/atom
```

Description:

Define a computation that calculates the number of contacts for each atom in a group.

The contact number is defined for finite-size spherical particles as the number of neighbor atoms which overlap the central particle, meaning that their distance of separation is less than or equal to the sum of the radii of the two particles.

The value of the contact number will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, whose values can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be a number >= 0.0, as explained above.

Restrictions:

This compute requires that atoms store a radius as defined by the atom_style sphere command.

Related commands:

compute coord/atom

Default: none

compute coord/atom command

Syntax:

```
compute ID group-ID coord/atom cutoff type1 type2 ...
```

- ID, group-ID are documented in compute command
- coord/atom = style name of this compute command
- cutoff = distance within which to count coordination neighbors (distance units)
- typeN = atom type for Nth coordination count (see asterisk form below)

Examples:

```
compute 1 all coord/atom 2.0
compute 1 all coord/atom 6.0 1 2
compute 1 all coord/atom 6.0 2*4 5*8 *
```

Description:

Define a computation that calculates one or more coordination numbers for each atom in a group.

A coordination number is defined as the number of neighbor atoms with specified atom type(s) that are within the specified cutoff distance from the central atom. Atoms not in the group are included in a coordination number of atoms in the group.

The *typeN* keywords allow you to specify which atom types contribute to each coordination number. One coordination number is computed for each of the *typeN* keywords listed. If no *typeN* keywords are listed, a single coordination number is calculated, which includes atoms of all types (same as the "*" format, see below).

The *typeN* keywords can be specified in one of two ways. An explicit numeric value can be used, as in the 2nd example above. Or a wild-card asterisk can be used to specify a range of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

The value of all coordination numbers will be 0.0 for atoms not in the specified compute group.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently.

NOTE: If you have a bonded system, then the settings of special_bonds command can remove pairwise interactions between atoms in the same bond, angle, or dihedral. This is the default setting for the special_bonds command, and means those pairwise interactions do not appear in the neighbor list. Because this fix uses the neighbor list, it also means those pairs will not be included in the coordination count. One way to get around this, is to write a dump file, and use the rerun command to compute the coordination for snapshots in the dump file. The rerun script can use a special_bonds command that includes all pairs in the neighbor list.

Output info:

If single *type1* keyword is specified (or if none are specified), this compute calculates a per-atom vector. If multiple *typeN* keywords are specified, this compute calculates a per-atom array, with N columns. These values

can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector or array values will be a number >= 0.0, as explained above.

Restrictions: none

Related commands:

compute cluster/atom

Default: none

compute damage/atom command

Syntax:

```
compute ID group-ID damage/atom
```

- ID, group-ID are documented in compute command
- damage/atom = style name of this compute command

Examples:

```
compute 1 all damage/atom
```

Description:

Define a computation that calculates the per-atom damage for each atom in a group. This is a quantity relevant for Peridynamics models. See this document for an overview of LAMMPS commands for Peridynamics modeling.

The "damage" of a Peridymaics particles is based on the bond breakage between the particle and its neighbors. If all the bonds are broken the particle is considered to be fully damaged.

See the PDLAMMPS user guide for a formal definition of "damage" and more details about Peridynamics as it is implemented in LAMMPS.

This command can be used with all the Peridynamic pair styles.

The damage value will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values are unitlesss numbers (damage) >= 0.0.

Restrictions:

This compute is part of the PERI package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

compute dilatation, compute plasticity

Default: none

compute dihedral/local command

Syntax:

```
compute ID group-ID dihedral/local input1 input2 ...
```

- ID, group-ID are documented in compute command
- dihedral/local = style name of this compute command
- one or more keywords may be appended
- keyword = *phi*

```
  phi = tabulate dihedral angles
```

Examples:

```
compute 1 all dihedral/local phi
```

Description:

Define a computation that calculates properties of individual dihedral interactions. The number of datums generated, aggregated across all processors, equals the number of angles in the system, modified by the group parameter as explained below.

The local data stored by this command is generated by looping over all the atoms owned on a processor and their dihedrals. A dihedral will only be included if all 4 atoms in the dihedral are in the specified compute group.

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For example, dihedral output from the compute property/local command can be combined with data from this command and output by the dump local command in a consistent way.

Output info:

This compute calculates a local vector or local array depending on the number of keywords. The length of the vector or number of rows in the array is the number of dihedrals. If a single keyword is specified, a local vector is produced. If two or more keywords are specified, a local array is produced where the number of columns = the number of keywords. The vector or array can be accessed by any command that uses local values from a compute as input. See this section for an overview of LAMMPS output options.

The output for *phi* will be in degrees.

Restrictions: none

Related commands:

dump local, compute property/local

Default: none

compute dilatation/atom command

Syntax:

```
compute ID group-ID dilatation/atom
```

- ID, group-ID are documented in compute command
- dilation/atom = style name of this compute command

Examples:

```
compute 1 all dilatation/atom
```

Description:

Define a computation that calculates the per-atom dilatation for each atom in a group. This is a quantity relevant for Peridynamics models. See this document for an overview of LAMMPS commands for Peridynamics modeling.

For small deformation, dilatation of is the measure of the volumetric strain.

The dilatation "theta" for each peridynamic particle I is calculated as a sum over its neighbors with unbroken bonds, where the contribution of the IJ pair is a function of the change in bond length (versus the initial length in the reference state), the volume fraction of the particles and an influence function. See the PDLAMMPS user guide for a formal definition of dilatation.

This command can only be used with a subset of the Peridynamic pair styles: peri/lps, peri/ves and peri/eps.

The dilatation value will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values are unitlesss numbers (theta) >= 0.0.

Restrictions:

This compute is part of the PERI package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

compute damage, compute plasticity

Default: none

compute displace/atom command

Syntax:

```
compute ID group-ID displace/atom
```

- ID, group-ID are documented in compute command
- displace/atom = style name of this compute command

Examples:

```
compute 1 all displace/atom
```

Description:

Define a computation that calculates the current displacement of each atom in the group from its original coordinates, including all effects due to atoms passing thru periodic boundaries.

A vector of four quantites per atom is calculated by this compute. The first 3 elements of the vector are the dx,dy,dz displacements. The 4th component is the total displacement, i.e. sqrt(dx*dx + dy*dy + dz*dz).

The displacement of an atom is from its original position at the time the compute command was issued. The value of the displacement will be 0.0 for atoms not in the specified compute group.

NOTE: Initial coordinates are stored in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

NOTE: If you want the quantities calculated by this compute to be continuous when running from a restart file, then you should use the same ID for this compute, as in the original run. This is so that the fix this compute creates to store per-atom quantities will also have the same ID, and thus be initialized correctly with time=0 atom coordinates from the restart file.

Output info:

This compute calculates a per-atom array with 4 columns, which can be accessed by indices 1-4 by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom array values will be in distance units.

Restrictions: none

Related commands:

compute msd, dump custom, fix store/state

Default: none

compute dpd command

Syntax:

```
compute ID group-ID dpd
```

- ID, group-ID are documented in compute command
- dpd = style name of this compute command

Examples:

```
compute 1 all dpd
```

Description:

Define a computation that accumulates the total internal conductive energy (U_cond), the total internal mechanical energy (U_mech), the total internal energy (U) and the *harmonic* average of the internal temperature (dpdTheta) for the entire system of particles. See the compute dpd/atom command if you want per-particle internal energies and internal temperatures.

The system internal properties are computed according to the following relations:

$$U^{cond} = \sum_{i=1}^{N} u_i^c$$

$$U^{mech} = \sum_{i=1}^{N} u_i^m$$

$$U = \sum_{i=1}^{N} (u_i^{cond} + u_i^{me}$$

$$\theta_{avg} = (\frac{1}{N} \sum_{i=1}^{N} \frac{1}{\theta_i}$$

where N is the number of particles in the system

Output info:

This compute calculates a global vector of length 5 (U_cond, U_mech, U, dpdTheta, N_particles), which can be accessed by indices 1-5. See this section for an overview of LAMMPS output options.

The vector values will be in energy and temperature units.

Restrictions:

The compute *dpd* is only available if LAMMPS is built with the USER-DPD package and requires the atom_style dpd.

Related commands:

compute dpd/atom, thermo_style

Default: none

(Larentzos) J.P. Larentzos, J.K. Brennan, J.D. Moore, and W.D. Mattson, "LAMMPS Implementation of Constant Energy Dissipative Particle Dynamics (DPD-E)", ARL-TR-6863, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD (2014).

compute dpd/atom command

Syntax:

```
compute ID group-ID dpd/atom
```

- ID, group-ID are documented in compute command
- dpd/atom = style name of this compute command

Examples:

compute 1 all dpd/atom

Description:

Define a computation that accesses the per-particle internal conductive energy (u_cond), internal mechanical energy (u_mech) and internal temperatures (dpdTheta) for each particle in a group. See the compute dpd command if you want the total internal conductive energy, the total internal mechanical energy, and average internal temperature of the entire system or group of dpd particles.

Output info:

This compute calculates a per-particle array with 3 columns (u_cond, u_mech, dpdTheta), which can be accessed by indices 1-3 by any command that uses per-particle values from a compute as input. See Section_howto15 for an overview of LAMMPS output options.

The per-particle array values will be in energy (u_cond, u_mech) and temperature (dpdTheta) units.

Restrictions:

The compute *dpd/atom* is only available if LAMMPS is built with the USER-DPD package.

Related commands:

dump custom, compute dpd

Default: none

(Larentzos) J.P. Larentzos, J.K. Brennan, J.D. Moore, and W.D. Mattson, "LAMMPS Implementation of Constant Energy Dissipative Particle Dynamics (DPD-E)", ARL-TR-6863, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD (2014).

compute erotate/asphere command

Syntax:

```
compute ID group-ID erotate/asphere
```

- ID, group-ID are documented in compute command
- erotate/asphere = style name of this compute command

Examples:

```
compute 1 all erotate/asphere
```

Description:

Define a computation that calculates the rotational kinetic energy of a group of aspherical particles. The aspherical particles can be ellipsoids, or line segments, or triangles. See the atom_style and read_data commands for descriptions of these options.

For all 3 types of particles, the rotational kinetic energy is computed as 1/2 I w^2, where I is the inertia tensor for the aspherical particle and w is its angular velocity, which is computed from its angular momentum if needed.

NOTE: For 2d models, ellipsoidal particles are treated as ellipsoids, not ellipses, meaning their moments of inertia will be the same as in 3d.

Output info:

This compute calculates a global scalar (the KE). This value can be used by any command that uses a global scalar value from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy units.

Restrictions:

This compute requires that ellipsoidal particles atoms store a shape and quaternion orientation and angular momentum as defined by the atom_style ellipsoid command.

This compute requires that line segment particles atoms store a length and orientation and angular velocity as defined by the atom_style line command.

This compute requires that triangular particles atoms store a size and shape and quaternion orientation and angular momentum as defined by the atom_style tri command.

All particles in the group must be finite-size. They cannot be point particles.

Related commands: none

compute erotate/sphere

Default: none

compute erotate/rigid command

Syntax:

```
compute ID group-ID erotate/rigid fix-ID
```

- ID, group-ID are documented in compute command
- erotate/rigid = style name of this compute command
- fix-ID = ID of rigid body fix

Examples:

```
compute 1 all erotate/rigid myRigid
```

Description:

Define a computation that calculates the rotational kinetic energy of a collection of rigid bodies, as defined by one of the fix rigid command variants.

The rotational energy of each rigid body is computed as 1/2 I Wbody^2, where I is the inertia tensor for the rigid body, and Wbody is its angular velocity vector. Both I and Wbody are in the frame of reference of the rigid body, i.e. I is diagonalized.

The *fix-ID* should be the ID of one of the fix rigid commands which defines the rigid bodies. The group specified in the compute command is ignored. The rotational energy of all the rigid bodies defined by the fix rigid command in included in the calculation.

Output info:

This compute calculates a global scalar (the summed rotational energy of all the rigid bodies). This value can be used by any command that uses a global scalar value from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy units.

Restrictions:

This compute is part of the RIGID package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

compute ke/rigid

Default: none

compute erotate/sphere command

Syntax:

```
compute ID group-ID erotate/sphere
```

- ID, group-ID are documented in compute command
- erotate/sphere = style name of this compute command

Examples:

```
compute 1 all erotate/sphere
```

Description:

Define a computation that calculates the rotational kinetic energy of a group of spherical particles.

The rotational energy is computed as 1/2 I w^2, where I is the moment of inertia for a sphere and w is the particle's angular velocity.

NOTE: For 2d models, particles are treated as spheres, not disks, meaning their moment of inertia will be the same as in 3d.

Output info:

This compute calculates a global scalar (the KE). This value can be used by any command that uses a global scalar value from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy units.

Restrictions:

This compute requires that atoms store a radius and angular velocity (omega) as defined by the atom_style sphere command.

All particles in the group must be finite-size spheres or point particles. They cannot be aspherical. Point particles will not contribute to the rotational energy.

Related commands:

compute erotate/asphere

Default: none

compute erotate/sphere/atom command

Syntax:

```
compute ID group-ID erotate/sphere/atom
```

- ID, group-ID are documented in compute command
- erotate/sphere/atom = style name of this compute command

Examples:

```
compute 1 all erotate/sphere/atom
```

Description:

Define a computation that calculates the rotational kinetic energy for each particle in a group.

The rotational energy is computed as 1/2 I w^2, where I is the moment of inertia for a sphere and w is the particle's angular velocity.

NOTE: For 2d models, particles are treated as spheres, not disks, meaning their moment of inertia will be the same as in 3d.

The value of the rotational kinetic energy will be 0.0 for atoms not in the specified compute group or for point particles with a radius = 0.0.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be in energy units.

Restrictions: none

Related commands:

dump custom

Default: none

compute event/displace command

Syntax:

```
compute ID group-ID event/displace threshold
```

- ID, group-ID are documented in compute command
- event/displace = style name of this compute command
- threshold = minimum distance anyparticle must move to trigger an event (distance units)

Examples:

```
compute 1 all event/displace 0.5
```

Description:

Define a computation that flags an "event" if any particle in the group has moved a distance greater than the specified threshold distance when compared to a previously stored reference state (i.e. the previous event). This compute is typically used in conjunction with the prd and tad commands, to detect if a transition to a new minimum energy basin has occurred.

This value calculated by the compute is equal to 0 if no particle has moved far enough, and equal to 1 if one or more particles have moved further than the threshold distance.

NOTE: If the system is undergoing significant center-of-mass motion, due to thermal motion, an external force, or an initial net momentum, then this compute will not be able to distinguish that motion from local atom displacements and may generate "false postives."

Output info:

This compute calculates a global scalar (the flag). This value can be used by any command that uses a global scalar value from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The scalar value will be a 0 or 1 as explained above.

Restrictions:

This command can only be used if LAMMPS was built with the REPLICA package. See the Making LAMMPS section for more info on packages.

Related commands:

prd, tad

Default: none

compute fep command

Syntax:

```
compute ID group-ID fep temp attribute args ... keyword value ...
```

- ID, group-ID are documented in the compute command
- fep = name of this compute command
- temp = external temperature (as specified for constant-temperature run)
- one or more attributes with args may be appended
- attribute = *pair* or *atom*

```
  pair args = pstyle pparam I J v_delta
      pstyle = pair style name, e.g. lj/cut
      pparam = parameter to perturb
      I,J = type pair(s) to set parameter for
      v_delta = variable with perturbation to apply (in the units of the parameter)
    atom args = aparam I v_delta
      aparam = parameter to perturb
      I = type to set parameter for
      v_delta = variable with perturbation to apply (in the units of the parameter)
```

- zero or more keyword/value pairs may be appended
- keyword = *tail* or *volume*

```
  tail value = no or yes
      no = ignore tail correction to pair energies (usually small in fep)
      yes = include tail correction to pair energies
    volume value = no or yes
      no = ignore volume changes (e.g. in NVE or NVT trajectories)
      yes = include volume changes (e.g. in NpT trajectories)
```

Examples:

```
compute 1 all fep 298 pair lj/cut epsilon 1 * v_delta pair lj/cut sigma 1 * v_delta volume yes
compute 1 all fep 300 atom charge 2 v_delta
```

Description:

Apply a perturbation to parameters of the interaction potential and recalculate the pair potential energy without changing the atomic coordinates from those of the reference, unperturbed system. This compute can be used to calculate free energy differences using several methods, such as free-energy perturbation (FEP), finite-difference thermodynamic integration (FDTI) or Bennet's acceptance ratio method (BAR).

The potential energy of the system is decomposed in three terms: a background term corresponding to interaction sites whose parameters remain constant, a reference term U_0 corresponding to the initial interactions of the atoms that will undergo perturbation, and a term U_1 corresponding to the final interactions of these atoms:

$$U(\lambda) = U_{\mathrm{bg}} + U_1(\lambda) + U_0(\lambda)$$

A coupling parameter varying from 0 to 1 connects the reference and perturbed systems:

$$\begin{aligned} \lambda = 0 \quad &\Rightarrow \quad U = U_{\mathrm{bg}} + U_0 \\ \lambda = 1 \quad &\Rightarrow \quad U = U_{\mathrm{bg}} + U_1 \end{aligned}$$

It is possible but not necessary that the coupling parameter (or a function thereof) appears as a multiplication factor of the potential energy. Therefore, this compute can apply perturbations to interaction parameters that are not directly proportional to the potential energy (e.g. in Lennard-Jones potentials).

This command can be combined with fix adapt to perform multistage free-energy perturbation calculations along stepwise alchemical transformations during a simulation run:

$$\Delta_0^1 A = \sum_{i=0}^{n-1} \Delta_{\lambda_i}^{\lambda_{i+1}} A = -kT \sum_{i=0}^{n-1} \ln \left\langle \exp\left(-\frac{U(\lambda_{i+1}) - U(\lambda_i)}{kT}\right)\right\rangle_{\lambda_i}$$

This compute is suitable for the finite-difference thermodynamic integration (FDTI) method (Mezei), which is based on an evaluation of the numerical derivative of the free energy by a perturbation method using a very small :

$$\Delta_0^1 A = \int_{\lambda=0}^{\lambda=1} \left(\frac{\partial A(\lambda)}{\partial \lambda}\right)_\lambda \mathrm{d}\lambda \approx \sum_{i=0}^{n-1} w_i \frac{A(\lambda_i + \delta) - A(\lambda_i)}{\delta}$$

where w_i are weights of a numerical quadrature. The fix adapt command can be used to define the stages of at which the derivative is calculated and averaged.

The compute fep calculates the exponential Boltzmann term and also the potential energy difference U_1-U_0. By choosing a very small perturbation the thermodynamic integration method can be implemented using a numerical evaluation of the derivative of the potential energy with respect to :

$$\Delta_0^1 A = \int_{\lambda=0}^{\lambda=1} \left\langle \frac{\partial U(\lambda)}{\partial \lambda} \right\rangle_\lambda \mathrm{d}\lambda \approx \sum_{i=0}^{n-1} w_i \left\langle \frac{U(\lambda_i + \delta) - U(\lambda_i)}{\delta} \right\rangle_{\lambda_i}$$

Another technique to calculate free energy differences is the acceptance ratio method (Bennet), which can be implemented by calculating the potential energy differences with = 1.0 on both the forward and reverse routes:

$$\left\langle \frac{1}{1 + \exp\left[\left(U_1 - U_0 - \Delta_0^1 A\right)/kT\right]} \right\rangle_0 = \left\langle \frac{1}{1 + \exp\left[\left(U_0 - U_1 + \Delta_0^1 A\right)/kT\right]} \right\rangle_1$$

The value of the free energy difference is determined by numerical root finding to establish the equality.

Concerning the choice of how the atomic parameters are perturbed in order to setup an alchemical transformation route, several strategies are available, such as single-topology or double-topology strategies (Pearlman). The latter does not require modification of bond lengths, angles or other internal coordinates.

NOTES: This compute command does not take kinetic energy into account, therefore the masses of the particles should not be modified between the reference and perturbed states, or along the alchemical transformation route. This compute command does not change bond lengths or other internal coordinates (Boresch, Karplus).

The *pair* attribute enables various parameters of potentials defined by the pair_style and pair_coeff commands to be changed, if the pair style supports it.

The *pstyle* argument is the name of the pair style. For example, *pstyle* could be specified as "lj/cut". The *pparam* argument is the name of the parameter to change. This is a (non-exclusive) list of pair styles and parameters that can be used with this compute. See the doc pages for individual pair styles and their energy formulas for the

meaning of these parameters:

lj/cut	epsilon,sigma	type pairs
lj/cut/coul/cut	epsilon,sigma	type pairs
lj/cut/coul/long	epsilon,sigma	type pairs
lj/cut/soft	epsilon,sigma,lambda	type pairs
coul/cut/soft	lambda	type pairs
coul/long/soft	lambda	type pairs
lj/cut/coul/cut/soft	epsilon,sigma,lambda	type pairs
lj/cut/coul/long/soft	epsilon,sigma,lambda	type pairs
lj/cut/tip4p/long/soft	epsilon,sigma,lambda	type pairs
tip4p/long/soft	lambda	type pairs
lj/charmm/coul/long/soft	epsilon,sigma,lambda	type pairs
born	a,b,c	type pairs
buck	a,c	type pairs

Note that it is easy to add new potentials and their parameters to this list. All it typically takes is adding an extract() method to the pair_*.cpp file associated with the potential.

Similar to the pair_coeff command, I and J can be specified in one of two ways. Explicit numeric values can be used for each, as in the 1st example above. I <= J is required. LAMMPS sets the coefficients for the symmetric J,I interaction to the same values. A wild-card asterisk can be used in place of or in conjunction with the I,J arguments to set the coefficients for multiple pairs of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that only type pairs with I <= J are considered; if asterisks imply type pairs where J < I, they are ignored.

If pair_style hybrid or hybrid/overlay is being used, then the *pstyle* will be a sub-style name. You must specify I,J arguments that correspond to type pair values defined (via the pair_coeff command) for that sub-style.

The *v_name* argument for keyword *pair* is the name of an equal-style variable which will be evaluated each time this compute is invoked. It should be specified as v_name, where name is the variable name.

The *atom* attribute enables atom properties to be changed. The *aparam* argument is the name of the parameter to change. This is the current list of atom parameters that can be used with this compute:

- charge = charge on particle

The *v_name* argument for keyword *pair* is the name of an equal-style variable which will be evaluated each time this compute is invoked. It should be specified as v_name, where name is the variable name.

The *tail* keyword controls the calculation of the tail correction to "van der Waals" pair energies beyond the cutoff, if this has been activated via the pair_modify command. If the perturbation is small, the tail contribution to the energy difference between the reference and perturbed systems should be negligible.

If the keyword *volume* = *yes*, then the Boltzmann term is multiplied by the volume so that correct ensemble averaging can be performed over trajectories during which the volume fluctuates or changes (Allen and Tildesley):

$$\Delta_0^1 A = -kT \sum_{i=0}^{n-1} \ln \frac{\left\langle V \exp\left(-\frac{U(\lambda_{i+1})-U(\lambda_i)}{kT}\right)\right\rangle_{\lambda_i}}{\langle V \rangle_{\lambda_i}}$$

Output info:

This compute calculates a global vector of length 3 which contains the energy difference (U_1-U_0) as c_ID[1], the Boltzmann factor exp(-(U_1-U_0)/*kT*), or *V*exp(-(U_1-U_0)/*kT*), as c_ID[2] and the volume of the simulation box *V* as c_ID[3]. U_1 is the pair potential energy obtained with the perturbed parameters and U_0 is the pair potential energy obtained with the unperturbed parameters. The energies include kspace terms if these are used in the simulation.

These output results can be used by any command that uses a global scalar or vector from a compute as input. See Section_howto 15 for an overview of LAMMPS output options. For example, the computed values can be averaged using fix ave/time.

The values calculated by this compute are "extensive".

Restrictions:

This compute is distributed as the USER-FEP package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix adapt/fep, fix ave/time, pair_lj_soft_coul_soft

Default:

The option defaults are *tail* = *no*, *volume* = *no*.

(Pearlman) Pearlman, J Chem Phys, 98, 1487 (1994)

(Mezei) Mezei, J Chem Phys, 86, 7084 (1987)

(Bennet) Bennet, J Comput Phys, 22, 245 (1976)

(BoreschKarplus) Boresch and Karplus, J Phys Chem A, 103, 103 (1999)

(AllenTildesley) Allen and Tildesley, Computer Simulation of Liquids, Oxford University Press (1987)

compute group/group command

Syntax:

```
compute ID group-ID group/group group2-ID keyword value ...
```

- ID, group-ID are documented in compute command
- group/group = style name of this compute command
- group2-ID = group ID of second (or same) group
- zero or more keyword/value pairs may be appended
- keyword = *pair* or *kspace* or *boundary*

```
pair value = yes or no
  kspace value = yes or no
  boundary value = yes or no
```

Examples:

```
compute 1 lower group/group upper
compute 1 lower group/group upper kspace yes
compute mine fluid group/group wall
```

Description:

Define a computation that calculates the total energy and force interaction between two groups of atoms: the compute group and the specified group2. The two groups can be the same.

If the *pair* keyword is set to *yes*, which is the default, then the the interaction energy will include a pair component which is defined as the pairwise energy between all pairs of atoms where one atom in the pair is in the first group and the other is in the second group. Likewise, the interaction force calculated by this compute will include the force on the compute group atoms due to pairwise interactions with atoms in the specified group2.

If the *kspace* keyword is set to *yes*, which is not the default, and if a kspace_style is defined, then the interaction energy will include a Kspace component which is the long-range Coulombic energy between all the atoms in the first group and all the atoms in the 2nd group. Likewise, the interaction force calculated by this compute will include the force on the compute group atoms due to long-range Coulombic interactions with atoms in the specified group2.

Normally the long-range Coulombic energy converges only when the net charge of the unit cell is zero. However, one can assume the net charge of the system is neutralized by a uniform background plasma, and a correction to the system energy can be applied to reduce artifacts. For more information see (Bogusz). If the *boundary* keyword is set to *yes*, which is the default, and *kspace* contributions are included, then this energy correction term will be added to the total group-group energy. This correction term does not affect the force calculation and will be zero if one or both of the groups are charge neutral. This energy correction term is the same as that included in the regular Ewald and PPPM routines.

This compute does not calculate any bond or angle or dihedral or improper interactions between atoms in the two groups.

The pairwise contributions to the group-group interactions are calculated by looping over a neighbor list. The Kspace contribution to the group-group interactions require essentially the same amount of work (FFTs, Ewald

summation) as computing long-range forces for the entire system. Thus it can be costly to invoke this compute too frequently.

If you desire a breakdown of the interactions into a pairwise and Kspace component, simply invoke the compute twice with the appropriate yes/no settings for the *pair* and *kspace* keywords. This is no more costly than using a single compute with both keywords set to *yes*. The individual contributions can be summed in a variable if desired.

This document describes how the long-range group-group calculations are performed.

Output info:

This compute calculates a global scalar (the energy) and a global vector of length 3 (force), which can be accessed by indices 1-3. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

Both the scalar and vector values calculated by this compute are "extensive". The scalar value will be in energy units. The vector values will be in force units.

Restrictions:

Not all pair styles can be evaluated in a pairwise mode as required by this compute. For example, 3-body and other many-body potentials, such as Tersoff and Stillinger-Weber cannot be used. EAM potentials only include the pair potential portion of the EAM interaction when used by this compute, not the embedding term.

Not all Kspace styles support calculation of group/group interactions. The *ewald* and *pppm* styles do.

Related commands: none

Default:

The option defaults are pair = yes, kspace = no, and boundary = yes.

Bogusz et al, J Chem Phys, 108, 7070 (1998)

compute gyration command

Syntax:

```
compute ID group-ID gyration
```

- ID, group-ID are documented in compute command
- gyration = style name of this compute command

Examples:

```
compute 1 molecule gyration
```

Description:

Define a computation that calculates the radius of gyration Rg of the group of atoms, including all effects due to atoms passing thru periodic boundaries.

Rg is a measure of the size of the group of atoms, and is computed as the square root of the Rg^2 value in this formula

$$R_g{}^2 = \frac{1}{M} \sum_i m_i (r_i - r_{cm})^2$$

where M is the total mass of the group, Rcm is the center-of-mass position of the group, and the sum is over all atoms in the group.

A Rg^2 tensor, stored as a 6-element vector, is also calculated by this compute. The formula for the components of the tensor is the same as the above formula, except that (Ri - Rcm)^2 is replaced by (Rix - Rcmx) * (Riy - Rcmy) for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz. Note that unlike the scalar Rg, each of the 6 values of the tensor is effectively a "squared" value, since the cross-terms may be negative and taking a sqrt() would be invalid.

NOTE: The coordinates of an atom contribute to Rg in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

Output info:

This compute calculates a global scalar (Rg) and a global vector of length 6 (Rg^2 tensor), which can be accessed by indices 1-6. These values can be used by any command that uses a global scalar value or vector values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The scalar and vector values calculated by this compute are "intensive". The scalar and vector values will be in distance and distance^2 units respectively.

Restrictions: none

Related commands:

compute gyration/chunk

Default: none

compute gyration/chunk command

Syntax:

```
compute ID group-ID gyration/chunk chunkID keyword value ...
```

- ID, group-ID are documented in compute command
- gyration/chunk = style name of this compute command
- chunkID = ID of compute chunk/atom command
- zero or more keyword/value pairs may be appended
- keyword = *tensor*

```
  tensor value = none
```

Examples:

```
compute 1 molecule gyration/chunk molchunk
compute 2 molecule gyration/chunk molchunk tensor
```

Description:

Define a computation that calculates the radius of gyration Rg for multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a compute chunk/atom command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the compute chunk/atom doc page and "Section_howto 23 for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates the radius of gyration Rg for each chunk, which includes all effects due to atoms passing thru periodic boundaries.

Rg is a measure of the size of a chunk, and is computed by this formula

$$R_g{}^2 = \frac{1}{M} \sum_i m_i (r_i - r_{cm})^2$$

where M is the total mass of the chunk, Rcm is the center-of-mass position of the chunk, and the sum is over all atoms in the chunk.

Note that only atoms in the specified group contribute to the calculation. The compute chunk/atom command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

If the *tensor* keyword is specified, then the scalar Rg value is not calculated, but an Rg tensor is instead calculated for each chunk. The formula for the components of the tensor is the same as the above formula, except that (Ri - Rcm)^2 is replaced by (Rix - Rcmx) * (Riy - Rcmy) for the xy component, etc. The 6 components of the tensor

are ordered xx, yy, zz, xy, xz, yz.

NOTE: The coordinates of an atom contribute to Rg in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

The simplest way to output the results of the compute gyration/chunk calculation to a file is to use the fix ave/time command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all gyration/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk file tmp.out mode vector
```

Output info:

This compute calculates a global vector if the *tensor* keyword is not specified and a global array if it is. The length of the vector or number of rows in the array = the number of chunks *Nchunk* as calculated by the specified compute chunk/atom command. If the *tensor* keyword is specified, the global array has 6 columns. The vector or array can be accessed by any command that uses global values from a compute as input. See this section for an overview of LAMMPS output options.

All the vector or array values calculated by this compute are "intensive". The vector or array values will be in distance units, since they are the square root of values represented by the formula above.

Restrictions: none

Related commands: none

compute gyration

Default: none

compute heat/flux command

Syntax:

```
compute ID group-ID heat/flux ke-ID pe-ID stress-ID
```

- ID, group-ID are documented in compute command
- heat/flux = style name of this compute command
- ke-ID = ID of a compute that calculates per-atom kinetic energy
- pe-ID = ID of a compute that calculates per-atom potential energy
- stress-ID = ID of a compute that calculates per-atom stress

Examples:

```
compute myFlux all heat/flux myKE myPE myStress
```

Description:

Define a computation that calculates the heat flux vector based on contributions from atoms in the specified group. This can be used by itself to measure the heat flux into or out of a reservoir of atoms, or to calculate a thermal conductivity using the Green-Kubo formalism.

See the fix thermal/conductivity command for details on how to compute thermal conductivity in an alternate way, via the Muller-Plathe method. See the fix heat command for a way to control the heat added or subtracted to a group of atoms.

The compute takes three arguments which are IDs of other computes. One calculates per-atom kinetic energy (*ke-ID*), one calculates per-atom potential energy (*pe-ID)*, and the third calcualtes per-atom stress (*stress-ID*). These should be defined for the same group used by compute heat/flux, though LAMMPS does not check for this.

The Green-Kubo formulas relate the ensemble average of the auto-correlation of the heat flux J to the thermal conductivity kappa:

$$\begin{aligned}
\mathbf{J} &= \frac{1}{V}\left[\sum_i e_i \mathbf{v}_i - \sum_i \mathbf{S}_i \mathbf{v}_i\right] \\
&= \frac{1}{V}\left[\sum_i e_i \mathbf{v}_i + \sum_{i<j} \left(\mathbf{f}_{ij} \cdot \mathbf{v}_j\right) \mathbf{x}_{ij}\right] \\
&= \frac{1}{V}\left[\sum_i e_i \mathbf{v}_i + \frac{1}{2}\sum_{i<j} \left(\mathbf{f}_{ij} \cdot \left(\mathbf{v}_i + \mathbf{v}_j\right)\right) \mathbf{x}_{ij}\right]
\end{aligned}$$

$$\kappa = \frac{V}{k_B T^2} \int_0^\infty \langle J_x(0) J_x(t) \rangle \, dt = \frac{V}{3 k_B T^2} \int_0^\infty \langle \mathbf{J}(0) \cdot \mathbf{J}(t) \rangle \, dt$$

Ei in the first term of the equation for J is the per-atom energy (potential and kinetic). This is calculated by the computes *ke-ID* and *pe-ID*. Si in the second term of the equation for J is the per-atom stress tensor calculated by the compute *stress-ID*. The tensor multiplies Vi as a 3x3 matrix-vector multiply to yield a vector. Note that as discussed below, the 1/V scaling factor in the equation for J is NOT included in the calculation performed by this compute; you need to add it for a volume appropriate to the atoms included in the calculation.

NOTE: The compute pe/atom and compute stress/atom commands have options for which terms to include in their calculation (pair, bond, etc). The heat flux calculation will thus include exactly the same terms. Normally you should use compute stress/atom virial so as not to include a kinetic energy term in the heat flux.

This compute calculates 6 quantities and stores them in a 6-component vector. The first 3 components are the x, y, z components of the full heat flux vector, i.e. (Jx, Jy, Jz). The next 3 components are the x, y, z components of just the convective portion of the flux, i.e. the first term in the equation for J above.

The heat flux can be output every so many timesteps (e.g. via the thermo_style custom command). Then as a post-processing operation, an autocorrelation can be performed, its integral estimated, and the Green-Kubo formula above evaluated.

The fix ave/correlate command can calclate the autocorrelation. The trap() function in the variable command can calculate the integral.

An example LAMMPS input script for solid Ar is appended below. The result should be: average conductivity ~0.29 in W/mK.

Output info:

This compute calculates a global vector of length 6 (total heat flux vector, followed by convective heat flux vector), which can be accessed by indices 1-6. These values can be used by any command that uses global vector values from a compute as input. See this section for an overview of LAMMPS output options.

The vector values calculated by this compute are "extensive", meaning they scale with the number of atoms in the simulation. They can be divided by the appropriate volume to get a flux, which would then be an "intensive" value, meaning independent of the number of atoms in the simulation. Note that if the compute is "all", then the appropriate volume to divide by is the simulation box volume. However, if a sub-group is used, it should be the volume containing those atoms.

The vector values will be in energy*velocity units. Once divided by a volume the units will be that of flux, namely energy/area/time units

Restrictions: none

Related commands:

fix thermal/conductivity, fix ave/correlate, variable

Default: none

```
# Sample LAMMPS input script for thermal conductivity of solid Ar

units       real
variable    T equal 70
variable    V equal vol
variable    dt equal 4.0
variable    p equal 200     # correlation length
variable    s equal 10      # sample interval
variable    d equal $p*$s   # dump interval

# convert from LAMMPS real units to SI

variable    kB equal 1.3806504e-23    # [J/K] Boltzmann
variable    kCal2J equal 4186.0/6.02214e23
variable    A2m equal 1.0e-10
variable    fs2s equal 1.0e-15
variable    convert equal ${kCal2J}*${kCal2J}/${fs2s}/${A2m}

# setup problem

dimension    3
boundary     p p p
lattice      fcc 5.376 orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
region       box block 0 4 0 4 0 4
create_box   1 box
create_atoms 1 box
mass         1 39.948
pair_style   lj/cut 13.0
pair_coeff   * * 0.2381 3.405
timestep     ${dt}
thermo       $d

# equilibration and thermalization

velocity     all create $T 102486 mom yes rot yes dist gaussian
fix          NVT all nvt temp $T $T 10 drag 0.2
run          8000

# thermal conductivity calculation, switch to NVE if desired

#unfix       NVT
#fix         NVE all nve

reset_timestep 0
compute      myKE all ke/atom
compute      myPE all pe/atom
compute      myStress all stress/atom NULL virial
compute      flux all heat/flux myKE myPE myStress
variable     Jx equal c_flux[1]/vol
variable     Jy equal c_flux[2]/vol
variable     Jz equal c_flux[3]/vol
fix          JJ all ave/correlate $s $p $d &
             c_flux[1] c_flux[2] c_flux[3] type auto file J0Jt.dat ave running
variable     scale equal ${convert}/${kB}/$T/$T/$V*$s*${dt}
variable     k11 equal trap(f_JJ[3])*${scale}
variable     k22 equal trap(f_JJ[4])*${scale}
variable     k33 equal trap(f_JJ[5])*${scale}
thermo_style custom step temp v_Jx v_Jy v_Jz v_k11 v_k22 v_k33
run          100000
variable     k equal (v_k11+v_k22+v_k33)/3.0
variable     ndens equal count(all)/vol
```

```
print        "average conductivity: $k[W/mK] @ $T K, ${ndens} /A^3"
```

compute hexorder/atom command

Syntax:

```
compute ID group-ID hexorder/atom keyword values ...
```

- ID, group-ID are documented in compute command
- hexorder/atom = style name of this compute command
- one or more keyword/value pairs may be appended

```
keyword = degree or nnn or cutoff
  cutoff value = distance cutoff
  nnn value = number of nearest neighbors
  degree value = degree n of order parameter
```

Examples:

```
compute 1 all hexorder/atom
compute 1 all hexorder/atom degree 4 nnn 4 cutoff 1.2
```

Description:

Define a computation that calculates *qn* the bond-orientational order parameter for each atom in a group. The hexatic (*n* = 6) order parameter was introduced by Nelson and Halperin as a way to detect hexagonal symmetry in two-dimensional systems. For each atom, *qn* is a complex number (stored as two real numbers) defined as follows:

$$q_n = \frac{1}{nnn} \sum_{j=1}^{nnn} e^{ni\theta(\mathbf{r}_{ij})}$$

where the sum is over the *nnn* nearest neighbors of the central atom. The angle theta is formed by the bond vector rij and the *x* axis. theta is calculated only using the *x* and *y* components, whereas the distance from the central atom is calculated using all three *x*, *y*, and *z* components of the bond vector. Neighbor atoms not in the group are included in the order parameter of atoms in the group.

The optional keyword *cutoff* defines the distance cutoff used when searching for neighbors. The default value, also the maximum allowable value, is the cutoff specified by the pair style.

The optional keyword *nnn* defines the number of nearest neighbors used to calculate *qn*. The default value is 6. If the value is NULL, then all neighbors up to the distance cutoff are used.

The optional keyword *degree* sets the degree *n* of the order parameter. The default value is 6. For a perfect hexagonal lattice with *nnn* = 6, *q*6 = exp(6 i phi) for all atoms, where the constant 0 < phi < pi/3 depends only on the orientation of the lattice relative to the *x* axis. In an isotropic liquid, local neighborhoods may still exhibit weak hexagonal symmetry, but because the orientational correlation decays quickly with distance, the value of phi will be different for different atoms, and so when *q*6 is averaged over all the atoms in the system, |<*q*6>| << 1.

The value of *qn* is set to zero for atoms not in the specified compute group, as well as for atoms that have less than *nnn* neighbors within the distance cutoff.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently.

NOTE: If you have a bonded system, then the settings of special_bonds command can remove pairwise interactions between atoms in the same bond, angle, or dihedral. This is the default setting for the special_bonds command, and means those pairwise interactions do not appear in the neighbor list. Because this fix uses the neighbor list, it also means those pairs will not be included in the order parameter. This difficulty can be circumvented by writing a dump file, and using the rerun command to compute the order parameter for snapshots in the dump file. The rerun script can use a special_bonds command that includes all pairs in the neighbor list.

Output info:

This compute calculates a per-atom array with 2 columns, giving the real and imaginary parts *qn*, a complex number restricted to the unit disk of the complex plane i.e. Re(*qn*)^2 + Im(*qn*)^2 <= 1 .

These values can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

Restrictions: none

Related commands:

compute orientorder/atom, compute coord/atom, compute centro/atom

Default:

The option defaults are *cutoff* = pair style cutoff, *nnn* = 6, *degree* = 6

(Nelson) Nelson, Halperin, Phys Rev B, 19, 2457 (1979).

compute improper/local command

Syntax:

```
compute ID group-ID improper/local input1 input2 ...
```

- ID, group-ID are documented in compute command
- improper/local = style name of this compute command
- one or more keywords may be appended
- keyword = *chi*

```
  chi = tabulate improper angles
```

Examples:

```
compute 1 all improper/local chi
```

Description:

Define a computation that calculates properties of individual improper interactions. The number of datums generated, aggregated across all processors, equals the number of impropers in the system, modified by the group parameter as explained below.

The local data stored by this command is generated by looping over all the atoms owned on a processor and their impropers. An improper will only be included if all 4 atoms in the improper are in the specified compute group.

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For example, improper output from the compute property/local command can be combined with data from this command and output by the dump local command in a consistent way.

Output info:

This compute calculates a local vector or local array depending on the number of keywords. The length of the vector or number of rows in the array is the number of impropers. If a single keyword is specified, a local vector is produced. If two or more keywords are specified, a local array is produced where the number of columns = the number of keywords. The vector or array can be accessed by any command that uses local values from a compute as input. See this section for an overview of LAMMPS output options.

The output for *chi* will be in degrees.

Restrictions: none

Related commands:

dump local, compute property/local

Default: none

compute inertia/chunk command

Syntax:

```
compute ID group-ID inertia/chunk chunkID
```

- ID, group-ID are documented in compute command
- inertia/chunk = style name of this compute command
- chunkID = ID of compute chunk/atom command

Examples:

```
compute 1 fluid inertia/chunk molchunk
```

Description:

Define a computation that calculates the inertia tensor for multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a compute chunk/atom command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the compute chunk/atom doc page and "Section_howto 23 for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates the 6 components of the symmetric intertia tensor for each chunk, ordered Ixx,Iyy,Izz,Ixy,Iyz,Ixz. The calculation includes all effects due to atoms passing thru periodic boundaries.

Note that only atoms in the specified group contribute to the calculation. The compute chunk/atom command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

NOTE: The coordinates of an atom contribute to the chunk's inertia tensor in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

The simplest way to output the results of the compute inertia/chunk calculation to a file is to use the fix ave/time command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all inertia/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk file tmp.out mode vector
```

Output info:

This compute calculates a global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified compute chunk/atom command. The number of columns = 6 for the 6 components of the inertia tensor for each chunk, ordered as listed above. These values can be accessed by any command that uses global array values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in mass*distance^2 units.

Restrictions: none

Related commands:

variable inertia() function

Default: none

compute ke command

Syntax:

```
compute ID group-ID ke
```

- ID, group-ID are documented in compute command
- ke = style name of this compute command

Examples:

```
compute 1 all ke
```

Description:

Define a computation that calculates the translational kinetic energy of a group of particles.

The kinetic energy of each particle is computed as 1/2 m v^2, where m and v are the mass and velocity of the particle.

There is a subtle difference between the quantity calculated by this compute and the kinetic energy calculated by the *ke* or *etotal* keyword used in thermodynamic output, as specified by the thermo_style command. For this compute, kinetic energy is "translational" kinetic energy, calculated by the simple formula above. For thermodynamic output, the *ke* keyword infers kinetic energy from the temperature of the system with 1/2 Kb T of energy for each degree of freedom. For the default temperature computation via the compute temp command, these are the same. But different computes that calculate temperature can subtract out different non-thermal components of velocity and/or include different degrees of freedom (translational, rotational, etc).

Output info:

This compute calculates a global scalar (the summed KE). This value can be used by any command that uses a global scalar value from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy units.

Restrictions: none

Related commands:

compute erotate/sphere

Default: none

compute ke/atom command

Syntax:

```
compute ID group-ID ke/atom
```

- ID, group-ID are documented in compute command
- ke/atom = style name of this compute command

Examples:

```
compute 1 all ke/atom
```

Description:

Define a computation that calculates the per-atom translational kinetic energy for each atom in a group.

The kinetic energy is simply 1/2 m v^2, where m is the mass and v is the velocity of each atom.

The value of the kinetic energy will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be in energy units.

Restrictions: none

Related commands:

dump custom

Default: none

compute ke/atom/eff command

Syntax:

```
compute ID group-ID ke/atom/eff
```

- ID, group-ID are documented in compute command
- ke/atom/eff = style name of this compute command

Examples:

```
compute 1 all ke/atom/eff
```

Description:

Define a computation that calculates the per-atom translational (nuclei and electrons) and radial kinetic energy (electron only) in a group. The particles are assumed to be nuclei and electrons modeled with the electronic force field.

The kinetic energy for each nucleus is computed as 1/2 m v^2, where m corresponds to the corresponding nuclear mass, and the kinetic energy for each electron is computed as 1/2 (me v^2 + 3/4 me s^2), where me and v correspond to the mass and translational velocity of each electron, and s to its radial velocity, respectively.

There is a subtle difference between the quantity calculated by this compute and the kinetic energy calculated by the *ke* or *etotal* keyword used in thermodynamic output, as specified by the thermo_style command. For this compute, kinetic energy is "translational" plus electronic "radial" kinetic energy, calculated by the simple formula above. For thermodynamic output, the *ke* keyword infers kinetic energy from the temperature of the system with 1/2 Kb T of energy for each (nuclear-only) degree of freedom in eFF.

NOTE: The temperature in eFF should be monitored via the compute temp/eff command, which can be printed with thermodynamic output by using the thermo_modify command, as shown in the following example:

```
compute         effTemp all temp/eff
thermo_style    custom step etotal pe ke temp press
thermo_modify   temp effTemp
```

The value of the kinetic energy will be 0.0 for atoms (nuclei or electrons) not in the specified compute group.

Output info:

This compute calculates a scalar quantity for each atom, which can be accessed by any command that uses per-atom computes as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be in energy units.

Restrictions:

This compute is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

dump custom

Default: none

compute ke/eff command

Syntax:

```
compute ID group-ID ke/eff
```

- ID, group-ID are documented in compute command
- ke/eff = style name of this compute command

Examples:

```
compute 1 all ke/eff
```

Description:

Define a computation that calculates the kinetic energy of motion of a group of eFF particles (nuclei and electrons), as modeled with the electronic force field.

The kinetic energy for each nucleus is computed as 1/2 m v^2 and the kinetic energy for each electron is computed as 1/2(me v^2 + 3/4 me s^2), where m corresponds to the nuclear mass, me to the electron mass, v to the translational velocity of each particle, and s to the radial velocity of the electron, respectively.

There is a subtle difference between the quantity calculated by this compute and the kinetic energy calculated by the *ke* or *etotal* keyword used in thermodynamic output, as specified by the thermo_style command. For this compute, kinetic energy is "translational" and "radial" (only for electrons) kinetic energy, calculated by the simple formula above. For thermodynamic output, the *ke* keyword infers kinetic energy from the temperature of the system with 1/2 Kb T of energy for each degree of freedom. For the eFF temperature computation via the compute temp_eff command, these are the same. But different computes that calculate temperature can subtract out different non-thermal components of velocity and/or include other degrees of freedom.

IMPRORTANT NOTE: The temperature in eFF models should be monitored via the compute temp/eff command, which can be printed with thermodynamic output by using the thermo_modify command, as shown in the following example:

```
compute         effTemp all temp/eff
thermo_style    custom step etotal pe ke temp press
thermo_modify   temp effTemp
```

See compute temp/eff.

Output info:

This compute calculates a global scalar (the KE). This value can be used by any command that uses a global scalar value from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy units.

Restrictions:

This compute is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands: none

Default: none

compute ke/rigid command

Syntax:

```
compute ID group-ID ke/rigid fix-ID
```

- ID, group-ID are documented in compute command
- ke = style name of this compute command
- fix-ID = ID of rigid body fix

Examples:

```
compute 1 all ke/rigid myRigid
```

Description:

Define a computation that calculates the translational kinetic energy of a collection of rigid bodies, as defined by one of the fix rigid command variants.

The kinetic energy of each rigid body is computed as 1/2 M Vcm^2, where M is the total mass of the rigid body, and Vcm is its center-of-mass velocity.

The *fix-ID* should be the ID of one of the fix rigid commands which defines the rigid bodies. The group specified in the compute command is ignored. The kinetic energy of all the rigid bodies defined by the fix rigid command in included in the calculation.

Output info:

This compute calculates a global scalar (the summed KE of all the rigid bodies). This value can be used by any command that uses a global scalar value from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy units.

Restrictions:

This compute is part of the RIGID package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

compute erotate/rigid

Default: none

compute meso/e/atom command

Syntax:

```
compute ID group-ID meso/e/atom
```

- ID, group-ID are documented in compute command
- meso/e/atom = style name of this compute command

Examples:

```
compute 1 all meso/e/atom
```

Description:

Define a computation that calculates the per-atom internal energy for each atom in a group.

The internal energy is the energy associated with the internal degrees of freedom of a mesoscopic particles, e.g. a Smooth-Particle Hydrodynamics particle.

See this PDF guide to using SPH in LAMMPS.

The value of the internal energy will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be in energy units.

Restrictions:

This compute is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

dump custom

Default: none

compute meso/rho/atom command

Syntax:

```
compute ID group-ID meso/rho/atom
```

- ID, group-ID are documented in compute command
- meso/rho/atom = style name of this compute command

Examples:

```
compute 1 all meso/rho/atom
```

Description:

Define a computation that calculates the per-atom mesoscopic density for each atom in a group.

The mesoscopic density is the mass density of a mesoscopic particle, calculated by kernel function interpolation using "pair style sph/rhosum".

See this PDF guide to using SPH in LAMMPS.

The value of the mesoscopic density will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be in mass/volume units.

Restrictions:

This compute is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

dump custom

Default: none

compute meso/t/atom command

Syntax:

```
compute ID group-ID meso/t/atom
```

- ID, group-ID are documented in compute command
- meso/t/atom = style name of this compute command

Examples:

```
compute 1 all meso/t/atom
```

Description:

Define a computation that calculates the per-atom internal temperature for each atom in a group.

The internal temperature is the ratio of internal energy over the heat capacity associated with the internal degrees of freedom of a mesoscopic particles, e.g. a Smooth-Particle Hydrodynamics particle.

T_*int* = E_*int* / C_*V, int*

See this PDF guide to using SPH in LAMMPS.

The value of the internal energy will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be in temperature units.

Restrictions:

This compute is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

dump custom

Default: none

compute_modify command

Syntax:

```
compute_modify compute-ID keyword value ...
```

- compute-ID = ID of the compute to modify
- one or more keyword/value pairs may be listed
- keyword = *extra* or *dynamic*

```
  extra value = N
      N = # of extra degrees of freedom to subtract
    dynamic value = yes or no
      yes/no = do or do not recompute the number of atoms contributing to the temperature
    thermo value = yes or no
      yes/no = do or do not add contributions from fixes to the potential energy
```

Examples:

```
compute_modify myTemp extra 0
compute_modify newtemp dynamic yes extra 600
```

Description:

Modify one or more parameters of a previously defined compute. Not all compute styles support all parameters.

The *extra* keyword refers to how many degrees-of-freedom are subtracted (typically from 3N) as a normalizing factor in a temperature computation. Only computes that compute a temperature use this option. The default is 2 or 3 for 2d or 3d systems which is a correction factor for an ensemble of velocities with zero total linear momentum. You can use a negative number for the *extra* parameter if you need to add degrees-of-freedom. See the compute temp/asphere command for an example.

The *dynamic* keyword determines whether the number of atoms N in the compute group is re-computed each time a temperature is computed. Only compute styles that compute a temperature use this option. By default, N is assumed to be constant. If you are adding atoms to the system (see the fix pour or fix deposit commands) or expect atoms to be lost (e.g. due to evaporation), then this option should be used to insure the temperature is correctly normalized.

The *thermo* keyword determines whether the potential energy contribution calculated by some fixes is added to the potential energy calculated by the compute. Currently, only the compute of style *pe* uses this option. See the doc pages for individual fixes for details.

Restrictions: none

Related commands:

compute

Default:

The option defaults are extra = 2 or 3 for 2d or 3d systems and dynamic = no. Thermo is *yes* if the compute of style *pe* was defined with no extra keywords; otherwise it is *no*.

compute msd command

Syntax:

```
compute ID group-ID msd keyword values ...
```

- ID, group-ID are documented in compute command
- msd = style name of this compute command
- zero or more keyword/value pairs may be appended
- keyword = *com* or *average*

```
com value = yes or no
  average value = yes or no
```

Examples:

```
compute 1 all msd
compute 1 upper msd com yes average yes
```

Description:

Define a computation that calculates the mean-squared displacement (MSD) of the group of atoms, including all effects due to atoms passing thru periodic boundaries. For computation of the non-Gaussian parameter of mean-squared displacement, see the compute msd/nongauss command.

A vector of four quantites is calculated by this compute. The first 3 elements of the vector are the squared dx,dy,dz displacements, summed and averaged over atoms in the group. The 4th element is the total squared displacement, i.e. (dx*dx + dy*dy + dz*dz), summed and averaged over atoms in the group.

The slope of the mean-squared displacement (MSD) versus time is proportional to the diffusion coefficient of the diffusing atoms.

The displacement of an atom is from its reference position. This is normally the original position at the time the compute command was issued, unless the *average* keyword is set to *yes*. The value of the displacement will be 0.0 for atoms not in the specified compute group.

If the *com* option is set to *yes* then the effect of any drift in the center-of-mass of the group of atoms is subtracted out before the displacment of each atom is calculated.

If the *average* option is set to *yes* then the reference position of an atom is based on the average position of that atom, corrected for center-of-mass motion if requested. The average position is a running average over all previous calls to the compute, including the current call. So on the first call it is current position, on the second call it is the arithmetic average of the current position and the position on the first call, and so on. Note that when using this option, the precise value of the mean square displacement will depend on the number of times the compute is called. So, for example, changing the frequency of thermo output may change the computed displacement. Also, the precise values will be changed if a single simulation is broken up into two parts, using either multiple run commands or a restart file. It only makes sense to use this option if the atoms are not diffusing, so that their average positions relative to the center of mass of the system are stationary. The most common case is crystalline solids undergoing thermal motion.

NOTE: Initial coordinates are stored in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

NOTE: If you want the quantities calculated by this compute to be continuous when running from a restart file, then you should use the same ID for this compute, as in the original run. This is so that the fix this compute creates to store per-atom quantities will also have the same ID, and thus be initialized correctly with atom reference positions from the restart file. When *average* is set to yes, then the atom reference positions are restored correctly, but not the number of samples used obtain them. As a result, the reference positions from the restart file are combined with subsequent positions as if they were from a single sample, instead of many, which will change the values of msd somewhat.

Output info:

This compute calculates a global vector of length 4, which can be accessed by indices 1-4 by any command that uses global vector values from a compute as input. See this section for an overview of LAMMPS output options.

The vector values are "intensive". The vector values will be in distance^2 units.

Restrictions: none

Related commands:

compute msd/nongauss, compute displace_atom, fix store/state, compute msd/chunk

Default:

The option default are com = no, average = no.

compute msd/chunk command

Syntax:

```
compute ID group-ID msd/chunk chunkID
```

- ID, group-ID are documented in compute command
- msd/chunk = style name of this compute command
- chunkID = ID of compute chunk/atom command

Examples:

```
compute 1 all msd/chunk molchunk
```

Description:

Define a computation that calculates the mean-squared displacement (MSD) for multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a compute chunk/atom command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the compute chunk/atom doc page and "Section_howto 23 for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

Four quantites are calculated by this compute for each chunk. The first 3 quantities are the squared dx,dy,dz displacements of the center-of-mass. The 4th component is the total squared displacement, i.e. (dx*dx + dy*dy + dz*dz) of the center-of-mass. These calculations include all effects due to atoms passing thru periodic boundaries.

Note that only atoms in the specified group contribute to the calculation. The compute chunk/atom command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

The slope of the mean-squared displacement (MSD) versus time is proportional to the diffusion coefficient of the diffusing chunks.

The displacement of the center-of-mass of the chunk is from its original center-of-mass position, calculated on the timestep this compute command was first invoked.

NOTE: The number of chunks *Nchunk* calculated by the compute chunk/atom command must remain constant each time this compute is invoked, so that the displacement for each chunk from its original position can be computed consistently. If *Nchunk* does not remain constant, an error will be generated. If needed, you can enforce a constant *Nchunk* by using the *nchunk once* or *ids once* options when specifying the compute chunk/atom command.

NOTE: This compute stores the original position (of the center-of-mass) of each chunk. When a displacement is calculated on a later timestep, it is assumed that the same atoms are assigned to the same chunk ID. However LAMMPS has no simple way to insure this is the case, though you can use the *ids once* option when specifying the compute chunk/atom command. Note that if this is not the case, the MSD calculation does not have a sensible meaning.

NOTE: The initial coordinates of the atoms in each chunk are stored in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

NOTE: If you want the quantities calculated by this compute to be continuous when running from a restart file, then you should use the same ID for this compute, as in the original run. This is so that the fix this compute creates to store per-chunk quantities will also have the same ID, and thus be initialized correctly with chunk reference positions from the restart file.

The simplest way to output the results of the compute com/msd calculation to a file is to use the fix ave/time command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all com/msd cc1
fix 1 all ave/time 100 1 100 c_myChunk file tmp.out mode vector
```

Output info:

This compute calculates a global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified compute chunk/atom command. The number of columns = 4 for dx,dy,dz and the total displacement. These values can be accessed by any command that uses global array values from a compute as input. See this section for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in distance^2 units.

Restrictions: none

Related commands:

compute msd

Default: none

compute msd/nongauss command

Syntax:

```
compute ID group-ID msd/nongauss keyword values ...
```

- ID, group-ID are documented in compute command
- msd/nongauss = style name of this compute command
- zero or more keyword/value pairs may be appended
- keyword = *com*

  ```
  com value = yes or no
  ```

Examples:

```
compute 1 all msd/nongauss
compute 1 upper msd/nongauss com yes
```

Description:

Define a computation that calculates the mean-squared displacement (MSD) and non-Gaussian parameter (NGP) of the group of atoms, including all effects due to atoms passing thru periodic boundaries.

A vector of three quantites is calculated by this compute. The first element of the vector is the total squared dx,dy,dz displacements drsquared = (dx*dx + dy*dy + dz*dz) of atoms, and the second is the fourth power of these displacements drfourth = (dx*dx + dy*dy + dz*dz)*(dx*dx + dy*dy + dz*dz), summed and averaged over atoms in the group. The 3rd component is the nonGaussian diffusion paramter NGP = 3*drfourth/(5*drsquared*drsquared), i.e.

$$NGP(t) = 3 < (r(t) - r(0))^4 > /(5 < (r(t) - r(0))^2 >^2) - 1$$

The NGP is a commonly used quantity in studies of dynamical heterogeneity. Its minimum theoretical value (-0.4) occurs when all atoms have the same displacement magnitude. NGP=0 for Brownian diffusion, while NGP > 0 when some mobile atoms move faster than others.

If the *com* option is set to *yes* then the effect of any drift in the center-of-mass of the group of atoms is subtracted out before the displacment of each atom is calcluated.

See the compute msd doc page for further important NOTEs, which also apply to this compute.

Output info:

This compute calculates a global vector of length 3, which can be accessed by indices 1-3 by any command that uses global vector values from a compute as input. See this section for an overview of LAMMPS output options.

The vector values are "intensive". The first vector value will be in distance^2 units, the second is in distance^4 units, and the 3rd is dimensionless.

Restrictions:

This compute is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

compute msd

Default:

The option default is com = no.

compute omega/chunk command

Syntax:

```
compute ID group-ID omega/chunk chunkID
```

- ID, group-ID are documented in compute command
- omega/chunk = style name of this compute command
- chunkID = ID of compute chunk/atom command

Examples:

```
compute 1 fluid omega/chunk molchunk
```

Description:

Define a computation that calculates the angular velocity (omega) of multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a compute chunk/atom command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the compute chunk/atom doc page and "Section_howto 23 for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates the 3 components of the angular velocity vector for each chunk, via the formula L = Iw where L is the angular momentum vector of the chunk, I is its moment of inertia tensor, and w is omega = angular velocity of the chunk. The calculation includes all effects due to atoms passing thru periodic boundaries.

Note that only atoms in the specified group contribute to the calculation. The compute chunk/atom command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

NOTE: The coordinates of an atom contribute to the chunk's angular velocity in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

The simplest way to output the results of the compute omega/chunk calculation to a file is to use the fix ave/time command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all omega/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk file tmp.out mode vector
```

Output info:

This compute calculates a global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified compute chunk/atom command. The number of columns = 3 for the 3 xyz components of the angular velocity for each chunk. These values can be accessed by any command that uses global array values

from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in velocity/distance units.

Restrictions: none

Related commands:

variable omega() function

Default: none

compute orientorder/atom command

Syntax:

```
compute ID group-ID orientorder/atom keyword values ...
```

- ID, group-ID are documented in compute command
- orientorder/atom = style name of this compute command
- one or more keyword/value pairs may be appended

```
keyword = cutoff or nnn or ql
  cutoff value = distance cutoff
  nnn value = number of nearest neighbors
  degrees values = nlvalues, l1, l2,...
```

Examples:

```
compute 1 all orientorder/atom
compute 1 all orientorder/atom degrees 5 4 6 8 10 12 nnn NULL cutoff 1.5
```

Description:

Define a computation that calculates a set of bond-orientational order parameters *Ql* for each atom in a group. These order parameters were introduced by Steinhardt et al. as a way to characterize the local orientational order in atomic structures. For each atom, *Ql* is a real number defined as follows:

$$\bar{Y}_{lm} = \frac{1}{nnn} \sum_{j=1}^{nnn} Y_{lm}(\theta(\mathbf{r}_{ij}), \phi(\mathbf{r}_{ij}))$$

$$Q_l = \sqrt{\frac{4\pi}{2l+1} \sum_{m=-l}^{m=l} \bar{Y}_{lm} \bar{Y}_{lm}^*}$$

The first equation defines the spherical harmonic order parameters. These are complex number components of the 3D analog of the 2D order parameter *qn*, which is implemented as LAMMPS compute hexorder/atom. The summation is over the *nnn* nearest neighbors of the central atom. The angles theta and phi are the standard spherical polar angles defining the direction of the bond vector *rij*. The second equation defines *Ql*, which is a rotationally invariant scalar quantity obtained by summing over all the components of degree *l*.

The optional keyword *cutoff* defines the distance cutoff used when searching for neighbors. The default value, also the maximum allowable value, is the cutoff specified by the pair style.

The optional keyword *nnn* defines the number of nearest neighbors used to calculate *Ql*. The default value is 12. If the value is NULL, then all neighbors up to the specified distance cutoff are used.

The optional keyword *degrees* defines the list of order parameters to be computed. The first argument *nlvalues* is the number of order parameters. This is followed by that number of integers giving the degree of each order parameter. Because $Q2$ and all odd-degree order parameters are zero for atoms in cubic crystals (see Steinhardt), the default order parameters are $Q4$, $Q6$, $Q8$, $Q10$, and $Q12$. For the FCC crystal with *nnn*=12, $Q4$ = sqrt(7/3)/8 = 0.19094.... The numerical values of all order parameters up to $Q12$ for a range of commonly encountered high-symmetry structures are given in Table I of Mickel et al..

The value of Ql is set to zero for atoms not in the specified compute group, as well as for atoms that have less than *nnn* neighbors within the distance cutoff.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently.

NOTE: If you have a bonded system, then the settings of special_bonds command can remove pairwise interactions between atoms in the same bond, angle, or dihedral. This is the default setting for the special_bonds command, and means those pairwise interactions do not appear in the neighbor list. Because this fix uses the neighbor list, it also means those pairs will not be included in the order parameter. This difficulty can be circumvented by writing a dump file, and using the rerun command to compute the order parameter for snapshots in the dump file. The rerun script can use a special_bonds command that includes all pairs in the neighbor list.

Output info:

This compute calculates a per-atom array with *nlvalues* columns, giving the Ql values for each atom, which are real numbers on the range $0 <= Ql <= 1$.

These values can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

Restrictions: none

Related commands:

compute coord/atom, compute centro/atom, compute hexorder/atom

Default:

The option defaults are *cutoff* = pair style cutoff, *nnn* = 12, *degrees* = 5 4 6 8 9 10 12 i.e. $Q4$, $Q6$, $Q8$, $Q10$, and $Q12$.

(Steinhardt) P. Steinhardt, D. Nelson, and M. Ronchetti, Phys. Rev. B 28, 784 (1983).

(Mickel) W. Mickel, S. C. Kapfer, G. E. Schroeder-Turkand, K. Mecke, J. Chem. Phys. 138, 044501 (2013).

compute pair command

Syntax:

```
compute ID group-ID pair pstyle evalue
```

- ID, group-ID are documented in compute command
- pair = style name of this compute command
- pstyle = style name of a pair style that calculates additional values
- evalue = *epair* or *evdwl* or *ecoul* or blank (optional setting)

Examples:

```
compute 1 all pair gauss
compute 1 all pair lj/cut/coul/cut ecoul
compute 1 all pair reax
```

Description:

Define a computation that extracts additional values calculated by a pair style, sums them across processors, and makes them accessible for output or further processing by other commands. The group specified for this command is ignored.

The specified *pstyle* must be a pair style used in your simulation either by itself or as a sub-style in a pair_style hybrid or hybrid/overlay command.

The *evalue* setting is optional; it may be left off the command. All pair styles tally a potential energy *epair* which may be broken into two parts: *evdwl* and *ecoul* such that *epair* = *evdwl* + *ecoul*. If the pair style calculates Coulombic interactions, their energy will be tallied in *ecoul*. Everything else (whether it is a Lennard-Jones style van der Waals interaction or not) is tallied in *evdwl*. If *evalue* is specified as *epair* or left out, then *epair* is stored as a global scalar by this compute. This is useful when using pair_style hybrid if you want to know the portion of the total energy contributed by one sub-style. If *evalue* is specfied as *evdwl* or *ecoul*, then just that portion of the energy is stored as a global scalar.

Some pair styles tally additional quantities, e.g. a breakdown of potential energy into a dozen or so components is tallied by the pair_style reax commmand. These values (1 or more) are stored as a global vector by this compute. See the doc page for individual pair styles for info on these values.

Output info:

This compute calculates a global scalar which is *epair* or *evdwl* or *ecoul*. If the pair style supports it, it also calculates a global vector of length >= 1, as determined by the pair style. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar and vector values calculated by this compute are "extensive".

The scalar value will be in energy units. The vector values will typically also be in energy units, but see the doc page for the pair style for details.

Restrictions: none

Related commands:

compute pe

Default:

The default for *evalue* is *epair*.

compute pair/local command

Syntax:

```
compute ID group-ID pair/local input1 input2 ...
```

- ID, group-ID are documented in compute command
- pair/local = style name of this compute command
- zero or more keywords may be appended
- keyword = *dist* or *eng* or *force* or *fx* or *fy* or *fz* or *pN*

```
  dist = pairwise distance
    eng = pairwise energy
    force = pairwise force
    fx,fy,fz = components of pairwise force
    pN = pair style specific quantities for allowed N values
```

Examples:

```
compute 1 all pair/local eng
compute 1 all pair/local dist eng force
compute 1 all pair/local dist eng fx fy fz
compute 1 all pair/local dist fx fy fz p1 p2 p3
```

Description:

Define a computation that calculates properties of individual pairwise interactions. The number of datums generated, aggregated across all processors, equals the number of pairwise interactions in the system.

The local data stored by this command is generated by looping over the pairwise neighbor list. Info about an individual pairwise interaction will only be included if both atoms in the pair are in the specified compute group, and if the current pairwise distance is less than the force cutoff distance for that interaction, as defined by the pair_style and pair_coeff commands.

The output *dist* is the distance bewteen the pair of atoms.

The output *eng* is the interaction energy for the pair of atoms.

The output *force* is the force acting between the pair of atoms, which is positive for a repulsive force and negative for an attractive force. The outputs *fx*, *fy*, and *fz* are the xyz components of *force* on atom I.

A pair style may define additional pairwise quantities which can be accessed as *p1* to *pN*, where N is defined by the pair style. Most pair styles do not define any additional quantities, so N = 0. An example of ones that do are the granular pair styles which calculate the tangential force between two particles and return its components and magnitude acting on atom I for N = 1,2,3,4. See individual pair styles for detils.

The output *dist* will be in distance units. The output *eng* will be in energy units. The outputs *force*, *fx*, *fy*, and *fz* will be in force units. The output *pN* will be in whatever units the pair style defines.

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For

example, pair output from the compute property/local command can be combined with data from this command and output by the dump local command in a consistent way.

NOTE: For pairs, if two atoms I,J are involved in 1-2, 1-3, 1-4 interactions within the molecular topology, their pairwise interaction may be turned off, and thus they may not appear in the neighbor list, and will not be part of the local data created by this command. More specifically, this will be true of I,J pairs with a weighting factor of 0.0; pairs with a non-zero weighting factor are included. The weighting factors for 1-2, 1-3, and 1-4 pairwise interactions are set by the special_bonds command. An exception is if long-range Coulombics are being computed via the kspace_style command, then atom pairs with weighting factors of zero are still included in the neighbor list, so that a portion of the long-range interaction contribution can be computed in the pair style. Hence in that case, those atom pairs will be part of the local data created by this command.

Output info:

This compute calculates a local vector or local array depending on the number of keywords. The length of the vector or number of rows in the array is the number of pairs. If a single keyword is specified, a local vector is produced. If two or more keywords are specified, a local array is produced where the number of columns = the number of keywords. The vector or array can be accessed by any command that uses local values from a compute as input. See this section for an overview of LAMMPS output options.

The output for *dist* will be in distance units. The output for *eng* will be in energy units. The output for *force* will be in force units.

Restrictions: none

Related commands:

dump local, compute property/local

Default: none

compute pe command

compute pe/cuda command

Syntax:

```
compute ID group-ID pe keyword ...
```

- ID, group-ID are documented in compute command
- pe = style name of this compute command
- zero or more keywords may be appended
- keyword = *pair* or *bond* or *angle* or *dihedral* or *improper* or *kspace*

Examples:

```
compute 1 all pe
compute molPE all pe bond angle dihedral improper
```

Description:

Define a computation that calculates the potential energy of the entire system of atoms. The specified group must be "all". See the compute pe/atom command if you want per-atom energies. These per-atom values could be summed for a group of atoms via the compute reduce command.

The energy is calculated by the various pair, bond, etc potentials defined for the simulation. If no extra keywords are listed, then the potential energy is the sum of pair, bond, angle, dihedral, improper, and kspace (long-range) energy. If any extra keywords are listed, then only those components are summed to compute the potential energy.

The Kspace contribution requires 1 extra FFT each timestep the energy is calculated, if using the PPPM solver via the kspace_style pppm command. Thus it can increase the cost of the PPPM calculation if it is needed on a large fraction of the simulation timesteps.

Various fixes can contribute to the total potential energy of the system. See the doc pages for individual fixes for details. The *thermo* option of the compute_modify command determines whether these contributions are added into the computed potential energy. If no keywords are specified the default is *yes*. If any keywords are specified, the default is *no*.

A compute of this style with the ID of "thermo_pe" is created when LAMMPS starts up, as if this command were in the input script:

```
compute thermo_pe all pe
```

See the "thermo_style" command for more details.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Output info:

This compute calculates a global scalar (the potential energy). This value can be used by any command that uses a global scalar value from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive". The scalar value will be in energy units.

Restrictions: none

Related commands:

compute pe/atom

Default: none

compute pe/atom command

Syntax:

```
compute ID group-ID pe/atom keyword ...
```

- ID, group-ID are documented in compute command
- pe/atom = style name of this compute command
- zero or more keywords may be appended
- keyword = *pair* or *bond* or *angle* or *dihedral* or *improper* or *kspace*

Examples:

```
compute 1 all pe/atom
compute 1 all pe/atom pair
compute 1 all pe/atom pair bond
```

Description:

Define a computation that computes the per-atom potential energy for each atom in a group. See the compute pe command if you want the potential energy of the entire system.

The per-atom energy is calculated by the various pair, bond, etc potentials defined for the simulation. If no extra keywords are listed, then the potential energy is the sum of pair, bond, angle, dihedral,improper, and kspace energy. If any extra keywords are listed, then only those components are summed to compute the potential energy.

Note that the energy of each atom is due to its interaction with all other atoms in the simulation, not just with other atoms in the group.

For an energy contribution produced by a small set of atoms (e.g. 4 atoms in a dihedral or 3 atoms in a Tersoff 3-body interaction), that energy is assigned in equal portions to each atom in the set. E.g. 1/4 of the dihedral energy to each of the 4 atoms.

The dihedral_style charmm style calculates pairwise interactions between 1-4 atoms. The energy contribution of these terms is included in the pair energy, not the dihedral energy.

The KSpace contribution is calculated using the method in (Heyes) for the Ewald method and a related method for PPPM, as specified by the kspace_style pppm command. For PPPM, the calcluation requires 1 extra FFT each timestep that per-atom energy is calculated. Thie document describes how the long-range per-atom energy calculation is performed.

As an example of per-atom potential energy compared to total potential energy, these lines in an input script should yield the same result in the last 2 columns of thermo output:

```
compute         peratom all pe/atom
compute         pe all reduce sum c_peratom
thermo_style    custom step temp etotal press pe c_pe
```

NOTE: The per-atom energy does not any Lennard-Jones tail corrections invoked by the pair_modify tail yes command, since those are global contributions to the system energy.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values will be in energy units.

Restrictions:

Related commands:

compute pe, compute stress/atom

Default: none

(Heyes) Heyes, Phys Rev B 49, 755 (1994),

compute plasticity/atom command

Syntax:

```
compute ID group-ID plasticity/atom
```

- ID, group-ID are documented in compute command
- plasticity/atom = style name of this compute command

Examples:

```
compute 1 all plasticity/atom
```

Description:

Define a computation that calculates the per-atom plasticity for each atom in a group. This is a quantity relevant for Peridynamics models. See this document for an overview of LAMMPS commands for Peridynamics modeling.

The plasticity for a Peridynamic particle is the so-called consistency parameter (lambda). For elastic deformation lambda = 0, otherwise lambda > 0 for plastic deformation. For details, see (Mitchell) and the PDF doc included in the LAMMPS distro in doc/PDF/PDLammps_EPS.pdf.

This command can be invoked for one of the Peridynamic pair styles: peri/eps.

The plasticity value will be 0.0 for atoms not in the specified compute group.

Output info:

This compute calculates a per-atom vector, which can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom vector values are unitlesss numbers (lambda) >= 0.0.

Restrictions:

This compute is part of the PERI package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

compute damage, compute dilatation

Default: none

(Mitchell) Mitchell, "A non-local, ordinary-state-based viscoelasticity model for peridynamics", Sandia National Lab Report, 8064:1-28 (2011).

compute pressure command

compute pressure/cuda command

Syntax:

```
compute ID group-ID pressure temp-ID keyword ...
```

- ID, group-ID are documented in compute command
- pressure = style name of this compute command
- temp-ID = ID of compute that calculates temperature, can be NULL if not needed
- zero or more keywords may be appended
- keyword = *ke* or *pair* or *bond* or *angle* or *dihedral* or *improper* or *kspace* or *fix* or *virial*

Examples:

```
compute 1 all pressure thermo_temp
compute 1 all pressure NULL pair bond
```

Description:

Define a computation that calculates the pressure of the entire system of atoms. The specified group must be "all". See the compute stress/atom command if you want per-atom pressure (stress). These per-atom values could be summed for a group of atoms via the compute reduce command.

The pressure is computed by the formula

$$P = \frac{Nk_BT}{V} + \frac{\sum_i^N r_i \bullet f_i}{dV}$$

where N is the number of atoms in the system (see discussion of DOF below), Kb is the Boltzmann constant, T is the temperature, d is the dimensionality of the system (2 or 3 for 2d/3d), V is the system volume (or area in 2d), and the second term is the virial, computed within LAMMPS for all pairwise as well as 2-body, 3-body, and 4-body, and long-range interactions. Fixes that impose constraints (e.g. the fix shake command) also contribute to the virial term.

A symmetric pressure tensor, stored as a 6-element vector, is also calculated by this compute. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz. The equation for the I,J components (where I and J = x,y,z) is similar to the above formula, except that the first term uses components of the kinetic energy tensor and the second term uses components of the virial tensor:

$$P_{IJ} = \frac{\sum_k^N m_k v_{k_I} v_{k_J}}{V} + \frac{\sum_k^N r_{k_I} f_{k_J}}{V}$$

If no extra keywords are listed, the entire equations above are calculated. This includes a kinetic energy (temperature) term and the virial as the sum of pair, bond, angle, dihedral, improper, kspace (long-range), and fix contributions to the force on each atom. If any extra keywords are listed, then only those components are summed to compute temperature or ke and/or the virial. The *virial* keyword means include all terms except the kinetic energy *ke*.

Details of how LAMMPS computes the virial efficiently for the entire system, including the effects of periodic boundary conditions is discussed in (Thompson).

The temperature and kinetic energy tensor is not calculated by this compute, but rather by the temperature compute specified with the command. If the kinetic energy is not included in the pressure, than the temperature compute is not used and can be specified as NULL. Normally the temperature compute used by compute pressure should calculate the temperature of all atoms for consistency with the virial term, but any compute style that calculates temperature can be used, e.g. one that excludes frozen atoms or other degrees of freedom.

Note that if desired the specified temperature compute can be one that subtracts off a bias to calculate a temperature using only the thermal velocity of the atoms, e.g. by subtracting a background streaming velocity. See the doc pages for individual compute commands to determine which ones include a bias.

Also note that the N in the first formula above is really degrees-of-freedom divided by d = dimensionality, where the DOF value is calcluated by the temperature compute. See the various compute temperature styles for details.

A compute of this style with the ID of "thermo_press" is created when LAMMPS starts up, as if this command were in the input script:

```
compute thermo_press all pressure thermo_temp
```

where "thermo_temp" is the ID of a similarly defined compute of style "temp". See the "thermo_style" command for more details.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Output info:

This compute calculates a global scalar (the pressure) and a global vector of length 6 (pressure tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar and vector values calculated by this compute are "intensive". The scalar and vector values will be in pressure units.

Restrictions: none

Related commands:

compute temp, compute stress/atom, thermo_style,

Default: none

(Thompson) Thompson, Plimpton, Mattson, J Chem Phys, 131, 154107 (2009).

compute property/atom command

Syntax:

```
compute ID group-ID property/atom input1 input2 ...
```

- ID, group-ID are documented in compute command
- property/atom = style name of this compute command
- input = one or more atom attributes

```
possible attributes = id, mol, proc, type, mass,
                      x, y, z, xs, ys, zs, xu, yu, zu, ix, iy, iz,
                      vx, vy, vz, fx, fy, fz,
                      q, mux, muy, muz, mu,
                      radius, diameter, omegax, omegay, omegaz,
                      angmomx, angmomy, angmomz,
                      shapex,shapey, shapez,
                      quatw, quati, quatj, quatk, tqx, tqy, tqz,
                      end1x, end1y, end1z, end2x, end2y, end2z,
                      corner1x, corner1y, corner1z,
                      corner2x, corner2y, corner2z,
                      corner3x, corner3y, corner3z,
                      nbonds,
                      vfrac, s0,
                      spin, eradius, ervel, erforce,
                      rho, drho, e, de, cv,
                      i_name, d_name

  id = atom ID
  mol = molecule ID
  proc = ID of processor that owns atom
  type = atom type
  mass = atom mass
  x,y,z = unscaled atom coordinates
  xs,ys,zs = scaled atom coordinates
  xu,yu,zu = unwrapped atom coordinates
  ix,iy,iz = box image that the atom is in
  vx,vy,vz = atom velocities
  fx,fy,fz = forces on atoms
  q = atom charge
  mux,muy,muz = orientation of dipole moment of atom
  mu = magnitude of dipole moment of atom
  radius,diameter = radius,diameter of spherical particle
  omegax,omegay,omegaz = angular velocity of spherical particle
  angmomx,angmomy,angmomz = angular momentum of aspherical particle
  shapex,shapey,shapez = 3 diameters of aspherical particle
  quatw,quati,quatj,quatk = quaternion components for aspherical or body particles
  tqx,tqy,tqz = torque on finite-size particles
  end12x, end12y, end12z = end points of line segment
  corner123x, corner123y, corner123z = corner points of triangle
  nbonds = number of bonds assigned to an atom

  PERI package per-atom properties:
  vfrac = ???
  s0 = ???

  USER-EFF and USER-AWPMD package per-atom properties:
  spin = electron spin
  eradius = electron radius
```

```
            ervel = electron radial velocity
            erforce = electron radial force

            USER-SPH package per-atom properties:
            rho = ???
            drho = ???
            e = ???
            de = ???
            cv = ???

      fix property/atom per-atom properties:
            i_name = custom integer vector with name
            d_name = custom integer vector with name
```

Examples:

```
compute 1 all property/atom xs vx fx mux
compute 2 all property/atom type
compute 1 all property/atom ix iy iz
```

Description:

Define a computation that simply stores atom attributes for each atom in the group. This is useful so that the values can be used by other output commands that take computes as inputs. See for example, the compute reduce, fix ave/atom, fix ave/histo, fix ave/spatial, and atom-style variable commands.

The list of possible attributes is the same as that used by the dump custom command, which describes their meaning, with some additional quantities that are only defined for certain atom styles. Basically, this augmented list gives an input script access to any per-atom quantity stored by LAMMPS.

The values are stored in a per-atom vector or array as discussed below. Zeroes are stored for atoms not in the specified group or for quantities that are not defined for a particular particle in the group (e.g. *shapex* if the particle is not an ellipsoid).

The additional quantities only accessible via this command, and not directly via the dump custom command, are as follows.

Shapex, *shapey*, and *shapez* are defined for ellipsoidal particles and define the 3d shape of each particle.

Quatw, *quati*, *quatj*, and *quatk* are defined for ellipsoidal particles and body particles and store the 4-vector quaternion representing the orientation of each particle. See the set command for an explanation of the quaternion vector.

End1x, *end1y*, *end1z*, *end2x*, *end2y*, *end2z*, are defined for line segment particles and define the end points of each line segment.

Corner1x, *corner1y*, *corner1z*, *corner2x*, *corner2y*, *corner2z*, *corner3x*, *corner3y*, *corner3z*, are defined for triangular particles and define the corner points of each triangle.

Nbonds is available for all molecular atom styles and refers to the number of explicit bonds assigned to an atom. Note that if the newton bond command is set to *on*, which is the default, then every bond in the system is assigned to only one of the two atoms in the bond. Thus a bond between atoms I,J may be tallied for either atom I or atom J. If newton bond off is set, it will be tallied with both atom I and atom J.

The *i_name* and *d_name* attributes refer to custom integer and floating-point properties that have been added to each atom via the fix property/atom command. When that command is used specific names are given to each attribute which are what is specified as the "name" portion of *i_name* or *d_name*.

Output info:

This compute calculates a per-atom vector or per-atom array depending on the number of input values. If a single input is specified, a per-atom vector is produced. If two or more inputs are specified, a per-atom array is produced where the number of columns = the number of inputs. The vector or array can be accessed by any command that uses per-atom values from a compute as input. See this section for an overview of LAMMPS output options.

The vector or array values will be in whatever units the corresponding attribute is in, e.g. velocity units for vx, charge units for q, etc.

Restrictions: none

Related commands:

dump custom, compute reduce, fix ave/atom, fix ave/spatial, fix property/atom

Default: none

compute property/chunk command

Syntax:

```
compute ID group-ID property/chunk chunkID input1 input2 ...
```

- ID, group-ID are documented in compute command
- property/chunk = style name of this compute command
- input = one or more attributes

```
attributes = count, id, coord1, coord2, coord3
  count = # of atoms in chunk
  id = original chunk IDs before compression by compute chunk/atom
  coord123 = coordinates for spatial bins calculated by compute chunk/atom
```

Examples:

```
compute 1 all property/chunk count
compute 1 all property/chunk ID coord1
```

Description:

Define a computation that stores the specified attributes of chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a compute chunk/atom command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the compute chunk/atom doc page and "Section_howto 23 for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates and stores the specified attributes of chunks as global data so they can be accessed by other output commands and used in conjunction with other commands that generate per-chunk data, such as compute com/chunk or compute msd/chunk.

Note that only atoms in the specified group contribute to the calculation of the *count* attribute. The compute chunk/atom command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

The *count* attribute is the number of atoms in the chunk.

The *id* attribute stores the original chunk ID for each chunk. It can only be used if the *compress* keyword was set to *yes* for the compute chunk/atom command referenced by chunkID. This means that the original chunk IDs (e.g. molecule IDs) will have been compressed to remove chunk IDs with no atoms assigned to them. Thus a compresed chunk ID of 3 may correspond to an original chunk ID (molecule ID in this case) of 415. The *id* attribute will then be 415 for the 3rd chunk.

The *coordN* attributes can only be used if a *binning* style was used in the compute chunk/atom command referenced by chunkID. For *bin/1d*, *bin/2d*, and *bin/3d* styles the attribute is the center point of the bin in the corresponding dimension. Style *bin/1d* only defines a *coord1* attribute. Style *bin/2d* adds a *coord2* attribute. Style *bin/3d* adds a *coord3* attribute.

Note that if the value of the *units* keyword used in the compute chunk/atom command is *box* or *lattice*, the *coordN* attributes will be in distance units. If the value of the *units* keyword is *reduced*, the *coordN* attributes will be in unitless reduced units (0-1).

The simplest way to output the results of the compute property/chunk calculation to a file is to use the fix ave/time command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk1 all property/chunk cc1
compute myChunk2 all com/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk1 c_myChunk2 file tmp.out mode vector
```

Output info:

This compute calculates a global vector or global array depending on the number of input values. The length of the vector or number of rows in the array is the number of chunks.

This compute calculates a global vector or global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified compute chunk/atom command. If a single input is specified, a global vector is produced. If two or more inputs are specified, a global array is produced where the number of columns = the number of inputs. The vector or array can be accessed by any command that uses global values from a compute as input. See this section for an overview of LAMMPS output options.

The vector or array values are "intensive". The values will be unitless or in the units discussed above.

Restrictions: none

Related commands:

fix ave/chunk

Default: none

compute property/local command

Syntax:

```
compute ID group-ID property/local input1 input2 ...
```

- ID, group-ID are documented in compute command
- property/local = style name of this compute command
- input = one or more attributes

```
possible attributes = natom1 natom2 ntype1 ntype2
                      patom1 patom2 ptype1 ptype2
                      batom1 batom2 btype
                      aatom1 aatom2 aatom3 atype
                      datom1 datom2 datom3 dtype
                      iatom1 iatom2 iatom3 itype

  natom1, natom2 = IDs of 2 atoms in each pair (within neighbor cutoff)
  ntype1, ntype2 = type of 2 atoms in each pair (within neighbor cutoff)
  patom1, patom2 = IDs of 2 atoms in each pair (within force cutoff)
  ptype1, ptype2 = type of 2 atoms in each pair (within force cutoff)
  batom1, batom2 = IDs of 2 atoms in each bond
  btype = bond type of each bond
  aatom1, aatom2, aatom3 = IDs of 3 atoms in each angle
  atype = angle type of each angle
  datom1, datom2, datom3, datom4 = IDs of 4 atoms in each dihedral
  dtype = dihedral type of each dihedral
  iatom1, iatom2, iatom3, iatom4 = IDs of 4 atoms in each improper
  itype = improper type of each improper
```

Examples:

```
compute 1 all property/local btype batom1 batom2
compute 1 all property/local atype aatom2
```

Description:

Define a computation that stores the specified attributes as local data so it can be accessed by other output commands. If the input attributes refer to bond information, then the number of datums generated, aggregated across all processors, equals the number of bonds in the system. Ditto for pairs, angles, etc.

If multiple input attributes are specified then they must all generate the same amount of information, so that the resulting local array has the same number of rows for each column. This means that only bond attributes can be specified together, or angle attributes, etc. Bond and angle attributes can not be mixed in the same compute property/local command.

If the inputs are pair attributes, the local data is generated by looping over the pairwise neighbor list. Info about an individual pairwise interaction will only be included if both atoms in the pair are in the specified compute group. For *natom1* and *natom2*, all atom pairs in the neighbor list are considered (out to the neighbor cutoff = force cutoff + neighbor skin). For *patom1* and *patom2*, the distance between the atoms must be less than the force cutoff distance for that pair to be included, as defined by the pair_style and pair_coeff commands.

If the inputs are bond, angle, etc attributes, the local data is generated by looping over all the atoms owned on a processor and extracting bond, angle, etc info. For bonds, info about an individual bond will only be included if

both atoms in the bond are in the specified compute group. Likewise for angles, dihedrals, etc.

For bonds and angles, a bonds/angles that have been broken by setting their bond/angle type to 0 will not be included. Bonds/angles that have been turned off (see the fix shake or delete_bonds commands) by setting their bond/angle type negative are written into the file. This is consistent with the compute bond/local and compute angle/local commands

Note that as atoms migrate from processor to processor, there will be no consistent ordering of the entries within the local vector or array from one timestep to the next. The only consistency that is guaranteed is that the ordering on a particular timestep will be the same for local vectors or arrays generated by other compute commands. For example, output from the compute bond/local command can be combined with bond atom indices from this command and output by the dump local command in a consistent way.

The *natom1* and *natom2*, or *patom1* and *patom2* attributes refer to the atom IDs of the 2 atoms in each pairwise interaction computed by the pair_style command. The *ntype1* and *ntype2*, or *ptype1* and *ptype2* attributes refer to the atom types of the 2 atoms in each pairwise interaction.

NOTE: For pairs, if two atoms I,J are involved in 1-2, 1-3, 1-4 interactions within the molecular topology, their pairwise interaction may be turned off, and thus they may not appear in the neighbor list, and will not be part of the local data created by this command. More specifically, this may be true of I,J pairs with a weighting factor of 0.0; pairs with a non-zero weighting factor are included. The weighting factors for 1-2, 1-3, and 1-4 pairwise interactions are set by the special_bonds command.

The *batom1* and *batom2* attributes refer to the atom IDs of the 2 atoms in each bond. The *btype* attribute refers to the type of the bond, from 1 to Nbtypes = # of bond types. The number of bond types is defined in the data file read by the read_data command.

The attributes that start with "a", "d", "i", refer to similar values for angles, dihedrals, and impropers.

Output info:

This compute calculates a local vector or local array depending on the number of input values. The length of the vector or number of rows in the array is the number of bonds, angles, etc. If a single input is specified, a local vector is produced. If two or more inputs are specified, a local array is produced where the number of columns = the number of inputs. The vector or array can be accessed by any command that uses local values from a compute as input. See this section for an overview of LAMMPS output options.

The vector or array values will be integers that correspond to the specified attribute.

Restrictions: none

Related commands:

dump local, compute reduce

Default: none

compute rdf command

Syntax:

```
compute ID group-ID rdf Nbin itype1 jtype1 itype2 jtype2 ...
```

- ID, group-ID are documented in compute command
- rdf = style name of this compute command
- Nbin = number of RDF bins
- itypeN = central atom type for Nth RDF histogram (see asterisk form below)
- jtypeN = distribution atom type for Nth RDF histogram (see asterisk form below)

Examples:

```
compute 1 all rdf 100
compute 1 all rdf 100 1 1
compute 1 all rdf 100 * 3
compute 1 fluid rdf 500 1 1 1 2 2 1 2 2
compute 1 fluid rdf 500 1*3 2 5 *10
```

Description:

Define a computation that calculates the radial distribution function (RDF), also called g(r), and the coordination number for a group of particles. Both are calculated in histogram form by binning pairwise distances into *Nbin* bins from 0.0 to the maximum force cutoff defined by the pair_style command. The bins are of uniform size in radial distance. Thus a single bin encompasses a thin shell of distances in 3d and a thin ring of distances in 2d.

NOTE: If you have a bonded system, then the settings of special_bonds command can remove pairwise interactions between atoms in the same bond, angle, or dihedral. This is the default setting for the special_bonds command, and means those pairwise interactions do not appear in the neighbor list. Because this fix uses the neighbor list, it also means those pairs will not be included in the RDF. This does not apply when using long-range coulomb (*coul/long*, *coul/msm*, *coul/wolf* or similar. One way to get around this would be to set special_bond scaling factors to very tiny numbers that are not exactly zero (e.g. 1.0e-50). Another workaround is to write a dump file, and use the rerun command to compute the RDF for snapshots in the dump file. The rerun script can use a special_bonds command that includes all pairs in the neighbor list.

The *itypeN* and *jtypeN* arguments are optional. These arguments must come in pairs. If no pairs are listed, then a single histogram is computed for g(r) between all atom types. If one or more pairs are listed, then a separate histogram is generated for each *itype*,*jtype* pair.

The *itypeN* and *jtypeN* settings can be specified in one of two ways. An explicit numeric value can be used, as in the 4th example above. Or a wild-card asterisk can be used to specify a range of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

If both *itypeN* and *jtypeN* are single values, as in the 4th example above, this means that a g(r) is computed where atoms of type *itypeN* are the central atom, and atoms of type *jtypeN* are the distribution atom. If either *itypeN* and *jtypeN* represent a range of values via the wild-card asterisk, as in the 5th example above, this means that a g(r) is computed where atoms of any of the range of types represented by *itypeN* are the central atom, and atoms of any of the range of types represented by *jtypeN* are the distribution atom.

Pairwise distances are generated by looping over a pairwise neighbor list, just as they would be in a pair_style computation. The distance between two atoms I and J is included in a specific histogram if the following criteria are met:

- atoms I,J are both in the specified compute group
- the distance between atoms I,J is less than the maximum force cutoff
- the type of the I atom matches itypeN (one or a range of types)
- the type of the J atom matches jtypeN (one or a range of types)

It is OK if a particular pairwise distance is included in more than one individual histogram, due to the way the *itypeN* and *jtypeN* arguments are specified.

The g(r) value for a bin is calculated from the histogram count by scaling it by the idealized number of how many counts there would be if atoms of type *jtypeN* were uniformly distributed. Thus it involves the count of *itypeN* atoms, the count of *jtypeN* atoms, the volume of the entire simulation box, and the volume of the bin's thin shell in 3d (or the area of the bin's thin ring in 2d).

A coordination number coord(r) is also calculated, which is the number of atoms of type *jtypeN* within the current bin or closer, averaged over atoms of type *itypeN*. This is calculated as the area- or volume-weighted sum of g(r) values over all bins up to and including the current bin, multiplied by the global average volume density of atoms of type jtypeN.

The simplest way to output the results of the compute rdf calculation to a file is to use the fix ave/time command, for example:

```
compute myRDF all rdf 50
fix 1 all ave/time 100 1 100 c_myRDF file tmp.rdf mode vector
```

Output info:

This compute calculates a global array with the number of rows = *Nbins*, and the number of columns = 1 + 2*Npairs, where Npairs is the number of I,J pairings specified. The first column has the bin coordinate (center of the bin), Each successive set of 2 columns has the g(r) and coord(r) values for a specific set of *itypeN* versus *jtypeN* interactions, as described above. These values can be used by any command that uses a global values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The array values calculated by this compute are all "intensive".

The first column of array values will be in distance units. The g(r) columns of array values are normalized numbers >= 0.0. The coordination number columns of array values are also numbers >= 0.0.

Restrictions:

The RDF is not computed for distances longer than the force cutoff, since processors (in parallel) don't know about atom coordinates for atoms further away than that distance. If you want an RDF for larger distances, you can use the rerun command to post-process a dump file and set the cutoff for the potential to be longer in the rerun script. Note that in the rerun context, the force cutoff is arbitrary, since you aren't running dynamics and thus are not changing your model. The definition of g(r) used by LAMMPS is only appropriate for characterizing atoms that are uniformly distributed throughout the simulation cell. In such cases, the coordination number is still correct and meaningful. As an example, if a large simulation cell contains only one atom of type *itypeN* and one of *jtypeN*, then g(r) will register an arbitrarily large spike at whatever distance they happen to be at, and zero everywhere else. Coord(r) will show a step change from zero to one at the location of the spike in g(r).

Related commands:

fix ave/time

Default: none

compute reduce command

compute reduce/region command

Syntax:

```
compute ID group-ID style arg mode input1 input2 ... keyword args ...
```

- ID, group-ID are documented in compute command
- style = *reduce* or *reduce/region*

```
reduce arg = none
  reduce/region arg = region-ID
    region-ID = ID of region to use for choosing atoms
```

- mode = *sum* or *min* or *max* or *ave* or *sumsq* or *avesq*
- one or more inputs can be listed
- input = x, y, z, vx, vy, vz, fx, fy, fz, c_ID, c_ID[N], f_ID, f_ID[N], v_name

```
x,y,z,vx,vy,vz,fx,fy,fz = atom attribute (position, velocity, force component)
c_ID = per-atom or local vector calculated by a compute with ID
c_ID[I] = Ith column of per-atom or local array calculated by a compute with ID
f_ID = per-atom or local vector calculated by a fix with ID
f_ID[I] = Ith column of per-atom or local array calculated by a fix with ID
v_name = per-atom vector calculated by an atom-style variable with name
```

- zero or more keyword/args pairs may be appended
- keyword = *replace*

```
replace args = vec1 vec2
    vec1 = reduced value from this input vector will be replaced
    vec2 = replace it with vec1[N] where N is index of max/min value from vec2
```

Examples:

```
compute 1 all reduce sum c_force
compute 1 all reduce/region subbox sum c_force
compute 2 all reduce min c_press[2] f_ave v_myKE
compute 3 fluid reduce max c_index[1] c_index[2] c_dist replace 1 3 replace 2 3
```

Description:

Define a calculation that "reduces" one or more vector inputs into scalar values, one per listed input. The inputs can be per-atom or local quantities; they cannot be global quantities. Atom attributes are per-atom quantities, computes and fixes may generate any of the three kinds of quantities, and atom-style variables generate per-atom quantities. See the variable command and its special functions which can perform the same operations as the compute reduce command on global vectors.

The reduction operation is specified by the *mode* setting. The *sum* option adds the values in the vector into a global total. The *min* or *max* options find the minimum or maximum value across all vector values. The *ave* setting adds the vector values into a global total, then divides by the number of values in the vector. The *sumsq* option sums the square of the values in the vector into a global total. The *avesq* setting does the same as *sumsq*, then divdes the sum of squares by the number of values. The last two options can be useful for calculating the variance of some quantity, e.g. variance = sumsq - ave^2.

Each listed input is operated on independently. For per-atom inputs, the group specified with this command means only atoms within the group contribute to the result. For per-atom inputs, if the compute reduce/region command is used, the atoms must also currently be within the region. Note that an input that produces per-atom quantities may define its own group which affects the quantities it returns. For example, if a compute is used as an input which generates a per-atom vector, it will generate values of 0.0 for atoms that are not in the group specified for that compute.

Each listed input can be an atom attribute (position, velocity, force component) or can be the result of a compute or fix or the evaluation of an atom-style variable.

The atom attribute values (x,y,z,vx,vy,vz,fx,fy,fz) are self-explanatory. Note that other atom attributes can be used as inputs to this fix by using the compute property/atom command and then specifying an input value from that compute.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. Computes can generate per-atom or local quantities. See the individual compute doc page for details. If no bracketed integer is appended, the vector calculated by the compute is used. If a bracketed integer is appended, the Ith column of the array calculated by the compute is used. Users can also write code for their own compute styles and add them to LAMMPS.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. Fixes can generate per-atom or local quantities. See the individual fix doc page for details. Note that some fixes only produce their values on certain timesteps, which must be compatible with when compute reduce references the values, else an error results. If no bracketed integer is appended, the vector calculated by the fix is used. If a bracketed integer is appended, the Ith column of the array calculated by the fix is used. Users can also write code for their own fix style and add them to LAMMPS.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. It must be an atom-style variable. Atom-style variables can reference thermodynamic keywords and various per-atom attributes, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of generating per-atom quantities to reduce.

If the *replace* keyword is used, two indices *vec1* and *vec2* are specified, where each index ranges from 1 to the # of input values. The replace keyword can only be used if the *mode* is *min* or *max*. It works as follows. A min/max is computed as usual on the *vec2* input vector. The index N of that value within *vec2* is also stored. Then, instead of performing a min/max on the *vec1* input vector, the stored index is used to select the Nth element of the *vec1* vector.

Thus, for example, if you wish to use this compute to find the bond with maximum stretch, you can do it as follows:

```
compute 1 all property/local batom1 batom2
compute 2 all bond/local dist
compute 3 all reduce max c_1[1] c_1[2] c_2 replace 1 3 replace 2 3
thermo_style custom step temp c_3[1] c_3[2] c_3[3]
```

The first two input values in the compute reduce command are vectors with the IDs of the 2 atoms in each bond, using the compute property/local command. The last input value is bond distance, using the compute bond/local command. Instead of taking the max of the two atom ID vectors, which does not yield useful information in this context, the *replace* keywords will extract the atom IDs for the two atoms in the bond of maximum stretch. These atom IDs and the bond stretch will be printed with thermodynamic output.

If a single input is specified this compute produces a global scalar value. If multiple inputs are specified, this compute produces a global vector of values, the length of which is equal to the number of inputs specified.

As discussed below, for the *sum* and *sumsq* modes, the value(s) produced by this compute are all "extensive", meaning their value scales linearly with the number of atoms involved. If normalized values are desired, this compute can be accessed by the thermo_style custom command with thermo_modify norm yes set as an option. Or it can be accessed by a variable that divides by the appropriate atom count.

Output info:

This compute calculates a global scalar if a single input value is specified or a global vector of length N where N is the number of inputs, and which can be accessed by indices 1 to N. These values can be used by any command that uses global scalar or vector values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

All the scalar or vector values calculated by this compute are "intensive", except when the *sum* or *sumsq* modes are used on per-atom or local vectors, in which case the calculated values are "extensive".

The scalar or vector values will be in whatever units the quantities being reduced are in.

Restrictions: none

Related commands:

compute, fix, variable

Default: none

compute saed command

Syntax:

```
compute ID group-ID saed lambda type1 type2 ... typeN keyword value ...
```

- ID, group-ID are documented in compute command
- saed = style name of this compute command
- lambda = wavelength of incident radiation (length units)
- type1 type2 ... typeN = chemical symbol of each atom type (see valid options below)
- zero or more keyword/value pairs may be appended
- keyword = *Kmax* or *Zone* or *dR_Ewald* or *c* or *manual* or *echo*

```
  Kmax value = Maximum distance explored from reciprocal space origin
                 (inverse length units)
    Zone values = z1 z2 z3
      z1,z2,z3 = Zone axis of incident radiation. If z1=z2=z3=0 all
                 reciprocal space will be meshed up to Kmax
    dR_Ewald value = Thickness of Ewald sphere slice intercepting
                     reciprocal space (inverse length units)
    c values = c1 c2 c3
      c1,c2,c3 = parameters to adjust the spacing of the reciprocal
                 lattice nodes in the h, k, and l directions respectively
    manual = flag to use manual spacing of reciprocal lattice points
             based on the values of the c parameters
    echo = flag to provide extra output for debugging purposes
```

Examples:

```
compute 1 all saed 0.0251 Al O Kmax 1.70 Zone 0 0 1 dR_Ewald 0.01 c 0.5 0.5 0.5
compute 2 all saed 0.0251 Ni Kmax 1.70 Zone 0 0 0 c 0.05 0.05 0.05 manual echo

fix saed/vtk 1 1 1 c_1 file Al2O3_001.saed
fix saed/vtk 1 1 1 c_2 file Ni_000.saed
```

Description:

Define a computation that calculates electron diffraction intensity as described in (Coleman) on a mesh of reciprocal lattice nodes defined by the entire simulation domain (or manually) using simulated radiation of wavelength lambda.

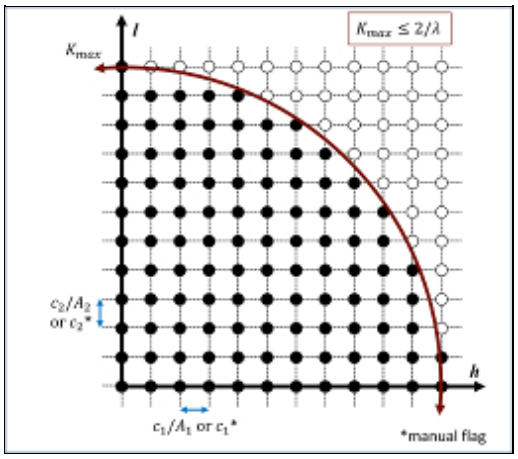
The electron diffraction intensity I at each reciprocal lattice point is computed from the structure factor F using the equations:

$$I = \frac{F^* F}{N}$$

$$F(\mathbf{k}) = \sum_{\mathbf{j}=\mathbf{1}}^{\mathbf{N}} \mathbf{f_j}(\theta)\mathbf{exp}(\mathbf{2\pi i k \cdot r_j})$$

Here, K is the location of the reciprocal lattice node, rj is the position of each atom, fj are atomic scattering factors.

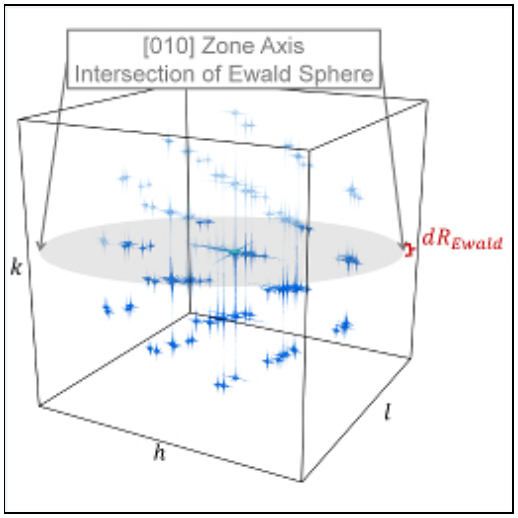
Diffraction intensities are calculated on a three-dimensional mesh of reciprocal lattice nodes. The mesh spacing is defined either (a) by the entire simulation domain or (b) manually using selected values as shown in the 2D diagram below.



For a mesh defined by the simulation domain, a rectilinear grid is constructed with spacing *c*inv(A) along each reciprocal lattice axis. Where A are the vectors corresponding to the edges of the simulation cell. If one or two directions has non-periodic boundary conditions, then the spacing in these directions is defined from the average of the (inversed) box lengths with periodic boundary conditions. Meshes defined by the simulation domain must contain at least one periodic boundary.

If the *manual* flag is included, the mesh of reciprocal lattice nodes will defined using the *c* values for the spacing along each reciprocal lattice axis. Note that manual mapping of the reciprocal space mesh is good for comparing diffraction results from multiple simulations; however it can reduce the likelihood that Bragg reflections will be satisfied unless small spacing parameters

The limits of the reciprocal lattice mesh are determined by the use of the *Kmax*, *Zone*, and *dR_Ewald* parameters. The rectilinear mesh created about the origin of reciprocal space is terminated at the boundary of a sphere of radius *Kmax* centered at the origin. If *Zone* parameters z1=z2=z3=0 are used, diffraction intensities are computed throughout the entire spherical volume - note this can greatly increase the cost of computation. Otherwise, *Zone* parameters will denote the z1=h, z2=k, and z3=l (in a global since) zone axis of an intersecting Ewald sphere. Diffraction intensities will only be computed at the intersection of the reciprocal lattice mesh and a *dR_Ewald* thick surface of the Ewald sphere. See the example 3D intestiety data and the intersection of a [010] zone axis in the below image.



The atomic scattering factors, fj, accounts for the reduction in diffraction intensity due to Compton scattering. Compute saed uses analytical approximations of the atomic scattering factors that vary for each atom type (type1 type2 ... typeN) and angle of diffraction. The analytic approximation is computed using the formula (Brown):

$$f_j\left(\frac{sin(\theta)}{\lambda}\right) = \sum_i^5 a_i exp\left(-b_i \frac{sin^2(\theta)}{\lambda^2}\right)$$

Coefficients parameterized by (Fox) are assigned for each atom type designating the chemical symbol and charge of each atom type. Valid chemical symbols for compute saed are:

H: He: Li: Be: B: C: N: O: F: Ne: Na: Mg: Al: Si: P: S: Cl: Ar: K: Ca: Sc: Ti: V: Cr: Mn: Fe: Co: Ni: Cu: Zn: Ga: Ge: As: Se: Br: Kr: Rb: Sr: Y: Zr: Nb: Mo: Tc: Ru: Rh: Pd: Ag: Cd: In: Sn: Sb: Te: I: Xe: Cs: Ba: La: Ce: Pr: Nd: Pm: Sm: Eu: Gd: Tb: Dy: Ho: Er: Tm: Yb: Lu: Hf: Ta: W: Re: Os: Ir: Pt: Au: Hg: Tl: Pb: Bi: Po: At: Rn: Fr: Ra: Ac: Th: Pa: U: Np: Pu: Am: Cm: Bk: Cf:tb(c=5,s=:)

If the *echo* keyword is specified, compute saed will provide extra reporting information to the screen.

Output info:

This compute calculates a global vector. The length of the vector is the number of reciprocal lattice nodes that are explored by the mesh. The entries of the global vector are the computed diffraction intensities as described above.

The vector can be accessed by any command that uses global values from a compute as input. See this section for an overview of LAMMPS output options.

All array values calculated by this compute are "intensive".

Restrictions:

This compute is part of the USER-DIFFRACTION package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The compute_saed command does not work for triclinic cells.

Related commands:

fix saed_vtk, compute xrd

Default:

The option defaults are Kmax = 1.70, Zone 1 0 0, c 1 1 1, dR_Ewald = 0.01.

(Coleman) Coleman, Spearot, Capolungo, MSMSE, 21, 055020 (2013).

(Brown) Brown et al. International Tables for Crystallography Volume C: Mathematical and Chemical Tables, 554-95 (2004).

(Fox) Fox, O'Keefe, Tabbernor, Acta Crystallogr. A, 45, 786-93 (1989).

compute slice command

Syntax:

```
compute ID group-ID slice Nstart Nstop Nskip input1 input2 ...
```

- ID, group-ID are documented in compute command
- slice = style name of this compute command
- Nstart = starting index within input vector(s)
- Nstop = stopping index within input vector(s)
- Nskip = extract every Nskip elements from input vector(s)
- input = c_ID, c_ID[N], f_ID, f_ID[N]

```
c_ID = global vector calculated by a compute with ID
c_ID[I] = Ith column of global array calculated by a compute with ID
f_ID = global vector calculated by a fix with ID
f_ID[I] = Ith column of global array calculated by a fix with ID
```

Examples:

```
compute 1 all slice 1 100 10 c_msdmol[4]
compute 1 all slice 301 400 1 c_msdmol[4]
```

Description:

Define a calculation that "slices" one or more vector inputs into smaller vectors, one per listed input. The inputs can be global quantities; they cannot be per-atom or local quantities. Computes and fixes may generate any of the three kinds of quantities. Variables do not generate global vectors. The group specified with this command is ignored.

The values extracted from the input vector(s) are determined by the *Nstart*, *Nstop*, and *Nskip* parameters. The elements of an input vector of length N are indexed from 1 to N. Starting at element *Nstart*, every Mth element is extracted, where M = *Nskip*, until element *Nstop* is reached. The extracted quantities are stored as a vector, which is typically shorter than the input vector.

Each listed input is operated on independently to produce one output vector. Each listed input must be a global vector or column of a global array calculated by another compute or fix.

If an input value begins with "c_", a compute ID must follow which has been previously defined in the input script and which generates a global vector or array. See the individual compute doc page for details. If no bracketed integer is appended, the vector calculated by the compute is used. If a bracketed integer is appended, the Ith column of the array calculated by the compute is used. Users can also write code for their own compute styles and add them to LAMMPS.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script and which generates a global vector or array. See the individual fix doc page for details. Note that some fixes only produce their values on certain timesteps, which must be compatible with when compute slice references the values, else an error results. If no bracketed integer is appended, the vector calculated by the fix is used. If a bracketed integer is appended, the Ith column of the array calculated by the fix is used. Users can also write code for their own fix style and add them to LAMMPS.

If a single input is specified this compute produces a global vector, even if the length of the vector is 1. If multiple inputs are specified, then a global array of values is produced, with the number of columns equal to the number of inputs specified.

Output info:

This compute calculates a global vector if a single input value is specified or a global array with N columns where N is the number of inputs. The length of the vector or the number of rows in the array is equal to the number of values extracted from each input vector. These values can be used by any command that uses global vector or array values from a compute as input. See this section for an overview of LAMMPS output options.

The vector or array values calculated by this compute are simply copies of values generated by computes or fixes that are input vectors to this compute. If there is a single input vector of intensive and/or extensive values, then each value in the vector of values calculated by this compute will be "intensive" or "extensive", depending on the corresponding input value. If there are multiple input vectors, and all the values in them are intensive, then the array values calculated by this compute are "intensive". If there are multiple input vectors, and any value in them is extensive, then the array values calculated by this compute are "extensive".

The vector or array values will be in whatever units the input quantities are in.

Restrictions: none

Related commands:

compute, fix, compute reduce

Default: none

compute smd/contact/radius command

Syntax:

```
compute ID group-ID smd/contact/radius
```

- ID, group-ID are documented in compute command
- smd/contact/radius = style name of this compute command

Examples:

```
compute 1 all smd/contact/radius
```

Description:

Define a computation which outputs the contact radius, i.e., the radius used to prevent particles from penetrating each other. The contact radius is used only to prevent particles belonging to different physical bodies from penetrating each other. It is used by the contact pair styles, e.g., smd/hertz and smd/tri_surface.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

The value of the contact radius will be 0.0 for particles not in the specified compute group.

Output info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-particle vector values will be in distance units.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

dump custom smd/hertz smd/tri_surface

Default: none

compute smd/damage command

Syntax:

```
compute ID group-ID smd/damage
```

- ID, group-ID are documented in compute command
- smd/damage = style name of this compute command

Examples:

```
compute 1 all smd/damage
```

Description:

Define a computation that calculates the damage status of SPH particles according to the damage model which is defined via the SMD SPH pair styles, e.g., the maximum plastic strain failure criterion.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Output Info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See How-to discussions, section 6.15 for an overview of LAMMPS output options.

The per-particle values are dimensionless an in the range of zero to one.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

smd/plastic_strain, smd/tlsph_stress

Default: none

compute smd/hourglass/error command

Syntax:

```
compute ID group-ID smd/hourglass/error
```

- ID, group-ID are documented in compute command
- smd/hourglass/error = style name of this compute command

Examples:

```
compute 1 all smd/hourglass/error
```

Description:

Define a computation which outputs the error of the approximated relative separation with respect to the actual relative separation of the particles i and j. Ideally, if the deformation gradient is exact, and there exists a unique mapping between all particles' positions within the neighborhood of the central node and the deformation gradient, the approximated relative separation will coincide with the actual relative separation of the particles i and j in the deformed configuration. This compute is only really useful for debugging the hourglass control mechanim which is part of the Total-Lagrangian SPH pair style.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Output Info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See How-to discussions, section 6.15 for an overview of LAMMPS output options.

The per-particle vector values will are dimensionless. See units.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This quantity will be computed only for particles which interact with tlsph pair style.

Related Commands:

smd/tlsph_defgrad

Default:

compute smd/internal/energy command

Syntax:

```
compute ID group-ID smd/internal/energy
```

- ID, group-ID are documented in compute command
- smd/smd/internal/energy = style name of this compute command

Examples:

```
compute 1 all smd/internal/energy
```

Description:

Define a computation which outputs the per-particle enthalpy, i.e., the sum of potential energy and heat.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Output Info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See How-to discussions, section 6.15 for an overview of LAMMPS output options.

The per-particle vector values will be given in units of energy.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info. This compute can only be used for particles which interact via the updated Lagrangian or total Lagrangian SPH pair styles.

Related Commands:

Default:

compute smd/plastic/strain command

Syntax:

```
compute ID group-ID smd/plastic/strain
```

- ID, group-ID are documented in compute command
- smd/plastic/strain = style name of this compute command

Examples:

```
compute 1 all smd/plastic/strain
```

Description:

Define a computation that outputs the equivalent plastic strain per particle. This command is only meaningful if a material model with plasticity is defined.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Output Info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See How-to discussions, section 6.15 for an overview of LAMMPS output options.

The per-particle values will be given dimensionless. See units.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info. This compute can only be used for particles which interact via the updated Lagrangian or total Lagrangian SPH pair styles.

Related commands:

smd/plastic/strain/rate, smd/tlsph/strain/rate, smd/tlsph/strain

Default: none

compute smd/plastic/strain/rate command

Syntax:

```
compute ID group-ID smd/plastic/strain/rate
```

- ID, group-ID are documented in compute command
- smd/plastic/strain/rate = style name of this compute command

Examples:

```
compute 1 all smd/plastic/strain/rate
```

Description:

Define a computation that outputs the time rate of the equivalent plastic strain. This command is only meaningful if a material model with plasticity is defined.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Output Info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See How-to discussions, section 6.15 for an overview of LAMMPS output options.

The per-particle values will be given in units of one over time.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info. This compute can only be used for particles which interact via the updated Lagrangian or total Lagrangian SPH pair styles.

Related commands:

smd/plastic/strain, smd/tlsph/strain/rate, smd/tlsph/strain

Default: none

compute smd/rho command

Syntax:

```
compute ID group-ID smd/rho
```

- ID, group-ID are documented in compute command
- smd/rho = style name of this compute command

Examples:

```
compute 1 all smd/rho
```

Description:

Define a computation that calculates the per-particle mass density. The mass density is the mass of a particle which is constant during the course of a simulation, divided by its volume, which can change due to mechanical deformation.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See How-to discussions, section 6.15 for an overview of LAMMPS output options.

The per-particle values will be in units of mass over volume.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

compute smd/vol

Default: none

compute smd/tlsph/defgrad command

Syntax:

```
compute ID group-ID smd/tlsph/defgrad
```

- ID, group-ID are documented in compute command
- smd/tlsph/defgrad = style name of this compute command

Examples:

```
compute 1 all smd/tlsph/defgrad
```

Description:

Define a computation that calculates the deformation gradient. It is only meaningful for particles which interact according to the Total-Lagrangian SPH pair style.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Output info:

This compute outputss a per-particle vector of vectors (tensors), which can be accessed by any command that uses per-particle values from a compute as input. See How-to discussions, section 6.15 for an overview of LAMMPS output options.

The per-particle vector values will be given dimensionless. See units. The per-particle vector has 10 entries. The first nine entries correspond to the xx, xy, xz, yx, yy, yz, zx, zy, zz components of the asymmetric deformation gradient tensor. The tenth entry is the determinant of the deformation gradient.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info. TThis compute can only be used for particles which interact via the total Lagrangian SPH pair style.

Related commands:

smd/hourglass/error

Default: none

compute smd/tlsph/dt command

Syntax:

```
compute ID group-ID smd/tlsph/dt
```

- ID, group-ID are documented in compute command
- smd/tlsph/dt = style name of this compute command

Examples:

```
compute 1 all smd/tlsph/dt
```

Description:

Define a computation that outputs the CFL-stable time increment per particle. This time increment is essentially given by the speed of sound, divided by the SPH smoothing length. Because both the speed of sound and the smoothing length typically change during the course of a simulation, the stable time increment needs to be recomputed every time step. This calculation is performed automatically in the relevant SPH pair styles and this compute only serves to make the stable time increment accessible for output purposes.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See How-to discussions, section 6.15 for an overview of LAMMPS output options.

The per-particle values will be given in units of time.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This compute can only be used for particles interacting with the Total-Lagrangian SPH pair style.

Related commands:

smd/adjust/dt

Default: none

compute smd/tlsph/num/neighs command

Syntax:

```
compute ID group-ID smd/tlsph/num/neighs
```

- ID, group-ID are documented in compute command
- smd/tlsph/num/neighs = style name of this compute command

Examples:

```
compute 1 all smd/tlsph/num/neighs
```

Description:

Define a computation that calculates the number of particles inside of the smoothing kernel radius for particles interacting via the Total-Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See How-to discussions, section 6.15 for an overview of LAMMPS output options.

The per-particle values are dimensionless. See units.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This quantity will be computed only for particles which interact with the Total-Lagrangian pair style.

Related commands:

smd/ulsph/num/neighs

Default: none

compute smd/tlsph/shape command

Syntax:

```
compute ID group-ID smd/tlsph/shape
```

- ID, group-ID are documented in compute command
- smd/tlsph/shape = style name of this compute command

Examples:

```
compute 1 all smd/tlsph/shape
```

Description:

Define a computation that outputs the current shape of the volume associated with a particle as a rotated ellipsoid. It is only meaningful for particles which interact according to the Total-Lagrangian SPH pair style.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector of vectors, which can be accessed by any command that uses per-particle values from a compute as input. See How-to discussions, section 6.15 for an overview of LAMMPS output options.

The per-particle vector has 7 entries. The first three entries correspond to the lengths of the ellipsoid's axes and have units of length. These axis valus are computed as the contact radius times the xx, yy, or zz components of the Green-Lagrange strain tensor associated with the particle. The next 4 values are quaternions (order: q, x, y, z) which describe the spatial rotation of the particle relative to its initial state.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This quantity will be computed only for particles which interact with the Total-Lagrangian SPH pair style.

Related commands:

smd/contact/radius

Default: none

compute smd/tlsph/strain command

Syntax:

```
compute ID group-ID smd/tlsph/strain
```

- ID, group-ID are documented in compute command
- smd/tlsph/strain = style name of this compute command

Examples:

```
compute 1 all smd/tlsph/strain
```

Description:

Define a computation that calculates the Green-Lagrange strain tensor for particles interacting via the Total-Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector of vectors (tensors), which can be accessed by any command that uses per-particle values from a compute as input. See How-to discussions, section 6.15 for an overview of LAMMPS output options.

The per-particle tensor values will be given dimensionless. See units.

The per-particle vector has 6 entries, corresponding to the xx, yy, zz, xy, xz, yz components of the symmetric strain tensor.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This quantity will be computed only for particles which interact with the Total-Lagrangian SPH pair style.

Related commands:

smd/tlsph/strain/rate, smd/tlsph/stress

Default: none

compute smd/tlsph/strain/rate command

Syntax:

```
compute ID group-ID smd/tlsph/strain/rate
```

- ID, group-ID are documented in compute command
- smd/tlsph/strain/rate = style name of this compute command

Examples:

```
compute 1 all smd/tlsph/strain/rate
```

Description:

Define a computation that calculates the rate of the strain tensor for particles interacting via the Total-Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector of vectors (tensors), which can be accessed by any command that uses per-particle values from a compute as input. See How-to discussions, section 6.15 for an overview of LAMMPS output options.

The values will be given in units of one over time.

The per-particle vector has 6 entries, corresponding to the xx, yy, zz, xy, xz, yz components of the symmetric strain rate tensor.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This quantity will be computed only for particles which interact with Total-Lagrangian SPH pair style.

Related commands:

compute smd/tlsph/strain, compute smd/tlsph/stress

Default: none

compute smd/tlsph/stress command

Syntax:

```
compute ID group-ID smd/tlsph/stress
```

- ID, group-ID are documented in compute command
- smd/tlsph/stress = style name of this compute command

Examples:

```
compute 1 all smd/tlsph/stress
```

Description:

Define a computation that outputs the Cauchy stress tensor for particles interacting via the Total-Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector of vectors (tensors), which can be accessed by any command that uses per-particle values from a compute as input. See How-to discussions, section 6.15 for an overview of LAMMPS output options.

The values will be given in units of pressure.

The per-particle vector has 7 entries. The first six entries correspond to the xx, yy, zz, xy, xz and yz components of the symmetric Cauchy stress tensor. The seventh entry is the second invariant of the stress tensor, i.e., the von Mises equivalent stress.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This quantity will be computed only for particles which interact with the Total-Lagrangian SPH pair style.

Related commands:

compute smd/tlsph/strain, cmopute smd/tlsph/strain/rate

Default: none

compute smd/triangle/mesh/vertices

Syntax:

```
compute ID group-ID smd/triangle/mesh/vertices
```

- ID, group-ID are documented in compute command
- smd/triangle/mesh/vertices = style name of this compute command

Examples:

```
compute 1 all smd/triangle/mesh/vertices
```

Description:

Define a computation that returns the coordinates of the vertices corresponding to the triangle-elements of a mesh created by the fix smd/wall_surface.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute returns a per-particle vector of vectors, which can be accessed by any command that uses per-particle values from a compute as input. See How-to discussions, section 6.15 for an overview of LAMMPS output options.

The per-particle vector has nine entries, (x1/y1/z1), (x2/y2/z2), and (x3/y3/z3) corresponding to the first, second, and third vertex of each triangle.

It is only meaningful to use this compute for a group of particles which is created via the fix smd/wall_surface command.

The output of this compute can be used with the dump2vtk_tris tool to generate a VTK representation of the smd/wall_surace mesh for visualization purposes.

The values will be given in units of distance.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

compute smd/move/tri/surf, compute smd/wall/surface

Default: none

compute smd/ulsph/num/neighs command

Syntax:

```
compute ID group-ID smd/ulsph/num/neighs
```

- ID, group-ID are documented in compute command
- smd/ulsph/num/neighs = style name of this compute command

Examples:

```
compute 1 all smd/ulsph/num/neighs
```

Description:

Define a computation that returns the number of neighbor particles inside of the smoothing kernel radius for particles interacting via the updated Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute returns a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-particle values will be given dimentionless, see units.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info. This compute can only be used for particles which interact with the updated Lagrangian SPH pair style.

Related commands:

compute smd/tlsph/num/neighs

Default: none

compute smd/ulsph/strain command

Syntax:

```
compute ID group-ID smd/ulsph/strain
```

- ID, group-ID are documented in compute command
- smd/ulsph/strain = style name of this compute command

Examples:

```
compute 1 all smd/ulsph/strain
```

Description:

Define a computation that outputs the logarithmic strain tensor. for particles interacting via the updated Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle tensor, which can be accessed by any command that uses per-particle values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-particle vector has 6 entries, corresponding to the xx, yy, zz, xy, xz, yz components of the symmetric strain rate tensor.

The per-particle tensor values will be given dimensionless, see units.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info. This compute can only be used for particles which interact with the updated Lagrangian SPH pair style.

Related commands:

compute smd/tlsph/strain

Default: none

compute smd/ulsph/strain/rate command

Syntax:

```
compute ID group-ID smd/ulsph/strain/rate
```

- ID, group-ID are documented in compute command
- smd/ulsph/strain/rate = style name of this compute command

Examples:

```
compute 1 all smd/ulsph/strain/rate
```

Description:

Define a computation that outputs the rate of the logarithmic strain tensor for particles interacting via the updated Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector of vectors (tensors), which can be accessed by any command that uses per-particle values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The values will be given in units of one over time.

The per-particle vector has 6 entries, corresponding to the xx, yy, zz, xy, xz, yz components of the symmetric strain rate tensor.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info. This compute can only be used for particles which interact with the updated Lagrangian SPH pair style.

Related commands:

compute smd/tlsph/strain/rate

Default: none

compute smd/ulsph/stress command

Syntax:

```
compute ID group-ID smd/ulsph/stress
```

- ID, group-ID are documented in compute command
- smd/ulsph/stress = style name of this compute command

Examples:

```
compute 1 all smd/ulsph/stress
```

Description:

Define a computation that outputs the Cauchy stress tensor.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector of vectors (tensors), which can be accessed by any command that uses per-particle values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The values will be given in units of pressure.

The per-particle vector has 7 entries. The first six entries correspond to the xx, yy, zz, xy, xz, yz components of the symmetric Cauchy stress tensor. The seventh entry is the second invariant of the stress tensor, i.e., the von Mises equivalent stress.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info. This compute can only be used for particles which interact with the updated Lagrangian SPH pair style.

Related commands:

compute smd/ulsph/strain, compute smd/ulsph/strain/rate compute smd/tlsph/stress

Default: none

compute smd/vol command

Syntax:

```
compute ID group-ID smd/vol
```

- ID, group-ID are documented in compute command
- smd/vol = style name of this compute command

Examples:

```
compute 1 all smd/vol
```

Description:

Define a computation that provides the per-particle volume and the sum of the per-particle volumes of the group for which the fix is defined.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Output info:

This compute calculates a per-particle vector, which can be accessed by any command that uses per-particle values from a compute as input. See How-to discussions, section 6.15 for an overview of LAMMPS output options.

The per-particle vector values will be given in units of volume.

Additionally, the compute returns a scalar, which is the sum of the per-particle volumes of the group for which the fix is defined.

Restrictions:

This compute is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

compute smd/rho

Default: none

compute sna/atom command

compute snad/atom command

compute snav/atom command

Syntax:

```
compute ID group-ID sna/atom ntypes rcutfac rfac0 twojmax R_1 R_2 ... w_1 w_2 ... keyword values ...
compute ID group-ID snad/atom ntypes rcutfac rfac0 twojmax R_1 R_2 ... w_1 w_2 ... keyword values ..
compute ID group-ID snav/atom ntypes rcutfac rfac0 twojmax R_1 R_2 ... w_1 w_2 ... keyword values ..
```

- ID, group-ID are documented in compute command
- sna/atom = style name of this compute command
- rcutfac = scale factor applied to all cutoff radii (positive real)
- rfac0 = parameter in distance to angle conversion (0 < rcutfac < 1)
- twojmax = band limit for bispectrum components (non-negative integer)
- R_1, R_2,... = list of cutoff radii, one for each type (distance units)
- w_1, w_2,... = list of neighbor weights, one for each type
- zero or more keyword/value pairs may be appended
- keyword = *diagonal* or *rmin0* or *switchflag*

```
  diagonal value = 0 or 1 or 2 or 3
       0 = all j1, j2, j <= twojmax, j2 <= j1
       1 = subset satisfying j1 == j2
       2 = subset satisfying j1 == j2 == j3
       3 = subset satisfying j2 <= j1 <= j
    rmin0 value = parameter in distance to angle conversion (distance units)
    switchflag value = 0 or 1
       0 = do not use switching function
       1 = use switching function
```

Examples:

```
compute b all sna/atom 1.4 0.99363 6 2.0 2.4 0.75 1.0 diagonal 3 rmin0 0.0
compute db all sna/atom 1.4 0.95 6 2.0 1.0
compute vb all sna/atom 1.4 0.95 6 2.0 1.0
```

Description:

Define a computation that calculates a set of bispectrum components for each atom in a group.

Bispectrum components of an atom are order parameters characterizing the radial and angular distribution of neighbor atoms. The detailed mathematical definition is given in the paper by Thompson et al. (Thompson)

The position of a neighbor atom *i'* relative to a central atom *i* is a point within the 3D ball of radius *R_ii'* = *rcutfac*(R_i + R_i')*

Bartok et al. (Bartok), proposed mapping this 3D ball onto the 3-sphere, the surface of the unit ball in a four-dimensional space. The radial distance *r* within *R_ii'* is mapped on to a third polar angle *theta0* defined by,

$$\theta_0 = \texttt{rfac0} \frac{r - r_{min0}}{R_{ii'} - r_{min0}} \pi$$

In this way, all possible neighbor positions are mapped on to a subset of the 3-sphere. Points south of the latitude *theta0max=rfac0*Pi* are excluded.

The natural basis for functions on the 3-sphere is formed by the 4D hyperspherical harmonics *U^j_m,m'(theta, phi, theta0).* These functions are better known as *D^j_m,m',* the elements of the Wigner *D*-matrices (Meremianin, Varshalovich).

The density of neighbors on the 3-sphere can be written as a sum of Dirac-delta functions, one for each neighbor, weighted by species and radial distance. Expanding this density function as a generalized Fourier series in the basis functions, we can write each Fourier coefficient as

$$u^j_{m,m'} = U^j_{m,m'}(0,0,0) + \sum_{r_{ii'}<R_{ii'}} f_c(r_{ii'}) w_{i'} U^j_{m,m'}(\theta_0, \theta, \phi)$$

The *w_i'* neighbor weights are dimensionless numbers that are chosen to distinguish atoms of different types, while the central atom is arbitrarily assigned a unit weight. The function *fc(r)* ensures that the contribution of each neighbor atom goes smoothly to zero at *R_ii'*:

$$\begin{aligned} f_c(r) &= \frac{1}{2}(\cos(\pi \frac{r - r_{min0}}{R_{ii'} - r_{min0}}) + 1), r \le R_{ii'} \\ &= 0, r > R_{ii'} \end{aligned}$$

The expansion coefficients *u^j_m,m'* are complex-valued and they are not directly useful as descriptors, because they are not invariant under rotation of the polar coordinate frame. However, the following scalar triple products of expansion coefficients can be shown to be real-valued and invariant under rotation (Bartok).

$$B_{j_1,j_2,j} = \sum_{m_1,m_1'=-j_1}^{j_1} \sum_{m_2,m_2'=-j_2}^{j_2} \sum_{m,m'=-j}^{j} (u^j_{m,m'})^* H^{jmm'}_{j_1 m_1 m_1' \; j_2 m_2 m_2'} u^{j_1}_{m_1,m_1'} u^{j_2}_{m_2,m_2'}$$

The constants *H^jmm'_j1m1m1'_j2m2m2'* are coupling coefficients, analogous to Clebsch-Gordan coefficients for rotations on the 2-sphere. These invariants are the components of the bispectrum and these are the quantities calculated by the compute *sna/atom*. They characterize the strength of density correlations at three points on the 3-sphere. The j2=0 subset form the power spectrum, which characterizes the correlations of two points. The lowest-order components describe the coarsest features of the density function, while higher-order components reflect finer detail. Note that the central atom is included in the expansion, so three point-correlations can be either due to three neighbors, or two neighbors and the central atom.

Compute *snad/atom* calculates the derivative of the bispectrum components summed separately for each atom type:

$$-\sum_{i' \in I} \frac{\partial B^{i'}_{j_1,j_2,j}}{\partial \mathbf{r}_i}$$

The sum is over all atoms *i'* of atom type *I*. For each atom *i*, this compute evaluates the above expression for each direction, each atom type, and each bispectrum component. See section below on output for a detailed explanation.

Compute *snav/atom* calculates the virial contribution due to the derivatives:

$$-\mathbf{r}_i \otimes \sum_{i' \in I} \frac{\partial B^{i'}_{j_1,j_2,j}}{\partial \mathbf{r}_i}$$

Again, the sum is over all atoms *i'* of atom type *I*. For each atom *i*, this compute evaluates the above expression for each of the six virial components, each atom type, and each bispectrum component. See section below on output for a detailed explanation.

The value of all bispectrum components will be zero for atoms not in the group. Neighbor atoms not in the group do not contribute to the bispectrum of atoms in the group.

The neighbor list needed to compute this quantity is constructed each time the calculation is performed (i.e. each time a snapshot of atoms is dumped). Thus it can be inefficient to compute/dump this quantity too frequently.

The argument *rcutfac* is a scale factor that controls the ratio of atomic radius to radial cutoff distance.

The argument *rfac0* and the optional keyword *rmin0* define the linear mapping from radial distance to polar angle *theta0* on the 3-sphere.

The argument *twojmax* and the keyword *diagonal* define which bispectrum components are generated. See section below on output for a detailed explanation of the number of bispectrum components and the ordered in which they are listed

The keyword *switchflag* can be used to turn off the switching function.

NOTE: If you have a bonded system, then the settings of special_bonds command can remove pairwise interactions between atoms in the same bond, angle, or dihedral. This is the default setting for the special_bonds command, and means those pairwise interactions do not appear in the neighbor list. Because this fix uses the neighbor list, it also means those pairs will not be included in the calculation. One way to get around this, is to write a dump file, and use the rerun command to compute the bispectrum components for snapshots in the dump file. The rerun script can use a special_bonds command that includes all pairs in the neighbor list.

;line

Output info:

Compute *sna/atom* calculates a per-atom array, each column corresponding to a particular bispectrum component. The total number of columns and the identities of the bispectrum component contained in each column depend on the values of *twojmax* and *diagonal*, as described by the following piece of python code:

```
for j1 in range(0,twojmax+1):
    if(diagonal==2):
        print j1/2,j1/2,j1/2
    elif(diagonal==1):
        for j in range(0,min(twojmax,2*j1)+1,2):
            print j1/2,j1/2,j/2
    elif(diagonal==0):
        for j2 in range(0,j1+1):
            for j in range(j1-j2,min(twojmax,j1+j2)+1,2):
                print j1/2,j2/2,j/2
    elif(diagonal==3):
        for j2 in range(0,j1+1):
            for j in range(j1-j2,min(twojmax,j1+j2)+1,2):
                if (j>=j1): print j1/2,j2/2,j/2
```

Compute *snad/atom* evaluates a per-atom array. The columns are arranged into *ntypes* blocks, listed in order of atom type *I*. Each block contains three sub-blocks corresponding to the *x*, *y*, and *z* components of the atom position. Each of these sub-blocks contains one column for each bispectrum component, the same as for compute *sna/atom*

Compute *snav/atom* evaluates a per-atom array. The columns are arranged into *ntypes* blocks, listed in order of atom type *I*. Each block contains six sub-blocks corresponding to the *xx*, *yy*, *zz*, *yz*, *xz*, and *xy* components of the virial tensor in Voigt notation. Each of these sub-blocks contains one column for each bispectrum component, the same as for compute *sna/atom*

These values can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

Restrictions:

These computes are part of the SNAP package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_style snap

Default:

The optional keyword defaults are *diagonal* = 0, *rmin0* = 0, *switchflag* = 1.

(Thompson) Thompson, Swiler, Trott, Foiles, Tucker, under review, preprint available at arXiv:1409.3880

(Bartok) Bartok, Payne, Risi, Csanyi, Phys Rev Lett, 104, 136403 (2010).

(Meremianin) Meremianin, J. Phys. A, 39, 3099 (2006).

(Varshalovich) Varshalovich, Moskalev, Khersonskii, Quantum Theory of Angular Momentum, World Scientific, Singapore (1987).

compute stress/atom command

Syntax:

```
compute ID group-ID stress/atom temp-ID keyword ...
```

- ID, group-ID are documented in compute command
- stress/atom = style name of this compute command
- temp-ID = ID of compute that calculates temperature, can be NULL if not needed
- zero or more keywords may be appended
- keyword = *ke* or *pair* or *bond* or *angle* or *dihedral* or *improper* or *kspace* or *fix* or *virial*

Examples:

```
compute 1 mobile stress/atom NULL
compute 1 mobile stress/atom myRamp
compute 1 all stress/atom NULL pair bond
```

Description:

Define a computation that computes the symmetric per-atom stress tensor for each atom in a group. The tensor for each atom has 6 components and is stored as a 6-element vector in the following order: xx, yy, zz, xy, xz, yz. See the compute pressure command if you want the stress tensor (pressure) of the entire system.

The stress tensor for atom *I* is given by the following formula, where *a* and *b* take on values x,y,z to generate the 6 components of the symmetric tensor:

$$
\begin{aligned}
S_{ab} = -\Bigg[& mv_a v_b + \frac{1}{2}\sum_{n=1}^{N_p}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b}) + \frac{1}{2}\sum_{n=1}^{N_b}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b}) + \\
& \frac{1}{3}\sum_{n=1}^{N_a}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b} + r_{3_a}F_{3_b}) + \frac{1}{4}\sum_{n=1}^{N_d}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b} + r_{3_a}F_{3_b} + r_{4_a}F_{4_b}) + \\
& \frac{1}{4}\sum_{n=1}^{N_i}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b} + r_{3_a}F_{3_b} + r_{4_a}F_{4_b}) + \mathrm{Kspace}(r_{i_a}, F_{i_b}) + \sum_{n=1}^{N_f} r_{i_a}F_{i_b} \Bigg]
\end{aligned}
$$

The first term is a kinetic energy contribution for atom *I*. See details below on how the specified *temp-ID* can affect the velocities used in this calculation. The second term is a pairwise energy contribution where *n* loops over the *Np* neighbors of atom *I*, *r1* and *r2* are the positions of the 2 atoms in the pairwise interaction, and *F1* and *F2* are the forces on the 2 atoms resulting from the pairwise interaction. The third term is a bond contribution of similar form for the *Nb* bonds which atom *I* is part of. There are similar terms for the *Na* angle, *Nd* dihedral, and *Ni* improper interactions atom *I* is part of. There is also a term for the KSpace contribution from long-range Coulombic interactions, if defined. Finally, there is a term for the *Nf* fixes that apply internal constraint forces to atom *I*. Currently, only the fix shake and fix rigid commands contribute to this term.

As the coefficients in the formula imply, a virial contribution produced by a small set of atoms (e.g. 4 atoms in a dihedral or 3 atoms in a Tersoff 3-body interaction) is assigned in equal portions to each atom in the set. E.g. 1/4 of the dihedral virial to each of the 4 atoms, or 1/3 of the fix virial due to SHAKE constraints applied to atoms in a a water molecule via the fix shake command.

If no extra keywords are listed, all of the terms in this formula are included in the per-atom stress tensor. If any extra keywords are listed, only those terms are summed to compute the tensor. The *virial* keyword means include all terms except the kinetic energy *ke*.

Note that the stress for each atom is due to its interaction with all other atoms in the simulation, not just with other atoms in the group.

Details of how LAMMPS computes the virial for individual atoms for either pairwise or manybody potentials, and including the effects of periodic boundary conditions is discussed in (Thompson). The basic idea for manybody potentials is to treat each component of the force computation between a small cluster of atoms in the same manner as in the formula above for bond, angle, dihedral, etc interactions. Namely the quantity R dot F is summed over the atoms in the interaction, with the R vectors unwrapped by periodic boundaries so that the cluster of atoms is close together. The total contribution for the cluster interaction is divided evenly among those atoms.

The dihedral_style charmm style calculates pairwise interactions between 1-4 atoms. The virial contribution of these terms is included in the pair virial, not the dihedral virial.

The KSpace contribution is calculated using the method in (Heyes) for the Ewald method and by the methodology described in (Sirk) for PPPM. The choice of KSpace solver is specified by the kspace_style pppm command. Note that for PPPM, the calcluation requires 6 extra FFTs each timestep that per-atom stress is calculated. Thus it can significantly increase the cost of the PPPM calculation if it is needed on a large fraction of the simulation timesteps.

The *temp-ID* argument can be used to affect the per-atom velocities used in the kinetic energy contribution to the total stress. If the kinetic energy is not included in the stress, than the temperature compute is not used and can be specified as NULL. If the kinetic energy is included and you wish to use atom velocities as-is, then *temp-ID* can also be specified as NULL. If desired, the specified temperature compute can be one that subtracts off a bias to leave each atom with only a thermal velocity to use in the formula above, e.g. by subtracting a background streaming velocity. See the doc pages for individual compute commands to determine which ones include a bias.

Note that as defined in the formula, per-atom stress is the negative of the per-atom pressure tensor. It is also really a stress*volume formulation, meaning the computed quantity is in units of pressure*volume. It would need to be divided by a per-atom volume to have units of stress (pressure), but an individual atom's volume is not well defined or easy to compute in a deformed solid or a liquid. See the compute voronoi/atom command for one possible way to estimate a per-atom volume.

Thus, if the diagonal components of the per-atom stress tensor are summed for all atoms in the system and the sum is divided by dV, where d = dimension and V is the volume of the system, the result should be -P, where P is the total pressure of the system.

These lines in an input script for a 3d system should yield that result. I.e. the last 2 columns of thermo output will be the same:

```
compute         peratom all stress/atom NULL
compute         p all reduce sum c_peratom[1] c_peratom[2] c_peratom[3]
variable        press equal -(c_p[1]+c_p[2]+c_p[3])/(3*vol)
thermo_style    custom step temp etotal press v_press
```

Output info:

This compute calculates a per-atom array with 6 columns, which can be accessed by indices 1-6 by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The per-atom array values will be in pressure*volume units as discussed above.

Restrictions: none

Related commands:

compute pe, compute pressure

Default: none

(Heyes) Heyes, Phys Rev B 49, 755 (1994),

(Sirk) Sirk, Moore, Brown, J Chem Phys, 138, 064505 (2013).

(Thompson) Thompson, Plimpton, Mattson, J Chem Phys, 131, 154107 (2009).

compute force/tally command

compute heat/flux/tally command

compute pe/tally command

compute stress/tally command

Syntax:

```
compute ID group-ID style group2-ID
```

- ID, group-ID are documented in compute command
- style = *force/tally* or *pe/tally* or *stress/tally*
- group2-ID = group ID of second (or same) group

Examples:

```
compute 1 lower force/tally upper
compute 1 left pe/tally right
compute 1 lower stress/tally lower
```

Description:

Define a computation that calculates properties between two groups of atoms by accumulating them from pairwise non-bonded computations. The two groups can be the same. This is similar to compute group/group only that the data is accumulated directly during the non-bonded force computation. The computes *force/tally*, *pe/tally*, *stress/tally*, and *heat/flux/tally* are primarily provided as example how to program additional, more sophisticated computes using the tally mechanism.

The pairwise contributions are computing via a callback that the compute registers with the non-bonded pairwise force computation. This limits the use to systems that have no bonds, no Kspace, and no manybody interactions. On the other hand, the computation does not have to compute forces or energies a second time and thus can be much more efficient. The callback mechanism allows to write more complex pairwise property computations.

Output info:

Compute *pe/tally* calculates a global scalar (the energy) and a per atom scalar (the contributions of the single atom to the global scalar). Compute *force/tally* calculates a global scalar (the force magnitude) and a per atom 3-element vector (force contribution from each atom). Compute *stress/tally* calculates a global scalar (average of the diagonal elements of the stress tensor) and a per atom vector (the 6 elements of stress tensor contributions from the individual atom).

Both the scalar and vector values calculated by this compute are "extensive".

Restrictions:

This compute is part of the USER-TALLY package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Not all pair styles can be evaluated in a pairwise mode as required by this compute. For example, 3-body and other many-body potentials, such as Tersoff and Stillinger-Weber cannot be used. EAM potentials only include the pair potential portion of the EAM interaction when used by this compute, not the embedding term. Also bonded or Kspace interactions do not contribute to this compute.

Related commands:

*compute group/group*_compute_group_group.html, *compute heat/flux*_compute_heat_flux.html

Default: none

compute temp command

compute temp/cuda command

compute temp/kk command

Syntax:

```
compute ID group-ID temp
```

- ID, group-ID are documented in compute command
- temp = style name of this compute command

Examples:

```
compute 1 all temp
compute myTemp mobile temp
```

Description:

Define a computation that calculates the temperature of a group of atoms. A compute of this style can be used by any command that computes a temperature, e.g. thermo_modify, fix temp/rescale, fix npt, etc.

The temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the compute_modify command if this is not the case.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the compute_modify command.

A compute of this style with the ID of "thermo_temp" is created when LAMMPS starts up, as if this command were in the input script:

```
compute thermo_temp all temp
```

See the "thermo_style" command for more details.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions: none

Related commands:

compute temp/partial, compute temp/region, compute pressure

Default: none

compute temp/asphere command

Syntax:

```
compute ID group-ID temp/asphere keyword value ...
```

- ID, group-ID are documented in compute command
- temp/asphere = style name of this compute command
- zero or more keyword/value pairs may be appended
- keyword = *bias* or *dof*

```
  bias value = bias-ID
      bias-ID = ID of a temperature compute that removes a velocity bias
    dof value = all or rotate
      all = compute temperature of translational and rotational degrees of freedom
      rotate = compute temperature of just rotational degrees of freedom
```

Examples:

```
compute 1 all temp/asphere
compute myTemp mobile temp/asphere bias tempCOM
compute myTemp mobile temp/asphere dof rotate
```

Description:

Define a computation that calculates the temperature of a group of aspherical particles, including a contribution from both their translational and rotational kinetic energy. This differs from the usual compute temp command, which assumes point particles with only translational kinetic energy.

Only finite-size particles (aspherical or spherical) can be included in the group. For 3d finite-size particles, each has 6 degrees of freedom (3 translational, 3 rotational). For 2d finite-size particles, each has 3 degrees of freedom (2 translational, 1 rotational).

NOTE: This choice for degrees of freedom (dof) assumes that all finite-size aspherical or spherical particles in your model will freely rotate, sampling all their rotational dof. It is possible to use a combination of interaction potentials and fixes that induce no torque or otherwise constrain some of all of your particles so that this is not the case. Then there are less dof and you should use the compute_modify extra command to adjust the dof accordingly.

For example, an aspherical particle with all three of its shape parameters the same is a sphere. If it does not rotate, then it should have 3 dof instead of 6 in 3d (or 2 instead of 3 in 2d). A uniaxial aspherical particle has two of its three shape parameters the same. If it does not rotate around the axis perpendicular to its circular cross section, then it should have 5 dof instead of 6 in 3d. The latter is the case for uniaxial ellipsoids in a GayBerne model since there is no induced torque around the optical axis. It will also be the case for biaxial ellipsoids when exactly two of the semiaxes have the same length and the corresponding relative well depths are equal.

The translational kinetic energy is computed the same as is described by the compute temp command. The rotational kinetic energy is computed as 1/2 I w^2, where I is the inertia tensor for the aspherical particle and w is its angular velocity, which is computed from its angular momentum.

NOTE: For 2d models, particles are treated as ellipsoids, not ellipses, meaning their moments of inertia will be the same as in 3d.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute. The formula for the components of the tensor is the same as the above formula, except that v^2 and w^2 are replaced by vx*vy and wx*wy for the xy component, and the appropriate elements of the inertia tensor are used. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the compute_modify command if this is not the case.

This compute subtracts out translational degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

The keyword/value option pairs are used in the following ways.

For the *bias* keyword, *bias-ID* refers to the ID of a temperature compute that removes a "bias" velocity from each atom. This allows compute temp/sphere to compute its thermal temperature after the translational kinetic energy components have been altered in a prescribed way, e.g. to remove a flow velocity profile. Thermostats that use this compute will work with this bias term. See the doc pages for individual computes that calculate a temperature and the doc pages for fixes that perform thermostatting for more details.

For the *dof* keyword, a setting of *all* calculates a temperature that includes both translational and rotational degrees of freedom. A setting of *rotate* calculates a temperature that includes only rotational degrees of freedom.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions:

This compute is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This compute requires that atoms store angular momementum and a quaternion as defined by the atom_style ellipsoid command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

Related commands:

compute temp

Default: none

compute temp/body command

Syntax:

```
compute ID group-ID temp/body keyword value ...
```

- ID, group-ID are documented in compute command
- temp/body = style name of this compute command
- zero or more keyword/value pairs may be appended
- keyword = *bias* or *dof*

```
  bias value = bias-ID
      bias-ID = ID of a temperature compute that removes a velocity bias
    dof value = all or rotate
      all = compute temperature of translational and rotational degrees of freedom
      rotate = compute temperature of just rotational degrees of freedom
```

Examples:

```
compute 1 all temp/body
compute myTemp mobile temp/body bias tempCOM
compute myTemp mobile temp/body dof rotate
```

Description:

Define a computation that calculates the temperature of a group of body particles, including a contribution from both their translational and rotational kinetic energy. This differs from the usual compute temp command, which assumes point particles with only translational kinetic energy.

Only body particles can be included in the group. For 3d particles, each has 6 degrees of freedom (3 translational, 3 rotational). For 2d body particles, each has 3 degrees of freedom (2 translational, 1 rotational).

NOTE: This choice for degrees of freedom (dof) assumes that all body particles in your model will freely rotate, sampling all their rotational dof. It is possible to use a combination of interaction potentials and fixes that induce no torque or otherwise constrain some of all of your particles so that this is not the case. Then there are less dof and you should use the compute_modify extra command to adjust the dof accordingly.

The translational kinetic energy is computed the same as is described by the compute temp command. The rotational kinetic energy is computed as 1/2 I w^2, where I is the inertia tensor for the aspherical particle and w is its angular velocity, which is computed from its angular momentum.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute. The formula for the components of the tensor is the same as the above formula, except that v^2 and w^2 are replaced by vx*vy and wx*wy for the xy component, and the appropriate elements of the inertia tensor are used. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the compute_modify command if this is not the case.

This compute subtracts out translational degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the

compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

The keyword/value option pairs are used in the following ways.

For the *bias* keyword, *bias-ID* refers to the ID of a temperature compute that removes a "bias" velocity from each atom. This allows compute temp/sphere to compute its thermal temperature after the translational kinetic energy components have been altered in a prescribed way, e.g. to remove a flow velocity profile. Thermostats that use this compute will work with this bias term. See the doc pages for individual computes that calculate a temperature and the doc pages for fixes that perform thermostatting for more details.

For the *dof* keyword, a setting of *all* calculates a temperature that includes both translational and rotational degrees of freedom. A setting of *rotate* calculates a temperature that includes only rotational degrees of freedom.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions:

This compute is part of the BODY package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This compute requires that atoms store angular momementum and a quaternion as defined by the atom_style body command.

Related commands:

compute temp

Default: none

compute temp/chunk command

Syntax:

```
compute ID group-ID temp/chunk chunkID value1 value2 ... keyword value ...
```

- ID, group-ID are documented in compute command
- temp/chunk = style name of this compute command
- chunkID = ID of compute chunk/atom command
- zero or more values can be listed as value1,value2,etc
- value = *temp* or *kecom* or *internal*

```
temp = temperature of each chunk
kecom = kinetic energy of each chunk based on velocity of center of mass
internal = internal kinetic energy of each chunk
```

- zero or more keyword/value pairs may be appended
- keyword = *com* or *bias* or *adof* or *cdof*

```
com value = yes or no
    yes = subtract center-of-mass velocity from each chunk before calculating temperature
    no = do not subtract center-of-mass velocity
  bias value = bias-ID
    bias-ID = ID of a temperature compute that removes a velocity bias
  adof value = dof_per_atom
    dof_per_atom = define this many degrees-of-freedom per atom
  cdof value = dof_per_chunk
    dof_per_chunk = define this many degrees-of-freedom per chunk
```

Examples:

```
compute 1 fluid temp/chunk molchunk
compute 1 fluid temp/chunk molchunk temp internal
compute 1 fluid temp/chunk molchunk bias tpartial adof 2.0
```

Description:

Define a computation that calculates the temperature of a group of atoms that are also in chunks, after optionally subtracting out the center-of-mass velocity of each chunk. By specifying optional values, it can also calulate the per-chunk temperature or energies of the multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a compute chunk/atom command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the compute chunk/atom doc page and "Section_howto 23 for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

The temperature is calculated by the formula KE = DOF/2 k T, where KE = total kinetic energy of all atoms assigned to chunks (sum of 1/2 m v^2), DOF = the total number of degrees of freedom for those atoms, k = Boltzmann constant, and T = temperature.

The DOF is calculated as N*adof + Nchunk*cdof, where N = number of atoms contributing to the KE, adof = degrees of freedom per atom, and cdof = degrees of freedom per chunk. By default adof = 2 or 3 = dimensionality of system, as set via the dimension command, and cdof = 0.0. This gives the usual formula for temperature.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

Note that the number of atoms contributing to the temperature is calculated each time the temperature is evaluated since it is assumed the atoms may be dynamically assigned to chunks. Thus there is no need to use the *dynamic* option of the compute_modify command for this compute style.

If any optional values are specified, then per-chunk quantities are also calculated and stored in a global array, as described below.

The *temp* value calculates the temperature for each chunk by the formula KE = DOF/2 k T, where KE = total kinetic energy of the chunk of atoms (sum of 1/2 m v^2), DOF = the total number of degrees of freedom for all atoms in the chunk, k = Boltzmann constant, and T = temperature.

The DOF in this case is calculated as N*adof + cdof, where N = number of atoms in the chunk, adof = degrees of freedom per atom, and cdof = degrees of freedom per chunk. By default adof = 2 or 3 = dimensionality of system, as set via the dimension command, and cdof = 0.0. This gives the usual formula for temperature.

The *kecom* value calculates the kinetic energy of each chunk as if all its atoms were moving with the velocity of the center-of-mass of the chunk.

The *internal* value calculates the internal kinetic energy of each chunk. The interal KE is summed over the atoms in the chunk using an internal "thermal" velocity for each atom, which is its velocity minus the center-of-mass velocity of the chunk.

Note that currently the global and per-chunk temperatures calculated by this compute only include translational degrees of freedom for each atom. No rotational degrees of freedom are included for finite-size particles. Also no degrees of freedom are subtracted for any velocity bias or constraints that are applied, such as compute temp/partial, or fix shake or fix rigid. This is because those degrees of freedom (e.g. a constrained bond) could apply to sets of atoms that are both included and excluded from a specific chunk, and hence the concept is somewhat ill-defined. In some cases, you can use the *adof* and *cdof* keywords to adjust the calculated degress of freedom appropriately, as explained below.

Note that the per-chunk temperature calulated by this compute and the fix ave/chunk temp command can be different. This compute calculates the temperature for each chunk for a single snapshot. Fix ave/chunk can do that but can also time average those values over many snapshots, or it can compute a temperature as if the atoms in the chunk on different timesteps were collected together as one set of atoms to calculate their temperature. This compute allows the center-of-mass velocity of each chunk to be subtracted before calculating the temperature; fix ave/chunk does not.

NOTE: Only atoms in the specified group contribute to the calculations performed by this compute. The compute chunk/atom command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

The simplest way to output the per-chunk results of the compute temp/chunk calculation to a file is to use the fix ave/time command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all temp/chunk cc1 temp
fix 1 all ave/time 100 1 100 c_myChunk file tmp.out mode vector
```

The keyword/value option pairs are used in the following ways.

The *com* keyword can be used with a value of *yes* to subtract the velocity of the center-of-mass for each chunk from the velocity of the atoms in that chunk, before calculating either the global or per-chunk temperature. This can be useful if the atoms are streaming or otherwise moving collectively, and you wish to calculate only the thermal temperature.

For the *bias* keyword, *bias-ID* refers to the ID of a temperature compute that removes a "bias" velocity from each atom. This also allows calculation of the global or per-chunk temperature using only the thermal temperature of atoms in each chunk after the translational kinetic energy components have been altered in a prescribed way, e.g. to remove a velocity profile. It also applies to the calculation of the other per-chunk values, such as *kecom* or *internal*, which involve the center-of-mass velocity of each chunk, which is calculated after the velocity bias is removed from each atom. Note that the temperature compute will apply its bias globally to the entire system, not on a per-chunk basis.

The *adof* and *cdof* keywords define the values used in the degree of freedom (DOF) formulas used for the global or per-chunk temperature, as described above. They can be used to calculate a more appropriate temperature for some kinds of chunks. Here are 3 examples:

If spatially binned chunks contain some number of water molecules and fix shake is used to make each molecule rigid, then you could calculate a temperature with 6 degrees of freedom (DOF) (3 translational, 3 rotational) per molecule by setting *adof* to 2.0.

If compute temp/partial is used with the *bias* keyword to only allow the x component of velocity to contribute to the temperature, then *adof* = 1.0 would be appropriate.

If each chunk consists of a large molecule, with some number of its bonds constrained by fix shake or the entire molecule by fix rigid/small, *adof* = 0.0 and *cdof* could be set to the remaining degrees of freedom for the entire molecule (entire chunk in this case), e.g. 6 for 3d, or 3 for 2d, for a rigid molecule.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

This compute also optionally calculates a global array, if one or more of the optional values are specified. The number of rows in the array = the number of chunks *Nchunk* as calculated by the specified compute chunk/atom command. The number of columns is the number of specifed values (1 or more). These values can be accessed by any command that uses global array values from a compute as input. Again, see Section_howto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive". The array values are "intensive".

The scalar value will be in temperature units. The vector values will be in energy units. The array values will be in temperature units for the *temp* value, and in energy units for the *kecom* and *internal* values.

Restrictions:

The *com* and *bias* keywords cannot be used together.

Related commands:

compute temp, fix ave/chunk temp

Default:

The option defaults are com no, no bias, adof = dimensionality of the system (2 or 3), and cdof = 0.0.

compute temp/com command

Syntax:

```
compute ID group-ID temp/com
```

- ID, group-ID are documented in compute command
- temp/com = style name of this compute command

Examples:

```
compute 1 all temp/com
compute myTemp mobile temp/com
```

Description:

Define a computation that calculates the temperature of a group of atoms, after subtracting out the center-of-mass velocity of the group. This is useful if the group is expected to have a non-zero net velocity for some reason. A compute of this style can be used by any command that computes a temperature, e.g. thermo_modify, fix temp/rescale, fix npt, etc.

After the center-of-mass velocity has been subtracted from each atom, the temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the compute_modify command if this is not the case.

The removal of the center-of-mass velocity by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include fix nvt, fix temp/rescale, fix temp/berendsen, and fix langevin.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions: none

Related commands:

compute temp

Default: none

compute temp/cs command

Syntax:

```
compute ID group-ID temp/cs group1 group2
```

- ID, group-ID are documented in compute command
- temp/cs = style name of this compute command
- group1 = group-ID of either cores or shells
- group2 = group-ID of either shells or cores

Examples:

```
compute oxygen_c-s all temp/cs O_core O_shell
compute core_shells all temp/cs cores shells
```

Description:

Define a computation that calculates the temperature of a system based on the center-of-mass velocity of atom pairs that are bonded to each other. This compute is designed to be used with the adiabatic core/shell model of (Mitchell and Finchham). See Section_howto 25 of the manual for an overview of the model as implemented in LAMMPS. Specifically, this compute enables correct temperature calculation and thermostatting of core/shell pairs where it is desirable for the internal degrees of freedom of the core/shell pairs to not be influenced by a thermostat. A compute of this style can be used by any command that computes a temperature via fix_modify e.g. fix temp/rescale, fix npt, etc.

Note that this compute does not require all ions to be polarized, hence defined as core/shell pairs. One can mix core/shell pairs and ions without a satellite particle if desired. The compute will consider the non-polarized ions according to the physical system.

For this compute, core and shell particles are specified by two respective group IDs, which can be defined using the group command. The number of atoms in the two groups must be the same and there should be one bond defined between a pair of atoms in the two groups. Non-polarized ions which might also be included in the treated system should not be included into either of these groups, they are taken into account by the *group-ID* (2nd argument) of the compute.

The temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature. Note that the velocity of each core or shell atom used in the KE calculation is the velocity of the center-of-mass (COM) of the core/shell pair the atom is part of.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz. In contrast to the temperature, the velocity of each core or shell atom is taken individually.

The change this fix makes to core/shell atom velocities is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. This "bias" is the velocity of the atom relative to the COM velocity of the core/shell pair. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining COM velocity will be performed, and the bias will

be added back in. This means the thermostating will effectively be performed on the core/shell pairs, instead of on the individual core and shell atoms. Thermostatting fixes that work in this way include fix nvt, fix temp/rescale, fix temp/berendsen, and fix langevin.

The internal energy of core/shell pairs can be calculated by the compute temp/chunk command, if chunks are defined as core/shell pairs. See Section_howto 25 for more discussion on how to do this.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions:

The number of core/shell pairs contributing to the temperature is assumed to be constant for the duration of the run. No fixes should be used which generate new molecules or atoms during a simulation.

Related commands:

compute temp, compute temp/chunk

Default: none

(Mitchell and Finchham) Mitchell, Finchham, J Phys Condensed Matter, 5, 1031-1038 (1993).

compute temp/deform command

Syntax:

```
compute ID group-ID temp/deform
```

- ID, group-ID are documented in compute command
- temp/deform = style name of this compute command

Examples:

```
compute myTemp all temp/deform
```

Description:

Define a computation that calculates the temperature of a group of atoms, after subtracting out a streaming velocity induced by the simulation box changing size and/or shape, for example in a non-equilibrium MD (NEMD) simulation. The size/shape change is induced by use of the fix deform command. A compute of this style is created by the fix nvt/sllod command to compute the thermal temperature of atoms for thermostatting purposes. A compute of this style can also be used by any command that computes a temperature, e.g. thermo_modify, fix temp/rescale, fix npt, etc.

The deformation fix changes the box size and/or shape over time, so each atom in the simulation box can be thought of as having a "streaming" velocity. For example, if the box is being sheared in x, relative to y, then atoms at the bottom of the box (low y) have a small x velocity, while atoms at the top of the box (hi y) have a large x velocity. This position-dependent streaming velocity is subtracted from each atom's actual velocity to yield a thermal velocity which is used to compute the temperature.

NOTE: Fix deform has an option for remapping either atom coordinates or velocities to the changing simulation box. When using this compute in conjunction with a deforming box, fix deform should NOT remap atom positions, but rather should let atoms respond to the changing box by adjusting their own velocities (or let fix deform remap the atom velocities, see it's remap option). If fix deform does remap atom positions, then they appear to move with the box but their velocity is not changed, and thus they do NOT have the streaming velocity assumed by this compute. LAMMPS will warn you if fix deform is defined and its remap setting is not consistent with this compute.

After the streaming velocity has been subtracted from each atom, the temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature. Note that v in the kinetic energy formula is the atom's thermal velocity.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the compute_modify command if this is not the case.

The removal of the box deformation velocity component by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include fix nvt, fix temp/rescale, fix temp/berendsen, and fix langevin.

NOTE: The temperature calculated by this compute is only accurate if the atoms are indeed moving with a stream velocity profile that matches the box deformation. If not, then the compute will subtract off an incorrect stream velocity, yielding a bogus thermal temperature. You should NOT assume that your atoms are streaming at the same rate the box is deforming. Rather, you should monitor their velocity profile, e.g. via the fix ave/spatial command. And you can compare the results of this compute to compute temp/profile, which actually calculates the stream profile before subtracting it. If the two computes do not give roughly the same temperature, then your atoms are not streaming consistent with the box deformation. See the fix deform command for more details on ways to get atoms to stream consistently with the box deformation.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions: none

Related commands:

compute temp/ramp, compute temp/profile, fix deform, fix nvt/sllod

Default: none

compute temp/deform/eff command

Syntax:

```
compute ID group-ID temp/deform/eff
```

- ID, group-ID are documented in compute command
- temp/deform/eff = style name of this compute command

Examples:

```
compute myTemp all temp/deform/eff
```

Description:

Define a computation that calculates the temperature of a group of nuclei and electrons in the electron force field model, after subtracting out a streaming velocity induced by the simulation box changing size and/or shape, for example in a non-equilibrium MD (NEMD) simulation. The size/shape change is induced by use of the fix deform/eff command. A compute of this style is created by the fix nvt/sllod/eff command to compute the thermal temperature of atoms for thermostatting purposes. A compute of this style can also be used by any command that computes a temperature, e.g. thermo_modify, fix npt/eff, etc.

The calculation performed by this compute is exactly like that described by the compute temp/deform command, except that the formula for the temperature includes the radial electron velocity contributions, as discussed by the compute temp/eff command. Note that only the translational degrees of freedom for each nuclei or electron are affected by the streaming velocity adjustment. The radial velocity component of the electrons is not affected.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions:

This compute is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

compute temp/ramp, fix deform/eff, fix nvt/sllod/eff

Default: none

compute temp/drude command

Syntax:

```
compute ID group-ID temp/drude
```

- ID, group-ID are documented in compute command
- temp/drude = style name of this compute command

Examples:

```
compute TDRUDE all temp/drude
```

Description:

Define a computation that calculates the temperatures of core-Drude pairs. This compute is designed to be used with the thermalized Drude oscillator model. Polarizable models in LAMMPS are described in this Section.

Drude oscillators consist of a core particle and a Drude particle connected by a harmonic bond, and the relative motion of these Drude oscillators is usually maintained cold by a specific thermostat that acts on the relative motion of the core-Drude particle pairs. Therefore, because LAMMPS considers Drude particles as normal atoms in its default temperature compute (compute temp command), the reduced temperature of the core-Drude particle pairs is not calculated correctly.

By contrast, this compute calculates the temperature of the cores using center-of-mass velocities of the core-Drude pairs, and the reduced temperature of the Drude particles using the relative velocities of the Drude particles with respect to their cores. Non-polarizable atoms are considered as cores. Their velocities contribute to the temperature of the cores.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6, which can be accessed by indices 1-6, whose components are

1. temperature of the centers of mass (temperature units)
2. temperature of the dipoles (temperature units)
3. number of degrees of freedom of the centers of mass
4. number of degrees of freedom of the dipoles
5. kinetic energy of the centers of mass (energy units)
6. kinetic energy of the dipoles (energy units)

These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

Both the scalar value and the first two values of the vector calculated by this compute are "intensive". The other 4 vector values are "extensive".

Restrictions:

The number of degrees of freedom contributing to the temperature is assumed to be constant for the duration of the run unless the *fix_modify* command sets the option *dynamic yes*.

Related commands:

fix drude, fix langevin/drude, fix drude/transform, pair_style thole, compute temp

Default: none

compute temp/eff command

Syntax:

```
compute ID group-ID temp/eff
```

- ID, group-ID are documented in compute command
- temp/eff = style name of this compute command

Examples:

```
compute 1 all temp/eff
compute myTemp mobile temp/eff
```

Description:

Define a computation that calculates the temperature of a group of nuclei and electrons in the electron force field model. A compute of this style can be used by commands that compute a temperature, e.g. thermo_modify, fix npt/eff, etc.

The temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2 for nuclei and sum of 1/2 (m v^2 + 3/4 m s^2) for electrons, where s includes the radial electron velocity contributions), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms (only total number of nuclei in the eFF (see the pair_eff command) in the group, k = Boltzmann constant, and T = temperature. This expression is summed over all nuclear and electronic degrees of freedom, essentially by setting the kinetic contribution to the heat capacity to 3/2k (where only nuclei contribute). This subtlety is valid for temperatures well below the Fermi temperature, which for densities two to five times the density of liquid H2 ranges from 86,000 to 170,000 K.

NOTE: For eFF models, in order to override the default temperature reported by LAMMPS in the thermodynamic quantities reported via the thermo command, the user should apply a thermo_modify command, as shown in the following example:

```
compute         effTemp all temp/eff
thermo_style    custom step etotal pe ke temp press
thermo_modify   temp effTemp
```

A 6-component kinetic energy tensor is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx * vy for the xy component, etc. For the eFF, again, the radial electronic velocities are also considered.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the compute_modify command if this is not the case.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

Output info:

The scalar value calculated by this compute is "intensive", meaning it is independent of the number of atoms in the simulation. The vector values are "extensive", meaning they scale with the number of atoms in the simulation.

Restrictions:

This compute is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

compute temp/partial, compute temp/region, compute pressure

Default: none

compute temp/partial command

compute temp/partial/cuda command

Syntax:

```
compute ID group-ID temp/partial xflag yflag zflag
```

- ID, group-ID are documented in compute command
- temp/partial = style name of this compute command
- xflag,yflag,zflag = 0/1 for whether to exclude/include this dimension

Examples:

```
compute newT flow temp/partial 1 1 0
```

Description:

Define a computation that calculates the temperature of a group of atoms, after excluding one or more velocity components. A compute of this style can be used by any command that computes a temperature, e.g. thermo_modify, fix temp/rescale, fix npt, etc.

The temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature. The calculation of KE excludes the x, y, or z dimensions if xflag, yflag, or zflag = 0. The dim parameter is adjusted to give the correct number of degrees of freedom.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the calculation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the compute_modify command if this is not the case.

The removal of velocity components by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include fix nvt, fix temp/rescale, fix temp/berendsen, and fix langevin.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions: none

Related commands:

compute temp, compute temp/region, compute pressure

Default: none

compute temp/profile command

Syntax:

```
compute ID group-ID temp/profile xflag yflag zflag binstyle args
```

- ID, group-ID are documented in compute command
- temp/profile = style name of this compute command
- xflag,yflag,zflag = 0/1 for whether to exclude/include this dimension
- binstyle = *x* or *y* or *z* or *xy* or *yz* or *xz* or *xyz*

```
  x arg = Nx
    y arg = Ny
    z arg = Nz
    xy args = Nx Ny
    yz args = Ny Nz
    xz args = Nx Nz
    xyz args = Nx Ny Nz
      Nx,Ny,Nz = number of velocity bins in x,y,z dimensions
```

- zero or more keyword/value pairs may be appended
- keyword = *out*

```
  out value = tensor or bin
```

Examples:

```
compute myTemp flow temp/profile 1 1 1 x 10
compute myTemp flow temp/profile 1 1 1 x 10 out bin
compute myTemp flow temp/profile 0 1 1 xyz 20 20 20
```

Description:

Define a computation that calculates the temperature of a group of atoms, after subtracting out a spatially-averaged center-of-mass velocity field, before computing the kinetic energy. This can be useful for thermostatting a collection of atoms undergoing a complex flow, e.g. via a profile-unbiased thermostat (PUT) as described in (Evans). A compute of this style can be used by any command that computes a temperature, e.g. thermo_modify, fix temp/rescale, fix npt, etc.

The *xflag*, *yflag*, *zflag* settings determine which components of average velocity are subtracted out.

The *binstyle* setting and its *Nx*, *Ny*, *Nz* arguments determine how bins are setup to perform spatial averaging. "Bins" can be 1d slabs, 2d pencils, or 3d bricks depending on which *binstyle* is used. The simulation box is partitioned conceptually into *Nx* by *Ny* by *Nz* bins. Depending on the *binstyle*, you may only specify one or two of these values; the others are effectively set to 1 (no binning in that dimension). For non-orthogonal (triclinic) simulation boxes, the bins are "tilted" slabs or pencils or bricks that are parallel to the tilted faces of the box. See the region prism command for a discussion of the geometry of tilted boxes in LAMMPS.

When a temperature is computed, the center-of-mass velocity for the set of atoms that are both in the compute group and in the same spatial bin is calculated. This bias velocity is then subtracted from the velocities of individual atoms in the bin to yield a thermal velocity for each atom. Note that if there is only one atom in the bin, its thermal velocity will thus be 0.0.

After the spatially-averaged velocity field has been subtracted from each atom, the temperature is calculated by the formula KE = (dim/2 N - dim*Nx*Ny*Nz) k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature. The dim*Nx*Ny*Nz term are degrees of freedom subtracted to adjust for the removal of the center-of-mass velocity in each of Nx*Ny*Nz bins, as discussed in the (Evans) paper.

If the *out* keyword is used with a *tensor* value, which is the default, a kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

If the *out* keyword is used with a *bin* value, the count of atoms and computed temperature for each bin are stored for output, as an array of values, as described below. The temperature of each bin is calculated as described above, where the bias velocity is subtracted and only the remaining thermal velocity of atoms in the bin contributes to the temperature. See the note below for how the temperature is normalized by the degrees-of-freedom of atoms in the bin.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the compute_modify command if this is not the case.

The removal of the spatially-averaged velocity field by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include fix nvt, fix temp/rescale, fix temp/berendsen, and fix langevin.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the compute_modify command.

NOTE: When using the *out* keyword with a value of *bin*, the calculated temperature for each bin does not include the degrees-of-freedom adjustment described in the preceeding paragraph, for fixes that constrain molecular motion. It does include the adjustment due to the *extra* option, which is applied to each bin.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting. Using this compute in conjunction with a thermostatting fix, as explained there, will effectively implement a profile-unbiased thermostat (PUT), as described in (Evans).

Output info:

This compute calculates a global scalar (the temperature). Depending on the setting of the *out* keyword, it also calculates a global vector or array. For *out* = *tensor*, it calculates a vector of length 6 (KE tensor), which can be accessed by indices 1-6. For *out* = *bin* it calculates a global array which has 2 columns and N rows, where N is the number of bins. The first column contains the number of atoms in that bin. The second contains the temperature of that bin, calculated as described above. The ordering of rows in the array is as follows. Bins in x vary fastest, then y, then z. Thus for a 10x10x10 3d array of bins, there will be 1000 rows. The bin with indices ix,iy,iz = 2,3,4 would map to row M = (iz-1)*10*10 + (iy-1)*10 + ix = 322, where the rows are numbered from 1 to 1000 and the bin indices are numbered from 1 to 10 in each dimension.

These values can be used by any command that uses global scalar or vector or array values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive". The array values are "intensive".

The scalar value will be in temperature units. The vector values will be in energy units. The first column of array values are counts; the values in the second column will be in temperature units.

Restrictions:

You should not use too large a velocity-binning grid, especially in 3d. In the current implementation, the binned velocity averages are summed across all processors, so this will be inefficient if the grid is too large, and the operation is performed every timestep, as it will be for most thermostats.

Related commands:

compute temp, compute temp/ramp, compute temp/deform, compute pressure

Default:

The option default is out = tensor.

(Evans) Evans and Morriss, Phys Rev Lett, 56, 2172-2175 (1986).

compute temp/ramp command

Syntax:

```
compute ID group-ID temp/ramp vdim vlo vhi dim clo chi keyword value ...
```

- ID, group-ID are documented in compute command
- temp/ramp = style name of this compute command
- vdim = *vx* or *vy* or *vz*
- vlo,vhi = subtract velocities between vlo and vhi (velocity units)
- dim = *x* or *y* or *z*
- clo,chi = lower and upper bound of domain to subtract from (distance units)
- zero or more keyword/value pairs may be appended
- keyword = *units*

```
units value = lattice or box
```

Examples:

```
compute 2nd middle temp/ramp vx 0 8 y 2 12 units lattice
```

Description:

Define a computation that calculates the temperature of a group of atoms, after subtracting out an ramped velocity profile before computing the kinetic energy. A compute of this style can be used by any command that computes a temperature, e.g. thermo_modify, fix temp/rescale, fix npt, etc.

The meaning of the arguments for this command which define the velocity ramp are the same as for the velocity ramp command which was presumably used to impose the velocity.

After the ramp velocity has been subtracted from the specified dimension for each atom, the temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature.

The *units* keyword determines the meaning of the distance units used for coordinates (c1,c2) and velocities (vlo,vhi). A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings; e.g. velocity = lattice spacings / tau. The lattice command must have been previously used to define the lattice spacing.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the compute_modify command if this is not the case.

The removal of the ramped velocity component by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs

thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include fix nvt, fix temp/rescale, fix temp/berendsen, and fix langevin.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions: none

Related commands:

compute temp, compute temp/profie, compute temp/deform, compute pressure

Default:

The option default is units = lattice.

compute temp/region command

Syntax:

```
compute ID group-ID temp/region region-ID
```

- ID, group-ID are documented in compute command
- temp/region = style name of this compute command
- region-ID = ID of region to use for choosing atoms

Examples:

```
compute mine flow temp/region boundary
```

Description:

Define a computation that calculates the temperature of a group of atoms in a geometric region. This can be useful for thermostatting one portion of the simulation box. E.g. a McDLT simulation where one side is cooled, and the other side is heated. A compute of this style can be used by any command that computes a temperature, e.g. thermo_modify, fix temp/rescale, etc.

Note that a *region*-style temperature can be used to thermostat with fix temp/rescale or fix langevin, but should probably not be used with Nose/Hoover style fixes (fix nvt, fix npt, or fix nph), if the degrees-of-freedom included in the computed T varies with time.

The temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in both the group and region, k = Boltzmann constant, and T = temperature.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is calculated each time the temperature is evaluated since it is assumed atoms can enter/leave the region. Thus there is no need to use the *dynamic* option of the compute_modify command for this compute style.

The removal of atoms outside the region by this fix is essentially computing the temperature after a "bias" has been removed, which in this case is the velocity of any atoms outside the region. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include fix nvt, fix temp/rescale, fix temp/berendsen, and fix langevin. This means that when this compute is used to calculate the temperature for any of the thermostatting fixes via the fix modify temp command, the thermostat will operate only on atoms that are currently in the geometric region.

Unlike other compute styles that calculate temperature, this compute does not subtract out degrees-of-freedom due to fixes that constrain motion, such as fix shake and fix rigid. This is because those degrees of freedom (e.g. a constrained bond) could apply to sets of atoms that straddle the region boundary, and hence the concept is somewhat ill-defined. If needed the number of subtracted degrees-of-freedom can be set explicitly using the *extra*

option of the compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions: none

Related commands:

compute temp, compute pressure

Default: none

compute temp/region/eff command

Syntax:

```
compute ID group-ID temp/region/eff region-ID
```

- ID, group-ID are documented in compute command
- temp/region/eff = style name of this compute command
- region-ID = ID of region to use for choosing atoms

Examples:

```
compute mine flow temp/region/eff boundary
```

Description:

Define a computation that calculates the temperature of a group of nuclei and electrons in the electron force field model, within a geometric region using the electron force field. A compute of this style can be used by commands that compute a temperature, e.g. thermo_modify.

The operation of this compute is exactly like that described by the compute temp/region command, except that the formula for the temperature itself includes the radial electron velocity contributions, as discussed by the compute temp/eff command.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions:

This compute is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

compute temp/region, compute temp/eff, compute pressure

Default: none

compute temp/rotate command

Syntax:

```
compute ID group-ID temp/rotate
```

- ID, group-ID are documented in compute command
- temp/rotate = style name of this compute command

Examples:

```
compute Tbead bead temp/rotate
```

Description:

Define a computation that calculates the temperature of a group of atoms, after subtracting out the center-of-mass velocity and angular velocity of the group. This is useful if the group is expected to have a non-zero net velocity and/or global rotation motion for some reason. A compute of this style can be used by any command that computes a temperature, e.g. thermo_modify, fix temp/rescale, fix npt, etc.

After the center-of-mass velocity and angular velocity has been subtracted from each atom, the temperature is calculated by the formula KE = dim/2 N k T, where KE = total kinetic energy of the group of atoms (sum of 1/2 m v^2), dim = 2 or 3 = dimensionality of the simulation, N = number of atoms in the group, k = Boltzmann constant, and T = temperature.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute for use in the computation of a pressure tensor. The formula for the components of the tensor is the same as the above formula, except that v^2 is replaced by vx*vy for the xy component, etc. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the compute_modify command if this is not the case.

The removal of the center-of-mass velocity and angular velocity by this fix is essentially computing the temperature after a "bias" has been removed from the velocity of the atoms. If this compute is used with a fix command that performs thermostatting then this bias will be subtracted from each atom, thermostatting of the remaining thermal velocity will be performed, and the bias will be added back in. Thermostatting fixes that work in this way include fix nvt, fix temp/rescale, fix temp/berendsen, and fix langevin.

This compute subtracts out degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions:

This compute is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

compute temp

Default: none

compute temp/sphere command

Syntax:

```
compute ID group-ID temp/sphere keyword value ...
```

- ID, group-ID are documented in compute command
- temp/sphere = style name of this compute command
- zero or more keyword/value pairs may be appended
- keyword = *bias* or *dof*

```
  bias value = bias-ID
      bias-ID = ID of a temperature compute that removes a velocity bias
    dof value = all or rotate
      all = compute temperature of translational and rotational degrees of freedom
      rotate = compute temperature of just rotational degrees of freedom
```

Examples:

```
compute 1 all temp/sphere
compute myTemp mobile temp/sphere bias tempCOM
compute myTemp mobile temp/sphere dof rotate
```

Description:

Define a computation that calculates the temperature of a group of spherical particles, including a contribution from both their translational and rotational kinetic energy. This differs from the usual compute temp command, which assumes point particles with only translational kinetic energy.

Both point and finite-size particles can be included in the group. Point particles do not rotate, so they have only 3 translational degrees of freedom. For 3d spherical particles, each has 6 degrees of freedom (3 translational, 3 rotational). For 2d spherical particles, each has 3 degrees of freedom (2 translational, 1 rotational).

NOTE: This choice for degrees of freedom (dof) assumes that all finite-size spherical particles in your model will freely rotate, sampling all their rotational dof. It is possible to use a combination of interaction potentials and fixes that induce no torque or otherwise constrain some of all of your particles so that this is not the case. Then there are less dof and you should use the compute_modify extra command to adjust the dof accordingly.

The translational kinetic energy is computed the same as is described by the compute temp command. The rotational kinetic energy is computed as 1/2 I w^2, where I is the moment of inertia for a sphere and w is the particle's angular velocity.

NOTE: For 2d models, particles are treated as spheres, not disks, meaning their moment of inertia will be the same as in 3d.

A kinetic energy tensor, stored as a 6-element vector, is also calculated by this compute. The formula for the components of the tensor is the same as the above formulas, except that v^2 and w^2 are replaced by vx*vy and wx*wy for the xy component. The 6 components of the vector are ordered xx, yy, zz, xy, xz, yz.

The number of atoms contributing to the temperature is assumed to be constant for the duration of the run; use the *dynamic* option of the compute_modify command if this is not the case.

This compute subtracts out translational degrees-of-freedom due to fixes that constrain molecular motion, such as fix shake and fix rigid. This means the temperature of groups of atoms that include these constraints will be computed correctly. If needed, the subtracted degrees-of-freedom can be altered using the *extra* option of the compute_modify command.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

The keyword/value option pairs are used in the following ways.

For the *bias* keyword, *bias-ID* refers to the ID of a temperature compute that removes a "bias" velocity from each atom. This allows compute temp/sphere to compute its thermal temperature after the translational kinetic energy components have been altered in a prescribed way, e.g. to remove a flow velocity profile. Thermostats that use this compute will work with this bias term. See the doc pages for individual computes that calculate a temperature and the doc pages for fixes that perform thermostatting for more details.

For the *dof* keyword, a setting of *all* calculates a temperature that includes both translational and rotational degrees of freedom. A setting of *rotate* calculates a temperature that includes only rotational degrees of freedom.

Output info:

This compute calculates a global scalar (the temperature) and a global vector of length 6 (KE tensor), which can be accessed by indices 1-6. These values can be used by any command that uses global scalar or vector values from a compute as input. See this section for an overview of LAMMPS output options.

The scalar value calculated by this compute is "intensive". The vector values are "extensive".

The scalar value will be in temperature units. The vector values will be in energy units.

Restrictions:

This fix requires that atoms store torque and angular velocity (omega) and a radius as defined by the atom_style sphere command.

All particles in the group must be finite-size spheres, or point particles with radius = 0.0.

Related commands:

compute temp, compute temp/asphere

Default:

The option defaults are no bias and dof = all.

compute ti command

Syntax:

```
compute ID group ti keyword args ...
```

- ID, group-ID are documented in compute command
- ti = style name of this compute command
- one or more attribute/arg pairs may be appended
- keyword = pair style (lj/cut, gauss, born, etc) or *tail* or *kspace*

```
pair style args = atype v_name1 v_name2
  atype = atom type (see asterisk form below)
  v_name1 = variable with name1 that is energy scale factor and function of lambda
  v_name2 = variable with name2 that is derivative of v_name1 with respect to lambda
tail args = atype v_name1 v_name2
  atype = atom type (see asterisk form below)
  v_name1 = variable with name1 that is energy tail correction scale factor and function of
  v_name2 = variable with name2 that is derivative of v_name1 with respect to lambda
kspace args = atype v_name1 v_name2
  atype = atom type (see asterisk form below)
  v_name1 = variable with name1 that is K-Space scale factor and function of lambda
  v_name2 = variable with name2 that is derivative of v_name1 with respect to lambda
```

Examples:

```
compute 1 all ti lj/cut 1 v_lj v_dlj coul/long 2 v_c v_dc kspace 1 v_ks v_dks
compute 1 all ti lj/cut 1*3 v_lj v_dlj coul/long * v_c v_dc kspace * v_ks v_dks
```

Description:

Define a computation that calculates the derivative of the interaction potential with respect to *lambda*, the coupling parameter used in a thermodynamic integration. This derivative can be used to infer a free energy difference resulting from an alchemical simulation, as described in Eike.

Typically this compute will be used in conjunction with the fix adapt command which can perform alchemical transformations by adusting the strength of an interaction potential as a simulation runs, as defined by one or more pair_style or kspace_style commands. This scaling is done via a prefactor on the energy, forces, virial calculated by the pair or K-Space style. The prefactor is often a function of a *lambda* parameter which may be adjusted from 0 to 1 (or vice versa) over the course of a run. The time-dependent adjustment is what the fix adapt command does.

Assume that the unscaled energy of a pair_style or kspace_style is given by U. Then the scaled energy is

```
Us = f(lambda) U
```

where f() is some function of lambda. What this compute calculates is

```
dUs / d(lambda) = U df(lambda)/dlambda = Us / f(lambda) df(lambda)/dlambda
```

which is the derivative of the system's scaled potential energy Us with respect to *lambda*.

To perform this calculation, you provide one or more atom types as *atype*. *Atype* can be specified in one of two ways. An explicit numeric values can be used, as in the 1st example above. Or a wildcard asterisk can be used in place of or in conjunction with the *atype* argument to select multiple atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

You also specify two functions, as equal-style variables. The first is specified as *v_name1*, where *name1* is the name of the variable, and is f(lambda) in the notation above. The second is specified as *v_name2*, where *name2* is the name of the variable, and is df(lambda) / dlambda in the notation above. I.e. it is the analytic derivative of f() with respect to lambda. Note that the *name1* variable is also typically given as an argument to the fix adapt command.

An alchemical simulation may use several pair potentials together, invoked via the pair_style hybrid or hybrid/overlay command. The total dUs/dlambda for the overall system is calculated as the sum of each contributing term as listed by the keywords in the compute ti command. Individual pair potentials can be listed, which will be sub-styles in the hybrid case. You can also include a K-space term via the *kspace* keyword. You can also include a pairwise long-range tail correction to the energy via the *tail* keyword.

For each term you can specify a different (or the same) scale factor by the two variables that you list. Again, these will typically correspond toe the scale factors applied to these various potentials and the K-Space contribution via the fix_adapt command.

More details about the exact functional forms for the computation of du/dl can be found in the paper by Eike.

Output info:

This compute calculates a global scalar, namely dUs/dlambda. This value can be used by any command that uses a global scalar value from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The scalar value calculated by this compute is "extensive".

The scalar value will be in energy units.

Restrictions:

This compute is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix adapt

Default: none

(Eike) Eike and Maginn, Journal of Chemical Physics, 124, 164503 (2006).

compute torque/chunk command

Syntax:

```
compute ID group-ID torque/chunk chunkID
```

- ID, group-ID are documented in compute command
- torque/chunk = style name of this compute command
- chunkID = ID of compute chunk/atom command

Examples:

```
compute 1 fluid torque/chunk molchunk
```

Description:

Define a computation that calculates the torque on multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a compute chunk/atom command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the compute chunk/atom doc page and "Section_howto 23 for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates the 3 components of the torque vector for eqch chunk, due to the forces on the individual atoms in the chunk around the center-of-mass of the chunk. The calculation includes all effects due to atoms passing thru periodic boundaries.

Note that only atoms in the specified group contribute to the calculation. The compute chunk/atom command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

NOTE: The coordinates of an atom contribute to the chunk's torque in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this compute by using the set image command.

The simplest way to output the results of the compute torque/chunk calculation to a file is to use the fix ave/time command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all torque/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk file tmp.out mode vector
```

Output info:

This compute calculates a global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified compute chunk/atom command. The number of columns = 3 for the 3 xyz components of the torque for each chunk. These values can be accessed by any command that uses global array values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in force-distance units.

Restrictions: none

Related commands:

variable torque() function

Default: none

compute vacf command

Syntax:

```
compute ID group-ID vacf
```

- ID, group-ID are documented in compute command
- vacf = style name of this compute command

Examples:

```
compute 1 all vacf
compute 1 upper vacf
```

Description:

Define a computation that calculates the velocity auto-correlation function (VACF), averaged over a group of atoms. Each atom's contribution to the VACF is its current velocity vector dotted into its initial velocity vector at the time the compute was specified.

A vector of four quantites is calculated by this compute. The first 3 elements of the vector are vx * vx0 (and similarly for the y and z components), summed and averaged over atoms in the group. Vx is the current x-component of velocity for the atom, vx0 is the initial x-component of velocity for the atom. The 4th element of the vector is the total VACF, i.e. (vx*vx0 + vy*vy0 + vz*vz0), summed and averaged over atoms in the group.

The integral of the VACF versus time is proportional to the diffusion coefficient of the diffusing atoms. This can be computed in the following manner, using the variable trap() function:

```
compute         2 all vacf
fix             5 all vector 1 c_2[4]
variable        diff equal dt*trap(f_5)
thermo_style    custom step v_diff
```

NOTE: If you want the quantities calculated by this compute to be continuous when running from a restart file, then you should use the same ID for this compute, as in the original run. This is so that the fix this compute creates to store per-atom quantities will also have the same ID, and thus be initialized correctly with time=0 atom velocities from the restart file.

Output info:

This compute calculates a global vector of length 4, which can be accessed by indices 1-4 by any command that uses global vector values from a compute as input. See this section for an overview of LAMMPS output options.

The vector values are "intensive". The vector values will be in velocity^2 units.

Restrictions: none

Related commands:

compute msd

Default: none

compute vcm/chunk command

Syntax:

```
compute ID group-ID vcm/chunk chunkID
```

- ID, group-ID are documented in compute command
- vcm/chunk = style name of this compute command
- chunkID = ID of compute chunk/atom command

Examples:

```
compute 1 fluid vcm/chunk molchunk
```

Description:

Define a computation that calculates the center-of-mass velocity for multiple chunks of atoms.

In LAMMPS, chunks are collections of atoms defined by a compute chunk/atom command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the compute chunk/atom doc page and "Section_howto 23 for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

This compute calculates the x,y,z components of the center-of-mass velocity for each chunk. This is done by summing mass*velocity for each atom in the chunk and dividing the sum by the total mass of the chunk.

Note that only atoms in the specified group contribute to the calculation. The compute chunk/atom command defines its own group; atoms will have a chunk ID = 0 if they are not in that group, signifying they are not assigned to a chunk, and will thus also not contribute to this calculation. You can specify the "all" group for this command if you simply want to include atoms with non-zero chunk IDs.

The simplest way to output the results of the compute vcm/chunk calculation to a file is to use the fix ave/time command, for example:

```
compute cc1 all chunk/atom molecule
compute myChunk all vcm/chunk cc1
fix 1 all ave/time 100 1 100 c_myChunk file tmp.out mode vector
```

Output info:

This compute calculates a global array where the number of rows = the number of chunks *Nchunk* as calculated by the specified compute chunk/atom command. The number of columns = 3 for the x,y,z center-of-mass velocity coordinates of each chunk. These values can be accessed by any command that uses global array values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options.

The array values are "intensive". The array values will be in velocity units.

Restrictions: none

Related commands: none

Default: none

compute voronoi/atom command

Syntax:

```
compute ID group-ID voronoi/atom keyword arg ...
```

- ID, group-ID are documented in compute command
- voronoi/atom = style name of this compute command
- zero or more keyword/value pairs may be appended
- keyword = *only_group* or *surface* or *radius* or *edge_histo* or *edge_threshold* or *face_threshold* or *neighbors* or *peratom*

```
only_group = no arg
  occupation = no arg
  surface arg = sgroup-ID
    sgroup-ID = compute the dividing surface between group-ID and sgroup-ID
      this keyword adds a third column to the compute output
  radius arg = v_r
    v_r = radius atom style variable for a poly-disperse Voronoi tessellation
  edge_histo arg = maxedge
    maxedge = maximum number of Voronoi cell edges to be accounted in the histogram
  edge_threshold arg = minlength
    minlength = minimum length for an edge to be counted
  face_threshold arg = minarea
    minarea = minimum area for a face to be counted
  neighbors value = yes or no = store list of all neighbors or no
  peratom value = yes or no = per-atom quantities accessible or no
```

Examples:

```
compute 1 all voronoi/atom
compute 2 precipitate voronoi/atom surface matrix
compute 3b precipitate voronoi/atom radius v_r
compute 4 solute voronoi/atom only_group

compute 5 defects voronoi/atom occupation
```

compute 6 all voronoi/atom neighbors yes

Description:

Define a computation that calculates the Voronoi tessellation of the atoms in the simulation box. The tessellation is calculated using all atoms in the simulation, but non-zero values are only stored for atoms in the group.

By default two per-atom quantities are calculated by this compute. The first is the volume of the Voronoi cell around each atom. Any point in an atom's Voronoi cell is closer to that atom than any other. The second is the number of faces of the Voronoi cell. This is equal to the number of nearest neighbors of the central atom, plus any exterior faces (see note below). If the *peratom* keyword is set to "no", the per-atom quantities are still calculated, but they are not accessible.

If the *only_group* keyword is specified the tessellation is performed only with respect to the atoms contained in the compute group. This is equivalent to deleting all atoms not contained in the group prior to evaluating the tessellation.

If the *surface* keyword is specified a third quantity per atom is computed: the Voronoi cell surface of the given atom. *surface* takes a group ID as an argument. If a group other than *all* is specified, only the Voronoi cell facets facing a neighbor atom from the specified group are counted towards the surface area.

In the example above, a precipitate embedded in a matrix, only atoms at the surface of the precipitate will have non-zero surface area, and only the outward facing facets of the Voronoi cells are counted (the hull of the precipitate). The total surface area of the precipitate can be obtained by running a "reduce sum" compute on c_2[3]

If the *radius* keyword is specified with an atom style variable as the argument, a poly-disperse Voronoi tessellation is performed. Examples for radius variables are

```
variable r1 atom (type==1)*0.1+(type==2)*0.4
compute radius all property/atom radius
variable r2 atom c_radius
```

Here v_r1 specifies a per-type radius of 0.1 units for type 1 atoms and 0.4 units for type 2 atoms, and v_r2 accesses the radius property present in atom_style sphere for granular models.

The *edge_histo* keyword activates the compilation of a histogram of number of edges on the faces of the Voronoi cells in the compute group. The argument *maxedge* of the this keyword is the largest number of edges on a single Voronoi cell face expected to occur in the sample. This keyword adds the generation of a global vector with *maxedge*+1 entries. The last entry in the vector contains the number of faces with with more than *maxedge* edges. Since the polygon with the smallest amount of edges is a triangle, entries 1 and 2 of the vector will always be zero.

The *edge_threshold* and *face_threshold* keywords allow the suppression of edges below a given minimum length and faces below a given minimum area. Ultra short edges and ultra small faces can occur as artifacts of the Voronoi tessellation. These keywords will affect the neighbor count and edge histogram outputs.

If the *occupation* keyword is specified the tessellation is only performed for the first invocation of the compute and then stored. For all following invocations of the compute the number of atoms in each Voronoi cell in the stored tessellation is counted. In this mode the compute returns a per-atom array with 2 columns. The first column is the number of atoms currently in the Voronoi volume defined by this atom at the time of the first invocation of the compute (note that the atom may have moved significantly). The second column contains the total number of atoms sharing the Voronoi cell of the stored tessellation at the location of the current atom. Numbers in column one can be any positive integer including zero, while column two values will always be greater than zero. Column one data can be used to locate vacancies (the coordinates are given by the atom coordinates at the time step when the compute was first invoked), while column two data can be used to identify interstitial atoms.

If the *neighbors* value is set to yes, then this compute creates a local array with 3 columns. There is one row for each face of each Voronoi cell. The 3 columns are the atom ID of the atom that owns the cell, the atom ID of the atom in the neighboring cell (or zero if the face is external), and the area of the face. The array can be accessed by any command that uses local values from a compute as input. See this section for an overview of LAMMPS output options. More specifically, the array can be accessed by a dump local command to write a file containing all the Voronoi neighbors in a system:

```
compute 6 all voronoi/atom neighbors yes
dump d2 all local 1 dump.neighbors index c_6[1] c_6[2] c_6[3]
```

If the *face_threshold* keyword is used, then only faces with areas greater than the threshold are stored.

The Voronoi calculation is performed by the freely available Voro++ package, written by Chris Rycroft at UC Berkeley and LBL, which must be installed on your system when building LAMMPS for use with this compute. See instructions on obtaining and installing the Voro++ software in the src/VORONOI/README file.

NOTE: The calculation of Voronoi volumes is performed by each processor for the atoms it owns, and includes the effect of ghost atoms stored by the processor. This assumes that the Voronoi cells of owned atoms are not affected by atoms beyond the ghost atom cut-off distance. This is usually a good assumption for liquid and solid systems, but may lead to underestimation of Voronoi volumes in low density systems. By default, the set of ghost atoms stored by each processor is determined by the cutoff used for pair_style interactions. The cutoff can be set explicitly via the comm_modify cutoff command. The Voronoi cells for atoms adjacent to empty regions will extend into those regions up to the communication cutoff in x, y, or z. In that situation, an exterior face is created at the cutoff distance normal to the x, y, or z direction. For triclinic systems, the exterior face is parallel to the corresponding reciprocal lattice vector.

NOTE: The Voro++ package performs its calculation in 3d. This will still work for a 2d LAMMPS simulation, provided all the atoms have the same z coordinate. The Voronoi cell of each atom will be a columnar polyhedron with constant cross-sectional area along the z direction and two exterior faces at the top and bottom of the simulation box. If the atoms do not all have the same z coordinate, then the columnar cells will be accordingly distorted. The cross-sectional area of each Voronoi cell can be obtained by dividing its volume by the z extent of the simulation box. Note that you define the z extent of the simulation box for 2d simulations when using the create_box or read_data commands.

Output info:

By default, this compute calculates a per-atom array with 2 columns. In regular dynamic tessellation mode the first column is the Voronoi volume, the second is the neighbor count, as described above (read above for the output data in case the *occupation* keyword is specified). These values can be accessed by any command that uses per-atom values from a compute as input. See Section_howto 15 for an overview of LAMMPS output options. If the *peratom* keyword is set to "no", the per-atom array is still created, but it is not accessible.

If the *edge_histo* keyword is used, then this compute generates a global vector of length *maxedge*+1, containing a histogram of the number of edges per face.

If the *neighbors* value is set to yes, then this compute calculates a local array with 3 columns. There is one row for each face of each Voronoi cell.

NOTE: Some LAMMPS commands such as the compute reduce command can accept either a per-atom or local quantity. If this compute produces both quantities, the command may access the per-atom quantity, even if you want to access the local quantity. This effect can be eliminated by using the *peratom* keyword to turn off the production of the per-atom quantities. For the default value *yes* both quantities are produced. For the value *no*, only the local array is produced.

The Voronoi cell volume will be in distance units cubed. The Voronoi face area will be in distance units squared.

Restrictions:

This compute is part of the VORONOI package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

dump custom, dump local

Default: *neighbors* no, *peratom* yes

compute xrd command

Syntax:

```
compute ID group-ID xrd lambda type1 type2 ... typeN keyword value ...
```

- ID, group-ID are documented in compute command
- xrd = style name of this compute command
- lambda = wavelength of incident radiation (length units)
- type1 type2 ... typeN = chemical symbol of each atom type (see valid options below)
- zero or more keyword/value pairs may be appended
- keyword = *2Theta* or *c* or *LP* or *manual* or *echo*

```
2Theta values = Min2Theta Max2Theta
    Min2Theta,Max2Theta = minimum and maximum 2 theta range to explore
    (radians or degrees)
  c values = c1 c2 c3
    c1,c2,c3 = parameters to adjust the spacing of the reciprocal
               lattice nodes in the h, k, and l directions respectively
  LP value = switch to apply Lorentz-polarization factor
    0/1 = off/on
  manual = flag to use manual spacing of reciprocal lattice points
           based on the values of the c parameters
  echo = flag to provide extra output for debugging purposes
```

Examples:

```
compute 1 all xrd 1.541838 Al O 2Theta 0.087 0.87 c 1 1 1 LP 1 echo
compute 2 all xrd 1.541838 Al O 2Theta 10 100 c 0.05 0.05 0.05 LP 1 manual

fix 1 all ave/histo/weight 1 1 1 0.087 0.87 250 c_1[1] c_1[2] mode vector file Rad2Theta.xrd
fix 2 all ave/histo/weight 1 1 1 10 100 250 c_2[1] c_2[2] mode vector file Deg2Theta.xrd
```

Description:

Define a computation that calculates x-ray diffraction intensity as described in (Coleman) on a mesh of reciprocal lattice nodes defined by the entire simulation domain (or manually) using a simulated radiation of wavelength lambda.

The x-ray diffraction intensity, I, at each reciprocal lattice point, k, is computed from the structure factor, F, using the equations:

$$I = Lp(\theta)\frac{F^* F}{N}$$

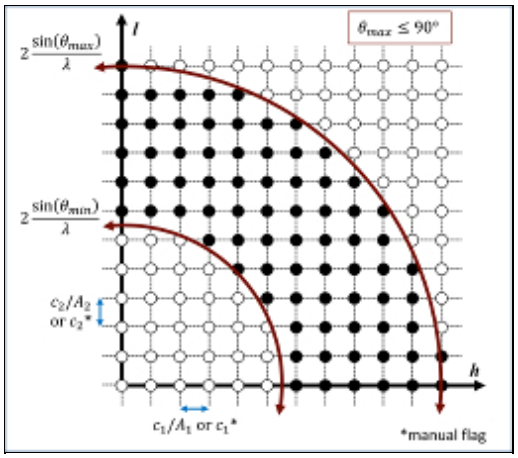
$$F(\mathbf{k}) = \sum_{\mathbf{j}=\mathbf{1}}^{\mathbf{N}} \mathbf{f_j}(\theta)\mathbf{exp}(\mathbf{2\pi i k \cdot r_j})$$

$$Lp(\theta) = \frac{1 + cos^2(2\theta)}{cos(\theta)sin^2(\theta)}$$

$$\frac{sin(\theta)}{\lambda} = \frac{|\mathbf{k}|}{2}$$

Here, K is the location of the reciprocal lattice node, rj is the position of each atom, fj are atomic scattering factors, LP is the Lorentz-polarization factor, and theta is the scattering angle of diffraction. The Lorentz-polarization factor can be turned off using the optional *LP* keyword.

Diffraction intensities are calculated on a three-dimensional mesh of reciprocal lattice nodes. The mesh spacing is defined either (a) by the entire simulation domain or (b) manually using selected values as shown in the 2D diagram below.



For a mesh defined by the simulation domain, a rectilinear grid is constructed with spacing *c*inv(A) along each reciprocal lattice axis. Where A are the vectors corresponding to the edges of the simulation cell. If one or two directions has non-periodic boundary conditions, then the spacing in these directions is defined from the average of the (inversed) box lengths with periodic boundary conditions. Meshes defined by the simulation domain must contain at least one periodic boundary.

If the *manual* flag is included, the mesh of reciprocal lattice nodes will defined using the *c* values for the spacing along each reciprocal lattice axis. Note that manual mapping of the reciprocal space mesh is good for comparing diffraction results from multiple simulations; however it can reduce the likelihood that Bragg reflections will be satisfied unless small spacing parameters (< 0.05 Angstrom^(-1)) are implemented. Meshes with manual spacing do not require a periodic boundary.

The limits of the reciprocal lattice mesh are determined by range of scattering angles explored. The *2Theta* parameters allows the user to reduce the scattering angle range to only the region of interest which reduces the

cost of the computation.

The atomic scattering factors, fj, accounts for the reduction in diffraction intensity due to Compton scattering. Compute xrd uses analytical approximations of the atomic scattering factors that vary for each atom type (type1 type2 ... typeN) and angle of diffraction. The analytic approximation is computed using the formula (Colliex):

$$f_j\left(\frac{sin(\theta)}{\lambda}\right) = \sum_i^4 a_i exp\left(-b_i \frac{sin^2(\theta)}{\lambda^2}\right) + c$$

Coefficients parameterized by (Peng) are assigned for each atom type designating the chemical symbol and charge of each atom type. Valid chemical symbols for compute xrd are:

H: He1-: He: Li: Li1+: Be: Be2+: B: C: Cval: N: O: O1-: F: F1-: Ne: Na: Na1+: Mg: Mg2+: Al: Al3+: Si: Sival: Si4+: P: S: Cl: Cl1-: Ar: K: Ca: Ca2+: Sc: Sc3+: Ti: Ti2+: Ti3+: Ti4+: V: V2+: V3+: V5+: Cr: Cr2+: Cr3+: Mn: Mn2+: Mn3+: Mn4+: Fe: Fe2+: Fe3+: Co: Co2+: Co: Ni: Ni2+: Ni3+: Cu: Cu1+: Cu2+: Zn: Zn2+: Ga: Ga3+: Ge: Ge4+: As: Se: Br: Br1-: Kr: Rb: Rb1+: Sr: Sr2+: Y: Y3+: Zr: Zr4+: Nb: Nb3+: Nb5+: Mo: Mo3+: Mo5+: Mo6+: Tc: Ru: Ru3+: Ru4+: Rh: Rh3+: Rh4+: Pd: Pd2+: Pd4+: Ag: Ag1+: Ag2+: Cd: Cd2+: In: In3+: Sn: Sn2+: Sn4+: Sb: Sb3+: Sb5+: Te: I: I1-: Xe: Cs: Cs1+: Ba: Ba2+: La: La3+: Ce: Ce3+: Ce4+: Pr: Pr3+: Pr4+: Nd: Nd3+: Pm: Pm3+: Sm: Sm3+: Eu: Eu2+: Eu3+: Gd: Gd3+: Tb: Tb3+: Dy: Dy3+: Ho: Ho3+: Er: Er3+: Tm: Tm3+: Yb: Yb2+: Yb3+: Lu: Lu3+: Hf: Hf4+: Ta: Ta5+: W: W6+: Re: Os: Os4+: Ir: Ir3+: Ir4+: Pt: Pt2+: Pt4+: Au: Au1+: Au3+: Hg: Hg1+: Hg2+: Tl: Tl1+: Tl3+: Pb: Pb2+: Pb4+: Bi: Bi3+: Bi5+: Po: At: Rn: Fr: Ra: Ra2+: Ac: Ac3+: Th: Th4+: Pa: U: U3+: U4+: U6+: Np: Np3+: Np4+: Np6+: Pu: Pu3+: Pu4+: Pu6+: Am: Cm: Bk: Cf:tb(c=5,s=:)

If the *echo* keyword is specified, compute xrd will provide extra reporting information to the screen.

Output info:

This compute calculates a global array. The number of rows in the array is the number of reciprocal lattice nodes that are explored which by the mesh. The global array has 2 columns.

The first column contains the diffraction angle in the units (radians or degrees) provided with the *2Theta* values. The second column contains the computed diffraction intensities as described above.

The array can be accessed by any command that uses global values from a compute as input. See this section for an overview of LAMMPS output options.

All array values calculated by this compute are "intensive".

Restrictions:

This compute is part of the USER-DIFFRACTION package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The compute_xrd command does not work for triclinic cells.

Related commands:

fix ave/histo, compute saed

Default:

The option defaults are 2Theta = 1 179 (degrees), c = 1 1 1, LP = 1, no manual flag, no echo flag.

(Coleman) Coleman, Spearot, Capolungo, MSMSE, 21, 055020 (2013).

(Colliex) Colliex et al. International Tables for Crystallography Volume C: Mathematical and Chemical Tables, 249-429 (2004).

(Peng) Peng, Ren, Dudarev, Whelan, Acta Crystallogr. A, 52, 257-76 (1996).

create_atoms command

Syntax:

```
create_atoms type style args keyword values ...
```

- type = atom type (1-Ntypes) of atoms to create (offset for molecule creation)
- style = *box* or *region* or *single* or *random*

```
  box args = none
    region args = region-ID
      region-ID = particles will only be created if contained in the region
    single args = x y z
      x,y,z = coordinates of a single particle (distance units)
    random args = N seed region-ID
      N = number of particles to create
      seed = random # seed (positive integer)
      region-ID = create atoms within this region, use NULL for entire simulation box
```

- zero or more keyword/value pairs may be appended
- keyword = *mol* or *basis* or *remap* or *var* or *set* or *units*

```
  mol value = template-ID seed
      template-ID = ID of molecule template specified in a separate molecule command
      seed = random # seed (positive integer)
    basis values = M itype
      M = which basis atom
      itype = atom type (1-N) to assign to this basis atom
    remap value = yes or no
    var value = name = variable name to evaluate for test of atom creation
    set values = dim vname
      dim = x or y or z
      name = name of variable to set with x,y,z atom position
    rotate values = Rx Ry Rz theta
      Rx,Ry,Rz = rotation vector for single molecule
      theta = rotation angle for single molecule (degrees)
    units value = lattice or box
      lattice = the geometry is defined in lattice units
      box = the geometry is defined in simulation box units
```

Examples:

```
create_atoms 1 box
create_atoms 3 region regsphere basis 2 3
create_atoms 3 single 0 0 5
create_atoms 1 box var v set x xpos set y ypos
```

Description:

This command creates atoms (or molecules) on a lattice, or a single atom (or molecule), or a random collection of atoms (or molecules), as an alternative to reading in their coordinates explicitly via a read_data or read_restart command. A simulation box must already exist, which is typically created via the create_box command. Before using this command, a lattice must also be defined using the lattice command, unless you specify the *single* style with units = box or the *random* style. For the remainder of this doc page, a created atom or molecule is referred to as a "particle".

If created particles are individual atoms, they are assigned the specified atom *type*, though this can be altered via the *basis* keyword as discussed below. If molecules are being created, the type of each atom in the created molecule is specified in the file read by the molecule command, and those values are added to the specified atom *type*. E.g. if *type* = 2, and the file specifies atom types 1,2,3, then each created molecule will have atom types 3,4,5.

For the *box* style, the create_atoms command fills the entire simulation box with particles on the lattice. If your simulation box is periodic, you should insure its size is a multiple of the lattice spacings, to avoid unwanted atom overlaps at the box boundaries. If your box is periodic and a multiple of the lattice spacing in a particular dimension, LAMMPS is careful to put exactly one particle at the boundary (on either side of the box), not zero or two.

For the *region* style, a geometric volume is filled with particles on the lattice. This volume what is inside the simulation box and is also consistent with the region volume. See the region command for details. Note that a region can be specified so that its "volume" is either inside or outside a geometric boundary. Also note that if your region is the same size as a periodic simulation box (in some dimension), LAMMPS does not implement the same logic described above as for the *box* style, to insure exactly one particle at periodic boundaries. if this is what you desire, you should either use the *box* style, or tweak the region size to get precisely the particles you want.

For the *single* style, a single particle is added to the system at the specified coordinates. This can be useful for debugging purposes or to create a tiny system with a handful of particles at specified positions.

For the *random* style, N particles are added to the system at randomly generated coordinates, which can be useful for generating an amorphous system. The particles are created one by one using the speficied random number *seed*, resulting in the same set of particles coordinates, independent of how many processors are being used in the simulation. If the *region-ID* argument is specified as NULL, then the created particles will be anywhere in the simulation box. If a *region-ID* is specified, a geometric volume is filled which is both inside the simulation box and is also consistent with the region volume. See the region command for details. Note that a region can be specified so that its "volume" is either inside or outside a geometric boundary.

NOTE: Particles generated by the *random* style will typically be highly overlapped which will cause many interatomic potentials to compute large energies and forces. Thus you should either perform an energy minimization or run dynamics with fix nve/limit to equilibrate such a system, before running normal dynamics.

Note that this command adds particles to those that already exist. This means it can be used to add particles to a system previously read in from a data or restart file. Or the create_atoms command can be used multiple times, to add multiple sets of particles to the simulation. For example, grain boundaries can be created, by interleaving create_atoms with lattice commands specifying different orientations. By using the create_atoms command in conjunction with the delete_atoms command, reasonably complex geometries can be created, or a protein can be solvated with a surrounding box of water molecules.

In all these cases, care should be taken to insure that new atoms do not overlap existing atoms inappropriately, especially if molecules are being added. The delete_atoms command can be used to remove overlapping atoms or molecules.

Individual atoms are inserted by this command, unless the *mol* keyword is used. It specifies a *template-ID* previously defined using the molecule command, which reads a file that defines the molecule. The coordinates, atom types, charges, etc, as well as any bond/angle/etc and special neighbor information for the molecule can be specified in the molecule file. See the molecule command for details. The only settings required to be in this file are the coordinates and types of atoms in the molecule.

Using a lattice to add molecules, e.g. via the *box* or *region* or *single* styles, is exactly the same as adding atoms on lattice points, except that entire molecules are added at each point, i.e. on the point defined by each basis atom in the unit cell as it tiles the simulation box or region. This is done by placing the geometric center of the molecule at the lattice point, and giving the molecule a random orientation about the point. The random *seed* specified with the *mol* keyword is used for this operation, and the random numbers generated by each processor are different. This means the coordinates of individual atoms (in the molecules) will be different when running on different numbers of processors, unlike when atoms are being created in parallel.

Also note that because of the random rotations, it may be important to use a lattice with a large enough spacing that adjacent molecules will not overlap, regardless of their relative orientations.

NOTE: If the create_box command is used to create the simulation box, followed by the create_atoms command with its *mol* option for adding molecules, then you typically need to use the optional keywords allowed by the create_box command for extra bonds (angles,etc) or extra special neighbors. This is because by default, the create_box command sets up a non-molecular system which doesn't allow molecules to be added.

This is the meaning of the other allowed keywords.

The *basis* keyword is only used when atoms (not molecules) are being created. It specifies an atom type that will be assigned to specific basis atoms as they are created. See the lattice command for specifics on how basis atoms are defined for the unit cell of the lattice. By default, all created atoms are assigned the argument *type* as their atom type.

The *remap* keyword only applies to the *single* style. If it is set to *yes*, then if the specified position is outside the simulation box, it will mapped back into the box, assuming the relevant dimensions are periodic. If it is set to *no*, no remapping is done and no particle is created if its position is outside the box.

The *var* and *set* keywords can be used to provide a criterion for accepting or rejecting the addition of an individual atom, based on its coordinates. The *vname* specified for the *var* keyword is the name of an equal-style variable which should evaluate to a zero or non-zero value based on one or two or three variables which will store the x, y, or z coordinates of an atom (one variable per coordinate). These other variables must be equal-style variables defined in the input script, but their formula can by anything. The *set* keyword is used to identify the names of these other variables, one variable for the x-coordinate of a created atom, one for y, and one for z.

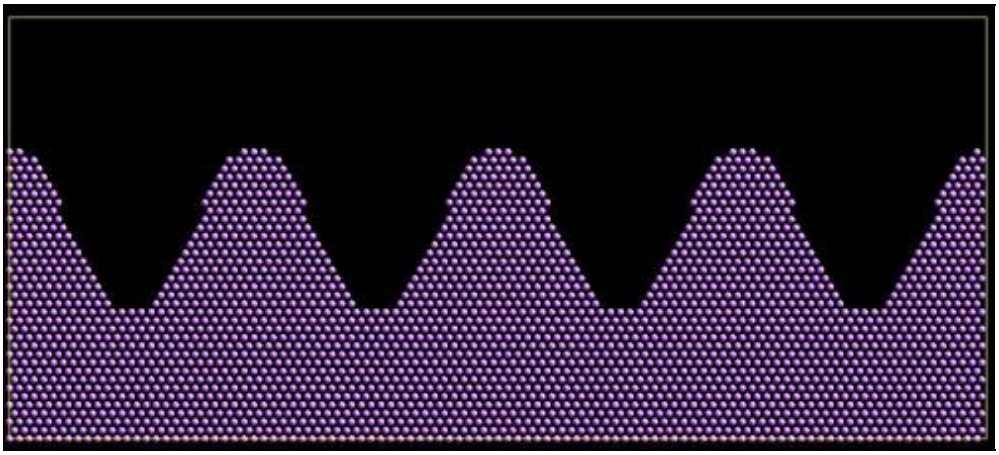
When an atom is created, its x, y, or z coordinates override the formula for any *set* variable that is defined. The *var* variable is then evaluated. If the returned value is 0.0, the atom is not created. If it is non-zero, the atom is created. After all atoms are created, the formulas defined for all of the *set* variables are restored to their original strings.

As an example, these commands can be used in a 2d simulation, to create a sinusoidal surface. Note that the surface is "rough" due to individual lattice points being "above" or "below" the mathematical expression for the sinusoidal curve. If a finer lattice were used, the sinusoid would appear to be "smoother". Also note the use of the "xlat" and "ylat" thermo_style keywords which converts lattice spacings to distance. Click on the image for a larger version.

```
variable        x equal 100
variable        y equal 25
lattice         hex 0.8442
region          box block 0 $x 0 $y -0.5 0.5
create_box      1 box

variable        xx equal 0.0
variable        yy equal 0.0
variable        v equal "(0.2*v_y*ylat * cos(v_xx/xlat * 2.0*PI*4.0/v_x) + 0.5*v_y*ylat - v_yy) > 0.
```

```
create_atoms    1 box var v set x xx set y yy
```



The *rotate* keyword can be used with the *single* style, when adding a single molecule to specify the orientation at which the molecule is inserted. The axis of rotation is determined by the rotation vector (Rx,Ry,Rz) that goes through the insertion point. The specified *theta* determines the angle of rotation around that axis. Note that the direction of rotation for the atoms around the rotation axis is consistent with the right-hand rule: if your right-hand's thumb points along *R*, then your fingers wrap around the axis in the direction of rotation.

The *units* keyword determines the meaning of the distance units used to specify the coordinates of the one particle created by the *single* style. A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings.

Atom IDs are assigned to created atoms in the following way. The collection of created atoms are assigned consecutive IDs that start immediately following the largest atom ID existing before the create_atoms command was invoked. When a simulation is performed on different numbers of processors, there is no guarantee a particular created atom will be assigned the same ID. If molecules are being created, molecule IDs are assigned to created molecules in a similar fashion.

Aside from their ID, atom type, and xyz position, other properties of created atoms are set to default values, depending on which quantities are defined by the chosen atom style. See the atom style command for more details. See the set and velocity commands for info on how to change these values.

- charge = 0.0
- dipole moment magnitude = 0.0
- diameter = 1.0
- shape = 0.0 0.0 0.0
- density = 1.0
- volume = 1.0
- velocity = 0.0 0.0 0.0
- angular velocity = 0.0 0.0 0.0
- angular momentum = 0.0 0.0 0.0
- quaternion = (1,0,0,0)
- bonds, angles, dihedrals, impropers = none

If molecules are being created, these defaults can be overridden by values specified in the file read by the molecule command. E.g. the file typically defines bonds (angles,etc) between atoms in the molecule, and can optionally define charges on each atom.

Note that the *sphere* atom style sets the default particle diameter to 1.0 as well as the density. This means the mass for the particle is not 1.0, but is PI/6 * diameter^3 = 0.5236.

Note that the *ellipsoid* atom style sets the default particle shape to (0.0 0.0 0.0) and the density to 1.0 which means it is a point particle, not an ellipsoid, and has a mass of 1.0.

Note that the *peri* style sets the default volume and density to 1.0 and thus also set the mass for the particle to 1.0.

The set command can be used to override many of these default settings.

Restrictions:

An atom_style must be previously defined to use this command.

A rotation vector specified for a single molecule must be in the z-direction for a 2d model.

Related commands:

lattice, region, create_box, read_data, read_restart

Default:

The default for the *basis* keyword is that all created atoms are assigned the argument *type* as their atom type (when single atoms are being created). The other defaults are *remap* = no, *rotate* = random, and *units* = lattice.

create_bonds command

Syntax:

```
create_bonds group-ID group2-ID btype rmin rmax
```

- group-ID = ID of first group
- group2-ID = ID of second group, bonds will be between atoms in the 2 groups
- btype = bond type of created bonds
- rmin = minimum distance between pair of atoms to bond together
- rmax = minimum distance between pair of atoms to bond together

Examples:

```
create_bonds all all 1 1.0 1.2
create_bonds surf solvent 3 2.0 2.4
```

Description:

Create bonds between pairs of atoms that meet specified distance criteria. The bond interactions can then be computed during a simulation by the bond potential defined by the bond_style and bond_coeff commands. This command is useful for adding bonds to a system, e.g. between nearest neighbors in a lattice of atoms, without having to enumerate all the bonds in the data file read by the read_data command.

Note that the flexibility of this command is limited. It can be used several times to create different types of bond at different distances. But it cannot typically create all the bonds that would normally be defined in a complex system of molecules. Also note that this command does not add any 3-body or 4-body interactions which, depending on your model, may be induced by added bonds, e.g. angle, dihedral, or improper interactions.

All created bonds will be between pairs of atoms I,J where I is in one of the two specified groups, and J is in the other. The two groups can be the same, e.g. group "all". The created bonds will be of bond type *btype*, where *btype* must be a value between 1 and the number of bond types defined. This maximum value is set by the "bond types" field in the header of the data file read by the read_data command, or via the optional "bond/types" argument of the create_box command.

For a bond to be created, an I,J pair of atoms must be a distance D apart such that *rmin* <= D <= *rmax*.

The following settings must have been made in an input script before this command is used:

- special_bonds weight for 1-2 interactions must be 0.0
- a pair_style must be defined
- no kspace_style defined
- minimum pair_style cutoff + neighbor skin >= *rmax*

These settings are required so that a neighbor list can be created to search for nearby atoms. Pairs of atoms that are already bonded cannot appear in the neighbor list, to avoid creation of duplicate bonds. The neighbor list for all atom type pairs must also extend to a distance that encompasses the *rmax* for new bonds to create.

An additional requirement is that your system must be ready to perform a simulation. This means, for example, that all pair_style coefficients be set via the pair_coeff command. A bond_style command and all bond

coefficients must also be set, even if no bonds exist before this command is invoked. This is because the building of neighbor list requires initialization and setup of a simulation, similar to what a run command would require.

Note that you can change any of these settings after this command executes, e.g. if you wish to use long-range Coulombic interactions via the kspace_style command for your subsequent simulation.

NOTE: If the system has no bonds to begin with, or if more bonds per atom are being added than currently exist, then you must insure that the number of bond types and the maximum number of bonds per atom are set to large enough values. Otherwise an error may occur when too many bonds are added to an atom. If the read_data command is used to define the system, these 2 parameters can be set via the "bond types" and "extra bond per atom" fields in the header section of the data file. If the create_box command is used to define the system, these 2 parameters can be set via its optional "bond/types" and "extra/bond/per/atom" arguments. See the doc pages for the 2 commands for details.

Restrictions:

This command cannot be used with molecular systems defined using molecule template files via the molecule and atom_style template commands.

Related commands:

create_atoms, delete_bonds

Default: none

create_box command

Syntax:

```
create_box N region-ID keyword value ...
```

- N = # of atom types to use in this simulation
- region-ID = ID of region to use as simulation domain
- zero or more keyword/value pairs may be appended
- keyword = *bond/types* or *angle/types* or *dihedral/types* or *improper/types* or *extra/bond/per/atom* or *extra/angle/per/atom* or *extra/dihedral/per/atom* or *extra/improper/per/atom*

```
  bond/types value = # of bond types
    angle/types value = # of angle types
    dihedral/types value = # of dihedral types
    improper/types value = # of improper types
    extra/bond/per/atom value = # of bonds per atom
    extra/angle/per/atom value = # of angles per atom
    extra/dihedral/per/atom value = # of dihedrals per atom
    extra/improper/per/atom value = # of impropers per atom
    extra/special/per/atom value = # of special neighbors per atom
```

Examples:

```
create_box 2 mybox
create_box 2 mybox bond/types 2 extra/bond/per/atom 1
```

Description:

This command creates a simulation box based on the specified region. Thus a region command must first be used to define a geometric domain. It also partitions the simulation box into a regular 3d grid of rectangular bricks, one per processor, based on the number of processors being used and the settings of the processors command. The partitioning can later be changed by the balance or fix balance commands.

The argument N is the number of atom types that will be used in the simulation.

If the region is not of style *prism*, then LAMMPS encloses the region (block, sphere, etc) with an axis-aligned orthogonal bounding box which becomes the simulation domain.

If the region is of style *prism*, LAMMPS creates a non-orthogonal simulation domain shaped as a parallelepiped with triclinic symmetry. As defined by the region prism command, the parallelepiped has its "origin" at (xlo,ylo,zlo) and is defined by 3 edge vectors starting from the origin given by A = (xhi-xlo,0,0); B = (xy,yhi-ylo,0); C = (xz,yz,zhi-zlo). *Xy,xz,yz* can be 0.0 or positive or negative values and are called "tilt factors" because they are the amount of displacement applied to faces of an originally orthogonal box to transform it into the parallelipiped.

By default, a *prism* region used with the create_box command must have tilt factors (xy,xz,yz) that do not skew the box more than half the distance of the parallel box length. For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = ..., -15, -5, 5, 15, 25, ... are all geometrically equivalent. If you wish to define a box with tilt factors that exceed these limits, you can use the box tilt command, with a setting of *large*; a

setting of *small* is the default.

See Section_howto 12 of the doc pages for a geometric description of triclinic boxes, as defined by LAMMPS, and how to transform these parameters to and from other commonly used triclinic representations.

When a prism region is used, the simulation domain should normally be periodic in the dimension that the tilt is applied to, which is given by the second dimension of the tilt factor (e.g. y for xy tilt). This is so that pairs of atoms interacting across that boundary will have one of them shifted by the tilt factor. Periodicity is set by the boundary command. For example, if the xy tilt factor is non-zero, then the y dimension should be periodic. Similarly, the z dimension should be periodic if xz or yz is non-zero. LAMMPS does not require this periodicity, but you may lose atoms if this is not the case.

Also note that if your simulation will tilt the box, e.g. via the fix deform command, the simulation box must be setup to be triclinic, even if the tilt factors are initially 0.0. You can also change an orthogonal box to a triclinic box or vice versa by using the change box command with its *ortho* and *triclinic* options.

NOTE: If the system is non-periodic (in a dimension), then you should not make the lo/hi box dimensions (as defined in your region command) radically smaller/larger than the extent of the atoms you eventually plan to create, e.g. via the create_atoms command. For example, if your atoms extend from 0 to 50, you should not specify the box bounds as -10000 and 10000. This is because as described above, LAMMPS uses the specified box size to layout the 3d grid of processors. A huge (mostly empty) box will be sub-optimal for performance when using "fixed" boundary conditions (see the boundary command). When using "shrink-wrap" boundary conditions (see the boundary command), a huge (mostly empty) box may cause a parallel simulation to lose atoms the first time that LAMMPS shrink-wraps the box around the atoms.

The optional keywords can be used to create a system that allows for bond (angle, dihedral, improper) interactions, or for molecules with special 1-2,1-3,1-4 neighbors to be added later. These optional keywords serve the same purpose as the analogous keywords that can be used in a data file which are recognized by the read_data command when it sets up a system.

Note that if these keywords are not used, then the create_box command creates an atomic (non-molecular) simulation that does not allow bonds between pairs of atoms to be defined, or a bond potential to be specified, or for molecules with special neighbors to be added to the system by commands such as create_atoms mol, fix deposit or fix pour.

As an example, see the examples/deposit/in.deposit.molecule script, which deposits molecules onto a substrate. Initially there are no molecules in the system, but they are added later by the fix deposit command. The create_box command in the script uses the bond/types and extra/bond/per/atom keywords to allow this. If the added molecule contained more than 1 special bond (allowed by default), an extra/special/per/atom keyword would also need to be specified.

Restrictions:

An atom_style and region must have been previously defined to use this command.

Related commands:

read_data, create_atoms, region

Default: none

delete_atoms command

Syntax:

```
delete_atoms style args keyword value ...
```

- style = *group* or *region* or *overlap* or *porosity*

```
  group args = group-ID
    region args = region-ID
    overlap args = cutoff group1-ID group2-ID
      cutoff = delete one atom from pairs of atoms within the cutoff (distance units)
      group1-ID = one atom in pair must be in this group
      group2-ID = other atom in pair must be in this group
    porosity args = region-ID fraction seed
      region-ID = region within which to perform deletions
      fraction = delete this fraction of atoms
      seed = random number seed (positive integer)
```

- zero or more keyword/value pairs may be appended
- keyword = *compress* or *bond* or *mol*

```
  compress value = no or yes
    bond value = no or yes
    mol value = no or yes
```

Examples:

```
delete_atoms group edge
delete_atoms region sphere compress no
delete_atoms overlap 0.3 all all
delete_atoms overlap 0.5 solvent colloid
delete_atoms porosity cube 0.1 482793 bond yes
```

Description:

Delete the specified atoms. This command can be used to carve out voids from a block of material or to delete created atoms that are too close to each other (e.g. at a grain boundary).

For style *group*, all atoms belonging to the group are deleted.

For style *region*, all atoms in the region volume are deleted. Additional atoms can be deleted if they are in a molecule for which one or more atoms were deleted within the region; see the *mol* keyword discussion below.

For style *overlap* pairs of atoms whose distance of separation is within the specified cutoff distance are searched for, and one of the 2 atoms is deleted. Only pairs where one of the two atoms is in the first group specified and the other atom is in the second group are considered. The atom that is in the first group is the one that is deleted.

Note that it is OK for the two group IDs to be the same (e.g. group *all*), or for some atoms to be members of both groups. In these cases, either atom in the pair may be deleted. Also note that if there are atoms which are members of both groups, the only guarantee is that at the end of the deletion operation, enough deletions will have occurred that no atom pairs within the cutoff will remain (subject to the group restriction). There is no guarantee that the minimum number of atoms will be deleted, or that the same atoms will be deleted when running on different numbers of processors.

For style *porosity* a specified *fraction* of atoms are deleted within the specified region. For example, if fraction is 0.1, then 10% of the atoms will be deleted. The atoms to delete are chosen randomly. There is no guarantee that the exact fraction of atoms will be deleted, or that the same atoms will be deleted when running on different numbers of processors.

If the *compress* keyword is set to *yes*, then after atoms are deleted, then atom IDs are re-assigned so that they run from 1 to the number of atoms in the system. Note that this is not done for molecular systems (see the atom_style command), regardless of the *compress* setting, since it would foul up the bond connectivity that has already been assigned.

A molecular system with fixed bonds, angles, dihedrals, or improper interactions, is one where the topology of the interactions is typically defined in the data file read by the read_data command, and where the interactions themselves are defined with the bond_style, angle_style, etc commands. If you delete atoms from such a system, you must be careful not to end up with bonded interactions that are stored by remaining atoms but which include deleted atoms. This will cause LAMMPS to generate a "missing atoms" error when the bonded interaction is computed. The *bond* and *mol* keywords offer two ways to do that.

It the *bond* keyword is set to *yes* then any bond or angle or dihedral or improper interaction that includes a deleted atom is also removed from the lists of such interactions stored by non-deleted atoms. Note that simply deleting interactions due to dangling bonds (e.g. at a surface) may result in a inaccurate or invalid model for the remaining atoms.

It the *mol* keyword is set to *yes*, then for every atom that is deleted, all other atoms in the same molecule (with the same molecule ID) will also be deleted. This is not done for atoms with molecule ID = 0, since such an ID is assumed to flag isolated atoms that are not part of molecules.

NOTE: The molecule deletion operation in invoked after all individual atoms have been deleted using the rules described above for each style. This means additional atoms may be deleted that are not in the group or region, that are not required by the overlap cutoff criterion, or that will create a higher fraction of porosity than was requested.

Restrictions:

The *overlap* styles requires inter-processor communication to acquire ghost atoms and build a neighbor list. This means that your system must be ready to perform a simulation before using this command (force fields setup, atom masses set, etc). Since a neighbor list is used to find overlapping atom pairs, it also means that you must define a pair style with the minimum force cutoff distance between any pair of atoms types (plus the neighbor skin) >= the specified overlap cutoff.

If the special_bonds command is used with a setting of 0, then a pair of bonded atoms (1-2, 1-3, or 1-4) will not appear in the neighbor list, and thus will not be considered for deletion by the *overlap* styles. You probably don't want to be deleting one atom in a bonded pair anyway.

The *bond yes* option cannot be used with molecular systems defined using molecule template files via the molecule and atom_style template commands.

Related commands:

create_atoms

Default:

The option defaults are compress = yes, bond = no, mol = no.

delete_bonds command

Syntax:

```
delete_bonds group-ID style arg keyword ...
```

- group-ID = group ID
- style = *multi* or *atom* or *bond* or *angle* or *dihedral* or *improper* or *stats*

```
  multi arg = none
    atom arg = an atom type or range of types (see below)
    bond arg = a bond type or range of types (see below)
    angle arg = an angle type or range of types (see below)
    dihedral arg = a dihedral type or range of types (see below)
    improper arg = an improper type or range of types (see below)
    stats arg = none
```

- zero or more keywords may be appended
- keyword = *any* or *undo* or *remove* or *special*

Examples:

```
delete_bonds frozen multi remove
delete_bonds all atom 4 special
delete_bonds all bond 0*3 special
delete_bonds all stats
```

Description:

Turn off (or on) molecular topology interactions, i.e. bonds, angles, dihedrals, impropers. This command is useful for deleting interactions that have been previously turned off by bond-breaking potentials. It is also useful for turning off topology interactions between frozen or rigid atoms. Pairwise interactions can be turned off via the neigh_modify exclude command. The fix shake command also effectively turns off certain bond and angle interactions.

For all styles, by default, an interaction is only turned off (or on) if all the atoms involved are in the specified group. See the *any* keyword to change the behavior.

Several of the styles (*atom*, *bond*, *angle*, *dihedral*, *improper*) take a *type* as an argument. The specified *type* should be an integer from 0 to N, where N is the number of relevant types (atom types, bond types, etc). A value of 0 is only relevant for style *bond*; see details below. In all cases, a wildcard asterisk can be used in place of or in conjunction with the *type* argument to specify a range of types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of types, then an asterisk with no numeric values means all types from 0 to N. A leading asterisk means all types from 0 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that it is fine to include a type of 0 for non-bond styles; it will simply be ignored.

For style *multi* all bond, angle, dihedral, and improper interactions of any type, involving atoms in the group, are turned off.

Style *atom* is the same as style *multi* except that in addition, one or more of the atoms involved in the bond, angle, dihedral, or improper interaction must also be of the specified atom type.

For style *bond*, only bonds are candidates for turn-off, and the bond must also be of the specified type. Styles *angle*, *dihedral*, and *improper* are treated similarly.

For style *bond*, you can set the type to 0 to delete bonds that have been previously broken by a bond-breaking potential (which sets the bond type to 0 when a bond is broken); e.g. see the bond_style quartic command.

For style *stats* no interactions are turned off (or on); the status of all interactions in the specified group is simply reported. This is useful for diagnostic purposes if bonds have been turned off by a bond-breaking potential during a previous run.

The default behavior of the delete_bonds command is to turn off interactions by toggling their type to a negative value, but not to permanently remove the interaction. E.g. a bond_type of 2 is set to -2. The neighbor list creation routines will not include such an interaction in their interaction lists. The default is also to not alter the list of 1-2, 1-3, 1-4 neighbors computed by the special_bonds command and used to weight pairwise force and energy calculations. This means that pairwise computations will proceed as if the bond (or angle, etc) were still turned on.

Several keywords can be appended to the argument list to alter the default behaviors.

The *any* keyword changes the requirement that all atoms in the bond (angle, etc) must be in the specified group in order to turn-off the interaction. Instead, if any of the atoms in the interaction are in the specified group, it will be turned off (or on if the *undo* keyword is used).

The *undo* keyword inverts the delete_bonds command so that the specified bonds, angles, etc are turned on if they are currently turned off. This means a negative value is toggled to positive. For example, for style *angle*, if *type* is specified as 2, then all angles with current type = -2, are reset to type = 2. Note that the fix shake command also sets bond and angle types negative, so this option should not be used on those interactions.

The *remove* keyword is invoked at the end of the delete_bonds operation. It causes turned-off bonds (angles, etc) to be removed from each atom's data structure and then adjusts the global bond (angle, etc) counts accordingly. Removal is a permanent change; removed bonds cannot be turned back on via the *undo* keyword. Removal does not alter the pairwise 1-2, 1-3, 1-4 weighting list.

The *special* keyword is invoked at the end of the delete_bonds operation, after (optional) removal. It re-computes the pairwise 1-2, 1-3, 1-4 weighting list. The weighting list computation treats turned-off bonds the same as turned-on. Thus, turned-off bonds must be removed if you wish to change the weighting list.

Note that the choice of *remove* and *special* options affects how 1-2, 1-3, 1-4 pairwise interactions will be computed across bonds that have been modified by the delete_bonds command.

Restrictions:

This command requires inter-processor communication to acquire ghost atoms, to coordinate the deleting of bonds, angles, etc between atoms shared by multiple processors. This means that your system must be ready to perform a simulation before using this command (force fields setup, atom masses set, etc). Just as would be needed to run dynamics, the force field you define should define a cutoff (e.g. through a pair_style command) which is long enough for a processor to acquire the ghost atoms its needs to compute bond, angle, etc interactions.

If deleted bonds (angles, etc) are removed but the 1-2, 1-3, 1-4 weighting list is not recomputed, this can cause a later fix shake command to fail due to an atom's bonds being inconsistent with the weighting list. This should only happen if the group used in the fix command includes both atoms in the bond, in which case you probably should be recomputing the weighting list.

Related commands:

neigh_modify exclude, special_bonds, fix shake

Default: none

dielectric command

Syntax:

```
dielectric value
```

- value = dielectric constant

Examples:

```
dielectric 2.0
```

Description:

Set the dielectric constant for Coulombic interactions (pairwise and long-range) to this value. The constant is unitless, since it is used to reduce the strength of the interactions. The value is used in the denominator of the formulas for Coulombic interactions - e.g. a value of 4.0 reduces the Coulombic interactions to 25% of their default strength. See the pair_style command for more details.

Restrictions: none

Related commands:

pair_style

Default:

```
dielectric 1.0
```

dihedral_style charmm command

dihedral_style charmm/intel command

dihedral_style charmm/kk command

dihedral_style charmm/omp command

Syntax:

```
dihedral_style charmm
```

Examples:

```
dihedral_style charmm
dihedral_coeff 1 120.0 1 60 0.5
```

Description:

The *charmm* dihedral style uses the potential

$$E = K[1 + \cos(n\phi - d)]$$

See (MacKerell) for a description of the CHARMM force field. This dihedral style can also be used for the AMBER force field (see comment on weighting factors below). See (Cornell) for a description of the AMBER force field.

The following coefficients must be defined for each dihedral type via the dihedral_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy)
- n (integer >= 0)
- d (integer value of degrees)
- weighting factor (0.0 to 1.0)

The weighting factor is applied to pairwise interaction between the 1st and 4th atoms in the dihedral, which are computed by a CHARMM pair_style with epsilon and sigma values specified with a pair_coeff command. Note that this weighting factor is unrelated to the weighting factor specified by the special bonds command which applies to all 1-4 interactions in the system.

For CHARMM force fields, the special_bonds 1-4 weighting factor should be set to 0.0. This is because the pair styles that contain "charmm" (e.g. pair_style lj/charmm/coul/long) define extra 1-4 interaction coefficients that are used by this dihedral style to compute those interactions explicitly. This means that if any of the weighting factors defined as dihedral coefficients (4th coeff above) are non-zero, then you must use a charmm pair style. Note that if you do not set the special_bonds 1-4 weighting factor to 0.0 (which is the default) then 1-4 interactions in dihedrals will be computed twice, once by the pair routine and once by the dihedral routine, which is probably not what you want.

For AMBER force fields, the special_bonds 1-4 weighting factor should be set to the AMBER defaults (1/2 and 5/6) and all the dihedral weighting factors (4th coeff above) should be set to 0.0. In this case, you can use any pair style you wish, since the dihedral does not need any 1-4 information.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This dihedral style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

dihedral_coeff

Default: none

(Cornell) Cornell, Cieplak, Bayly, Gould, Merz, Ferguson, Spellmeyer, Fox, Caldwell, Kollman, JACS 117, 5179-5197 (1995).

(MacKerell) MacKerell, Bashford, Bellott, Dunbrack, Evanseck, Field, Fischer, Gao, Guo, Ha, et al, J Phys Chem B, 102, 3586 (1998).

dihedral_style class2 command

dihedral_style class2/omp command

Syntax:

```
dihedral_style class2
```

Examples:

```
dihedral_style class2
dihedral_coeff 1 100 75 100 70 80 60
dihedral_coeff * mbt 3.5945 0.1704 -0.5490 1.5228
dihedral_coeff * ebt 0.3417 0.3264 -0.9036 0.1368 0.0 -0.8080 1.0119 1.1010
dihedral_coeff 2 at 0.0 -0.1850 -0.7963 -2.0220 0.0 -0.3991 110.2453 105.1270
dihedral_coeff * aat -13.5271 110.2453 105.1270
dihedral_coeff * bb13 0.0 1.0119 1.1010
```

Description:

The *class2* dihedral style uses the potential

$$
\begin{aligned}
E &= E_d + E_{mbt} + E_{ebt} + E_{at} + E_{aat} + E_{bb13} \\
E_d &= \sum_{n=1}^{3} K_n[1 - \cos(n\phi - \phi_n)] \\
E_{mbt} &= (r_{jk} - r_2)[A_1 \cos(\phi) + A_2 \cos(2\phi) + A_3 \cos(3\phi)] \\
E_{ebt} &= (r_{ij} - r_1)[B_1 \cos(\phi) + B_2 \cos(2\phi) + B_3 \cos(3\phi)] + \\
&\quad (r_{kl} - r_3)[C_1 \cos(\phi) + C_2 \cos(2\phi) + C_3 \cos(3\phi)] \\
E_{at} &= (\theta_{ijk} - \theta_1)[D_1 \cos(\phi) + D_2 \cos(2\phi) + D_3 \cos(3\phi)] + \\
&\quad (\theta_{jkl} - \theta_2)[E_1 \cos(\phi) + E_2 \cos(2\phi) + E_3 \cos(3\phi)] \\
E_{aat} &= M(\theta_{ijk} - \theta_1)(\theta_{jkl} - \theta_2) \cos(\phi) \\
E_{bb13} &= N(r_{ij} - r_1)(r_{kl} - r_3)
\end{aligned}
$$

where Ed is the dihedral term, Embt is a middle-bond-torsion term, Eebt is an end-bond-torsion term, Eat is an angle-torsion term, Eaat is an angle-angle-torsion term, and Ebb13 is a bond-bond-13 term.

Theta1 and theta2 are equilibrium angles and r1 r2 r3 are equilibrium bond lengths.

See (Sun) for a description of the COMPASS class2 force field.

Coefficients for the Ed, Embt, Eebt, Eat, Eaat, and Ebb13 formulas must be defined for each dihedral type via the dihedral_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands.

These are the 6 coefficients for the Ed formula:

- K1 (energy)
- phi1 (degrees)
- K2 (energy)
- phi2 (degrees)
- K3 (energy)
- phi3 (degrees)

For the Embt formula, each line in a dihedral_coeff command in the input script lists 5 coefficients, the first of which is "mbt" to indicate they are MiddleBondTorsion coefficients. In a data file, these coefficients should be listed under a "MiddleBondTorsion Coeffs" heading and you must leave out the "mbt", i.e. only list 4 coefficients after the dihedral type.

- mbt
- A1 (energy/distance)
- A2 (energy/distance)
- A3 (energy/distance)
- r2 (distance)

For the Eebt formula, each line in a dihedral_coeff command in the input script lists 9 coefficients, the first of which is "ebt" to indicate they are EndBondTorsion coefficients. In a data file, these coefficients should be listed under a "EndBondTorsion Coeffs" heading and you must leave out the "ebt", i.e. only list 8 coefficients after the dihedral type.

- ebt
- B1 (energy/distance)
- B2 (energy/distance)
- B3 (energy/distance)
- C1 (energy/distance)
- C2 (energy/distance)
- C3 (energy/distance)
- r1 (distance)
- r3 (distance)

For the Eat formula, each line in a dihedral_coeff command in the input script lists 9 coefficients, the first of which is "at" to indicate they are AngleTorsion coefficients. In a data file, these coefficients should be listed under a "AngleTorsion Coeffs" heading and you must leave out the "at", i.e. only list 8 coefficients after the dihedral type.

- at
- D1 (energy/radian)
- D2 (energy/radian)
- D3 (energy/radian)
- E1 (energy/radian)
- E2 (energy/radian)
- E3 (energy/radian)
- theta1 (degrees)

- theta2 (degrees)

Theta1 and theta2 are specified in degrees, but LAMMPS converts them to radians internally; hence the units of D and E are in energy/radian.

For the Eaat formula, each line in a dihedral_coeff command in the input script lists 4 coefficients, the first of which is "aat" to indicate they are AngleAngleTorsion coefficients. In a data file, these coefficients should be listed under a "AngleAngleTorsion Coeffs" heading and you must leave out the "aat", i.e. only list 3 coefficients after the dihedral type.

- aat
- M (energy/radian^2)
- theta1 (degrees)
- theta2 (degrees)

Theta1 and theta2 are specified in degrees, but LAMMPS converts them to radians internally; hence the units of M are in energy/radian^2.

For the Ebb13 formula, each line in a dihedral_coeff command in the input script lists 4 coefficients, the first of which is "bb13" to indicate they are BondBond13 coefficients. In a data file, these coefficients should be listed under a "BondBond13 Coeffs" heading and you must leave out the "bb13", i.e. only list 3 coefficients after the dihedral type.

- bb13
- N (energy/distance^2)
- r1 (distance)
- r3 (distance)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This dihedral style can only be used if LAMMPS was built with the CLASS2 package. See the Making LAMMPS section for more info on packages.

Related commands:

dihedral_coeff

Default: none

(Sun) Sun, J Phys Chem B 102, 7338-7364 (1998).

dihedral_coeff command

Syntax:

```
dihedral_coeff N args
```

- N = dihedral type (see asterisk form below)
- args = coefficients for one or more dihedral types

Examples:

```
dihedral_coeff 1 80.0 1 3
dihedral_coeff * 80.0 1 3 0.5
dihedral_coeff 2* 80.0 1 3 0.5
```

Description:

Specify the dihedral force field coefficients for one or more dihedral types. The number and meaning of the coefficients depends on the dihedral style. Dihedral coefficients can also be set in the data file read by the read_data command or in a restart file.

N can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to set the coefficients for multiple dihedral types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of dihedral types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

Note that using a dihedral_coeff command can override a previous setting for the same dihedral type. For example, these commands set the coeffs for all dihedral types, then overwrite the coeffs for just dihedral type 2:

```
dihedral_coeff * 80.0 1 3
dihedral_coeff 2 200.0 1 3
```

A line in a data file that specifies dihedral coefficients uses the exact same format as the arguments of the dihedral_coeff command in an input script, except that wild-card asterisks should not be used since coefficients for all N types must be listed in the file. For example, under the "Dihedral Coeffs" section of a data file, the line that corresponds to the 1st example above would be listed as

```
1 80.0 1 3
```

The dihedral_style class2 is an exception to this rule, in that an additional argument is used in the input script to allow specification of the cross-term coefficients. See its doc page for details.

NOTE: When comparing the formulas and coefficients for various LAMMPS dihedral styles with dihedral equations defined by other force fields, note that some force field implementations divide/multiply the energy prefactor *K* by the multiple number of torsions that contain the J-K bond in an I-J-K-L torsion. LAMMPS does not do this, i.e. the listed dihedral equation applies to each individual dihedral. Thus you need to define *K* appropriately to account for this difference if necessary.

Here is an alphabetic list of dihedral styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated dihedral_coeff command.

Note that there are also additional dihedral styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the dihedral section of this page.

- dihedral_style none - turn off dihedral interactions
- dihedral_style hybrid - define multiple styles of dihedral interactions

- dihedral_style charmm - CHARMM dihedral
- dihedral_style class2 - COMPASS (class 2) dihedral
- dihedral_style harmonic - harmonic dihedral
- dihedral_style helix - helix dihedral
- dihedral_style multi/harmonic - multi-harmonic dihedral
- dihedral_style opls - OPLS dihedral

Restrictions:

This command must come after the simulation box is defined by a read_data, read_restart, or create_box command.

A dihedral style must be defined before any dihedral coefficients are set, either in the input script or in a data file.

Related commands:

dihedral_style

Default: none

dihedral_style cosine/shift/exp command

dihedral_style cosine/shift/exp/omp command

Syntax:

```
dihedral_style cosine/shift/exp
```

Examples:

```
dihedral_style cosine/shift/exp
dihedral_coeff 1 10.0 45.0 2.0
```

Description:

The *cosine/shift/exp* dihedral style uses the potential

$$E = -U_{min}\frac{e^{-aU(\theta,\theta_0)}-1}{e^{a}-1} \quad \text{with} \quad U(\theta,\theta_0) = -0.5\left(1+\cos(\theta-\theta_0)\right)$$

where Umin, theta, and a are defined for each dihedral type.

The potential is bounded between [-Umin:0] and the minimum is located at the angle theta0. The a parameter can be both positive or negative and is used to control the spring constant at the equilibrium.

The spring constant is given by k=a exp(a) Umin/ [2 (Exp(a)-1)]. For a>3 k/Umin = a/2 to better than 5% relative error. For negative values of the a parameter, the spring constant is essentially zero, and anharmonic terms takes over. The potential is furthermore well behaved in the limit a->0, where it has been implemented to linear order in a for a < 0.001.

The following coefficients must be defined for each dihedral type via the dihedral_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- umin (energy)
- theta (angle)
- A (real number)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This dihedral style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

dihedral_coeff, angle_cosineshiftexp

Default: none

dihedral_style fourier command

dihedral_style fourier/omp command

Syntax:

```
dihedral_style fourier
```

Examples:

```
dihedral_style fourier
dihedral_coeff 1 3 -0.846200 3 0.0 7.578800 1 0 0.138000 2 -180.0
```

Description:

The *fourier* dihedral style uses the potential:

$$E = \sum_{i=1,m} K_i[1.0 + \cos(n_i\phi - d_i)]$$

The following coefficients must be defined for each dihedral type via the dihedral_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- m (integer >=1)
- K1 (energy)
- n1 (integer >= 0)
- d1 (degrees)
- ....
- Km (energy)
- nm (integer >= 0)
- dm (degrees)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the USER_MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

dihedral_coeff

Default: none

dihedral_style harmonic command

dihedral_style harmonic/intel command

dihedral_style harmonic/omp command

Syntax:

```
dihedral_style harmonic
```

Examples:

```
dihedral_style harmonic
dihedral_coeff 1 80.0 1 2
```

Description:

The *harmonic* dihedral style uses the potential

$$E = K[1 + d\cos(n\phi)]$$

The following coefficients must be defined for each dihedral type via the dihedral_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy)
- d (+1 or -1)
- n (integer >= 0)

NOTE: Here are important points to take note of when defining LAMMPS dihedral coefficients for the harmonic style, so that they are compatible with how harmonic dihedrals are defined by other force fields:

- The LAMMPS convention is that the trans position = 180 degrees, while in some force fields trans = 0 degrees.
- Some force fields reverse the sign convention on *d*.
- Some force fields let *n* be positive or negative which corresponds to *d* = 1 or -1 for the harmonic style.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input

script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This dihedral style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

dihedral_coeff

Default: none

dihedral_style helix command

dihedral_style helix/omp command

Syntax:

```
dihedral_style helix
```

Examples:

```
dihedral_style helix
dihedral_coeff 1 80.0 100.0 40.0
```

Description:

The *helix* dihedral style uses the potential

$$E = A[1 - \cos(\theta)] + B[1 + \cos(3\theta)] + C[1 + \cos(\theta + \frac{\pi}{4})]$$

This coarse-grain dihedral potential is described in (Guo). For dihedral angles in the helical region, the energy function is represented by a standard potential consisting of three minima, one corresponding to the trans (t) state and the other to gauche states (g+ and g-). The paper describes how the A,B,C parameters are chosen so as to balance secondary (largely driven by local interactions) and tertiary structure (driven by long-range interactions).

The following coefficients must be defined for each dihedral type via the dihedral_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- A (energy)
- B (energy)
- C (energy)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This dihedral style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

dihedral_coeff

Default: none

(Guo) Guo and Thirumalai, Journal of Molecular Biology, 263, 323-43 (1996).

dihedral_style hybrid command

Syntax:

```
dihedral_style hybrid style1 style2 ...
```

- style1,style2 = list of one or more dihedral styles

Examples:

```
dihedral_style hybrid harmonic helix
dihedral_coeff 1 harmonic 6.0 1 3
dihedral_coeff 2* helix 10 10 10
```

Description:

The *hybrid* style enables the use of multiple dihedral styles in one simulation. An dihedral style is assigned to each dihedral type. For example, dihedrals in a polymer flow (of dihedral type 1) could be computed with a *harmonic* potential and dihedrals in the wall boundary (of dihedral type 2) could be computed with a *helix* potential. The assignment of dihedral type to style is made via the dihedral_coeff command or in the data file.

In the dihedral_coeff commands, the name of a dihedral style must be added after the dihedral type, with the remaining coefficients being those appropriate to that style. In the example above, the 2 dihedral_coeff commands set dihedrals of dihedral type 1 to be computed with a *harmonic* potential with coefficients 6.0, 1, 3 for K, d, n. All other dihedral types (2-N) are computed with a *helix* potential with coefficients 10, 10, 10 for A, B, C.

If dihedral coefficients are specified in the data file read via the read_data command, then the same rule applies. E.g. "harmonic" or "helix", must be added after the dihedral type, for each line in the "Dihedral Coeffs" section, e.g.

```
Dihedral Coeffs

1 harmonic 6.0 1 3
2 helix 10 10 10
...
```

If *class2* is one of the dihedral hybrid styles, the same rule holds for specifying additional AngleTorsion (and EndBondTorsion, etc) coefficients either via the input script or in the data file. I.e. *class2* must be added to each line after the dihedral type. For lines in the AngleTorsion (or EndBondTorsion, etc) section of the data file for dihedral types that are not *class2*, you must use an dihedral style of *skip* as a placeholder, e.g.

```
AngleTorsion Coeffs

1 skip
2 class2 1.0 1.0 1.0 3.0 3.0 3.0 30.0 50.0
...
```

Note that it is not necessary to use the dihedral style *skip* in the input script, since AngleTorsion (or EndBondTorsion, etc) coefficients need not be specified at all for dihedral types that are not *class2*.

A dihedral style of *none* with no additional coefficients can be used in place of a dihedral style, either in a input script dihedral_coeff command or in the data file, if you desire to turn off interactions for specific dihedral types.

Restrictions:

This dihedral style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Unlike other dihedral styles, the hybrid dihedral style does not store dihedral coefficient info for individual sub-styles in a binary restart files. Thus when retarting a simulation from a restart file, you need to re-specify dihedral_coeff commands.

Related commands:

dihedral_coeff

Default: none

dihedral_style multi/harmonic command

dihedral_style multi/harmonic/omp command

Syntax:

```
dihedral_style multi/harmonic
```

Examples:

```
dihedral_style multi/harmonic
dihedral_coeff 1 20 20 20 20 20
```

Description:

The *multi/harmonic* dihedral style uses the potential

$$E = \sum_{n=1,5} A_n \cos^{n-1}(\phi)$$

The following coefficients must be defined for each dihedral type via the dihedral_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- A1 (energy)
- A2 (energy)
- A3 (energy)
- A4 (energy)
- A5 (energy)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This dihedral style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

dihedral_coeff

Default: none

dihedral_style nharmonic command

dihedral_style nharmonic/omp command

Syntax:

```
dihedral_style nharmonic
```

Examples:

```
dihedral_style nharmonic
dihedral_coeff 3 10.0 20.0 30.0
```

Description:

The *nharmonic* dihedral style uses the potential:

$$E = \sum_{n=1,n} A_n \cos^{n-1}(\phi)$$

The following coefficients must be defined for each dihedral type via the dihedral_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- n (integer >=1)
- A1 (energy)
- A2 (energy)
- ...
- An (energy)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the USER_MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

dihedral_coeff

Default: none

dihedral_style none command

Syntax:

```
dihedral_style none
```

Examples:

```
dihedral_style none
```

Description:

Using an dihedral style of none means dihedral forces are not computed, even if quadruplets of dihedral atoms were listed in the data file read by the read_data command.

Restrictions: none

Related commands: none

Default: none

dihedral_style opls command

dihedral_style opls/intel command

dihedral_style opls/kk command

dihedral_style opls/omp command

Syntax:

```
dihedral_style opls
```

Examples:

```
dihedral_style opls
dihedral_coeff 1 1.740 -0.157 0.279 0.00   # CT-CT-CT-CT
dihedral_coeff 2 0.000 0.000 0.366 0.000   # CT-CT-CT-HC
dihedral_coeff 3 0.000 0.000 0.318 0.000   # HC-CT-CT-HC
```

Description:

The *opls* dihedral style uses the potential

$$E = \frac{1}{2}K_1[1+\cos(\phi)] + \frac{1}{2}K_2[1-\cos(2\phi)] + \frac{1}{2}K_3[1+\cos(3\phi)] + \frac{1}{2}K_4[1-\cos(4\phi)$$

Note that the usual 1/2 factor is not included in the K values.

This dihedral potential is used in the OPLS force field and is described in (Watkins).

The following coefficients must be defined for each dihedral type via the dihedral_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K1 (energy)
- K2 (energy)
- K3 (energy)
- K4 (energy)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This dihedral style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

dihedral_coeff

Default: none

(Watkins) Watkins and Jorgensen, J Phys Chem A, 105, 4118-4125 (2001).

dihedral_style quadratic command

dihedral_style quadratic/omp command

Syntax:

```
dihedral_style quadratic
```

Examples:

```
dihedral_style quadratic
dihedral_coeff 100.0 80.0
```

Description:

The *quadratic* dihedral style uses the potential:

$$E = K(\phi - \phi_0)^2$$

This dihedral potential can be used to keep a dihedral in a predefined value (cis=zero, right-hand convention is used).

The following coefficients must be defined for each dihedral type via the dihedral_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/radian^2)
- phi0 (degrees)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the USER_MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

dihedral_coeff

Default: none

dihedral_style command

Syntax:

```
dihedral_style style
```

- style = *none* or *hybrid* or *charmm* or *class2* or *harmonic* or *helix* or *multi/harmonic* or *opls*

Examples:

```
dihedral_style harmonic
dihedral_style multi/harmonic
dihedral_style hybrid harmonic charmm
```

Description:

Set the formula(s) LAMMPS uses to compute dihedral interactions between quadruplets of atoms, which remain in force for the duration of the simulation. The list of dihedral quadruplets is read in by a read_data or read_restart command from a data or restart file.

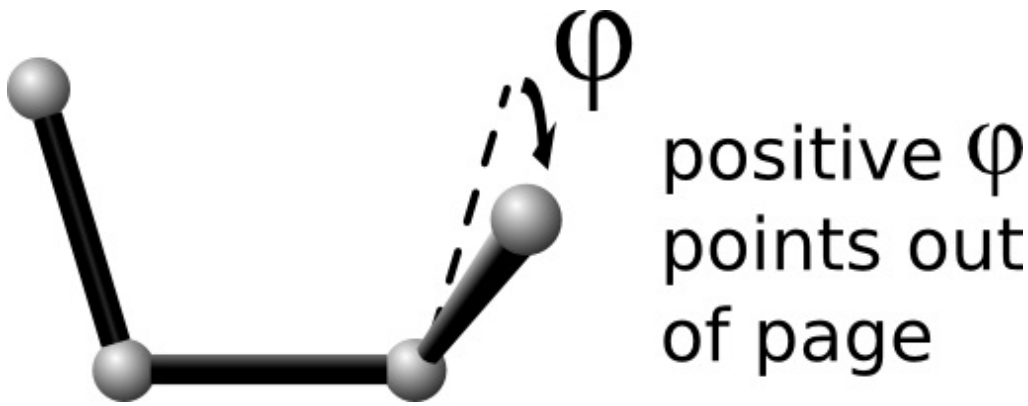
Hybrid models where dihedrals are computed using different dihedral potentials can be setup using the *hybrid* dihedral style.

The coefficients associated with a dihedral style can be specified in a data or restart file or via the dihedral_coeff command.

All dihedral potentials store their coefficient data in binary restart files which means dihedral_style and dihedral_coeff commands do not need to be re-specified in an input script that restarts a simulation. See the read_restart command for details on how to do this. The one exception is that dihedral_style *hybrid* only stores the list of sub-styles in the restart file; dihedral coefficients need to be re-specified.

NOTE: When both a dihedral and pair style is defined, the special_bonds command often needs to be used to turn off (or weight) the pairwise interaction that would otherwise exist between 4 bonded atoms.

In the formulas listed for each dihedral style, *phi* is the torsional angle defined by the quadruplet of atoms. This angle has a sign convention as shown in this diagram:



where the I,J,K,L ordering of the 4 atoms that define the dihedral is from left to right.

This sign convention effects several of the dihedral styles listed below (e.g. charmm, helix) in the sense that the energy formula depends on the sign of phi, which may be reflected in the value of the coefficients you specify.

NOTE: When comparing the formulas and coefficients for various LAMMPS dihedral styles with dihedral equations defined by other force fields, note that some force field implementations divide/multiply the energy prefactor *K* by the multiple number of torsions that contain the J-K bond in an I-J-K-L torsion. LAMMPS does not do this, i.e. the listed dihedral equation applies to each individual dihedral. Thus you need to define *K* appropriately via the dihedral_coeff command to account for this difference if necessary.

Here is an alphabetic list of dihedral styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated dihedral_coeff command.

Note that there are also additional dihedral styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the dihedral section of this page.

- dihedral_style none - turn off dihedral interactions
- dihedral_style hybrid - define multiple styles of dihedral interactions

- dihedral_style charmm - CHARMM dihedral
- dihedral_style class2 - COMPASS (class 2) dihedral
- dihedral_style harmonic - harmonic dihedral
- dihedral_style helix - helix dihedral
- dihedral_style multi/harmonic - multi-harmonic dihedral
- dihedral_style opls - OPLS dihedral

Restrictions:

Dihedral styles can only be set for atom styles that allow dihedrals to be defined.

Most dihedral styles are part of the MOLECULE package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info on packages. The doc pages for individual dihedral potentials tell if it is part of a package.

Related commands:

dihedral_coeff

Default:

dihedral_style none

dihedral_style table command

dihedral_style table/omp command

Syntax:

```
dihedral_style table style Ntable
```

- style = *linear* or *spline* = method of interpolation
- Ntable = size of the internal lookup table

Examples:

```
dihedral_style table spline 400
dihedral_style table linear 1000
dihedral_coeff 1 file.table DIH_TABLE1
dihedral_coeff 2 file.table DIH_TABLE2
```

Description:

The *table* dihedral style creates interpolation tables of length *Ntable* from dihedral potential and derivative values listed in a file(s) as a function of the dihedral angle "phi". The files are read by the dihedral_coeff command.

The interpolation tables are created by fitting cubic splines to the file values and interpolating energy and derivative values at each of *Ntable* dihedral angles. During a simulation, these tables are used to interpolate energy and force values on individual atoms as needed. The interpolation is done in one of 2 styles: *linear* or *spline*.

For the *linear* style, the dihedral angle (phi) is used to find 2 surrounding table values from which an energy or its derivative is computed by linear interpolation.

For the *spline* style, cubic spline coefficients are computed and stored at each of the *Ntable* evenly-spaced values in the interpolated table. For a given dihedral angle (phi), the appropriate coefficients are chosen from this list, and a cubic polynomial is used to compute the energy and the derivative at this angle.

The following coefficients must be defined for each dihedral type via the dihedral_coeff command as in the example above.

- filename
- keyword

The filename specifies a file containing tabulated energy and derivative values. The keyword specifies a section of the file. The format of this file is described below.

The format of a tabulated file is as follows (without the parenthesized comments). It can begin with one or more comment or blank lines.

```
# Table of the potential and its negative derivative

DIH_TABLE1                  (keyword is the first text on line)
N 30 DEGREES                (N, NOF, DEGREES, RADIANS, CHECKU/F)
```

```
                              (blank line)
1 -168.0 -1.40351172223 -0.0423346818422
2 -156.0 -1.70447981034 -0.00811786522531
3 -144.0 -1.62956100432 0.0184129719987
...
30 180.0 -0.707106781187 -0.0719306095245

# Example 2: table of the potential. Forces omitted

DIH_TABLE2
N 30 NOF CHECKU testU.dat CHECKF testF.dat

1 -168.0 -1.40351172223
2 -156.0 -1.70447981034
3 -144.0 -1.62956100432
...
30 180.0 -0.707106781187
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the dihedral_coeff command. The next line lists (in any order) one or more parameters for the table. Each parameter is a keyword followed by one or more numeric values.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is the angle value, the 3rd value is the energy (in energy units), and the 4th is -dE/d(phi) also in energy units). The 3rd term is the energy of the 4-atom configuration for the specified angle. The 4th term (when present) is the negative derivative of the energy with respect to the angle (in degrees, or radians depending on whether the user selected DEGREES or RADIANS). Thus the units of the last term are still energy, not force. The dihedral angle values must increase from one line to the next.

Dihedral table splines are cyclic. There is no discontinuity at 180 degrees (or at any other angle). Although in the examples above, the angles range from -180 to 180 degrees, in general, the first angle in the list can have any value (positive, zero, or negative). However the *range* of angles represented in the table must be *strictly* less than 360 degrees (2pi radians) to avoid angle overlap. (You may not supply entries in the table for both 180 and -180, for example.) If the user's table covers only a narrow range of dihedral angles, strange numerical behavior can occur in the large remaining gap.

Parameters:

The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the N specified in the dihedral_style table command. Let *Ntable* is the number of table entries requested dihedral_style command, and let *Nfile* be the parameter following "N" in the tabulated file ("30" in the sparse example above). What LAMMPS does is a preliminary interpolation by creating splines using the *Nfile* tabulated values as nodal points. It uses these to interpolate as needed to generate energy and derivative values at *Ntable* different points (which are evenly spaced over a 360 degree range, even if the angles in the file are not). The resulting tables of length *Ntable* are then used as described above, when computing energy and force for individual dihedral angles and their atoms. This means that if you want the interpolation tables of length *Ntable* to match exactly what is in the tabulated file (with effectively nopreliminary interpolation), you should set *Ntable* = *Nfile*. To insure the nodal points in the user's file are aligned with the interpolated table entries, the angles in the table should be integer multiples of 360/*Ntable* degrees, or 2*PI/*Ntable* radians (depending on your choice of angle units).

The optional "NOF" keyword allows the user to omit the forces (negative energy derivatives) from the table file (normally located in the 4th column). In their place, forces will be calculated automatically by differentiating the

potential energy function indicated by the 3rd column of the table (using either linear or spline interpolation).

The optional "DEGREES" keyword allows the user to specify angles in degrees instead of radians (default).

The optional "RADIANS" keyword allows the user to specify angles in radians instead of degrees. (Note: This changes the way the forces are scaled in the 4th column of the data file.)

The optional "CHECKU" keyword is followed by a filename. This allows the user to save all of the the *Ntable* different entries in the interpolated energy table to a file to make sure that the interpolated function agrees with the user's expectations. (Note: You can temporarily increase the *Ntable* parameter to a high value for this purpose. "*Ntable*" is explained above.)

The optional "CHECKF" keyword is analogous to the "CHECKU" keyword. It is followed by a filename, and it allows the user to check the interpolated force table. This option is available even if the user selected the "NOF" option.

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This dihedral style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

dihedral_coeff

Default: none

dimension command

Syntax:

```
dimension N
```

- N = 2 or 3

Examples:

```
dimension 2
```

Description:

Set the dimensionality of the simulation. By default LAMMPS runs 3d simulations. To run a 2d simulation, this command should be used prior to setting up a simulation box via the create_box or read_data commands. Restart files also store this setting.

See the discussion in Section_howto for additional instructions on how to run 2d simulations.

NOTE: Some models in LAMMPS treat particles as finite-size spheres or ellipsoids, as opposed to point particles. In 2d, the particles will still be spheres or ellipsoids, not circular disks or ellipses, meaning their moment of inertia will be the same as in 3d.

Restrictions:

This command must be used before the simulation box is defined by a read_data or create_box command.

Related commands:

fix enforce2d

Default:

```
dimension 3
```

displace_atoms command

Syntax:

```
displace_atoms group-ID style args keyword value ...
```

- group-ID = ID of group of atoms to displace
- style = *move* or *ramp* or *random* or *rotate*

```
  move args = delx dely delz
      delx,dely,delz = distance to displace in each dimension (distance units)
      any of delx,dely,delz can be a variable (see below)
    ramp args = ddim dlo dhi dim clo chi
      ddim = x or y or z
      dlo,dhi = displacement distance between dlo and dhi (distance units)
      dim = x or y or z
      clo,chi = lower and upper bound of domain to displace (distance units)
    random args = dx dy dz seed
      dx,dy,dz = random displacement magnitude in each dimension (distance units)
      seed = random # seed (positive integer)
    rotate args = Px Py Pz Rx Ry Rz theta
      Px,Py,Pz = origin point of axis of rotation (distance units)
      Rx,Ry,Rz = axis of rotation vector
      theta = angle of rotation (degrees)
```

- zero or more keyword/value pairs may be appended

```
  keyword = units
    value = box or lattice
```

Examples:

```
displace_atoms top move 0 -5 0 units box
displace_atoms flow ramp x 0.0 5.0 y 2.0 20.5
```

Description:

Displace a group of atoms. This can be used to move atoms a large distance before beginning a simulation or to randomize atoms initially on a lattice. For example, in a shear simulation, an initial strain can be imposed on the system. Or two groups of atoms can be brought into closer proximity.

The *move* style displaces the group of atoms by the specified 3d displacement vector. Any of the 3 quantities defining the vector components can be specified as an equal-style or atom-style variable. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated, and its value(s) used for the displacement(s). The scale factor implied by the *units* keyword will also be applied to the variable result.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates or per-atom values read from a file. Note that if the variable references other compute or fix commands, those values must be up-to-date for the current timestep. See the "Variable Accuracy" section of the variable doc page for more details.

The *ramp* style displaces atoms a variable amount in one dimension depending on the atom's coordinate in a (possibly) different dimension. For example, the second example command displaces atoms in the x-direction an amount between 0.0 and 5.0 distance units. Each atom's displacement depends on the fractional distance its y coordinate is between 2.0 and 20.5. Atoms with y-coordinates outside those bounds will be moved the minimum (0.0) or maximum (5.0) amount.

The *random* style independently moves each atom in the group by a random displacement, uniformly sampled from a value between -dx and +dx in the x dimension, and similarly for y and z. Random numbers are used in such a way that the displacement of a particular atom is the same, regardless of how many processors are being used.

The *rotate* style rotates each atom in the group by the angle *theta* around a rotation axis *R* = (Rx,Ry,Rz) that goes thru a point *P* = (Px,Py,Pz). The direction of rotation for the atoms around the rotation axis is consistent with the right-hand rule: if your right-hand thumb points along *R*, then your fingers wrap around the axis in the direction of positive theta.

If the defined atom_style assigns an orientation to each atom (atom styles ellipsoid, line, tri, body), then that property is also updated appropriately to correspond to the atom's rotation.

Distance units for displacements and the origin point of the *rotate* style are determined by the setting of *box* or *lattice* for the *units* keyword. *Box* means distance units as defined by the units command - e.g. Angstroms for *real* units. *Lattice* means distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacing.

NOTE: Care should be taken not to move atoms on top of other atoms. After the move, atoms are remapped into the periodic simulation box if needed, and any shrink-wrap boundary conditions (see the boundary command) are enforced which may change the box size. Other than this effect, this command does not change the size or shape of the simulation box. See the change_box command if that effect is desired.

NOTE: Atoms can be moved arbitrarily long distances by this command. If the simulation box is non-periodic and shrink-wrapped (see the boundary command), this can change its size or shape. This is not a problem, except that the mapping of processors to the simulation box is not changed by this command from its initial 3d configuration; see the processors command. Thus, if the box size/shape changes dramatically, the mapping of processors to the simulation box may not end up as optimal as the initial mapping attempted to be.

Restrictions:

You cannot rotate around any rotation vector except the z-axis for a 2d simulation.

Related commands:

lattice, change_box, fix_move

Default:

The option defaults are units = lattice.

dump command

dump h5md command

dump image command

dump movie command

dump molfile command

Syntax:

```
dump ID group-ID style N file args
```

- ID = user-assigned name for the dump
- group-ID = ID of the group of atoms to be dumped
- style = *atom* or *atom/gz* or *atom/mpiio* or *cfg* or *cfg/gz* or *cfg/mpiio* or *dcd* or *xtc* or *xyz* or *xyz/gz* or *xyz/mpiio* or *h5md* or *image* or *movie* or *molfile* or *local* or *custom* or *custom/gz* or *custom/mpiio*
- N = dump every this many timesteps
- file = name of file to write dump info to
- args = list of arguments for a particular style

```
atom args = none
  atom/gz args = none
  atom/mpiio args = none
  cfg args = same as custom args, see below
  cfg/gz args = same as custom args, see below
  cfg/mpiio args = same as custom args, see below
  dcd args = none
  xtc args = none
  xyz args = none

xyz/gz args = none

xyz/mpiio args = none

h5md args = discussed on dump h5md doc page

image args = discussed on dump image doc page

movie args = discussed on dump image doc page

molfile args = discussed on dump molfile doc page

local args = list of local attributes
    possible attributes = index, c_ID, c_ID[N], f_ID, f_ID[N]
      index = enumeration of local values
      c_ID = local vector calculated by a compute with ID
      c_ID[N] = Nth column of local array calculated by a compute with ID
      f_ID = local vector calculated by a fix with ID
      f_ID[N] = Nth column of local array calculated by a fix with ID

custom or custom/gz or custom/mpiio args = list of atom attributes
    possible attributes = id, mol, proc, procp1, type, element, mass,
```

```
                        x, y, z, xs, ys, zs, xu, yu, zu,
                        xsu, ysu, zsu, ix, iy, iz,
                        vx, vy, vz, fx, fy, fz,
                        q, mux, muy, muz, mu,
                        radius, diameter, omegax, omegay, omegaz,
                        angmomx, angmomy, angmomz, tqx, tqy, tqz,
                        c_ID, c_ID[N], f_ID, f_ID[N], v_name

      id = atom ID
      mol = molecule ID
      proc = ID of processor that owns atom
      procp1 = ID+1 of processor that owns atom
      type = atom type
      element = name of atom element, as defined by dump_modify command
      mass = atom mass
      x,y,z = unscaled atom coordinates
      xs,ys,zs = scaled atom coordinates
      xu,yu,zu = unwrapped atom coordinates
      xsu,ysu,zsu = scaled unwrapped atom coordinates
      ix,iy,iz = box image that the atom is in
      vx,vy,vz = atom velocities
      fx,fy,fz = forces on atoms
      q = atom charge
      mux,muy,muz = orientation of dipole moment of atom
      mu = magnitude of dipole moment of atom
      radius,diameter = radius,diameter of spherical particle
      omegax,omegay,omegaz = angular velocity of spherical particle
      angmomx,angmomy,angmomz = angular momentum of aspherical particle
      tqx,tqy,tqz = torque on finite-size particles
      c_ID = per-atom vector calculated by a compute with ID
      c_ID[N] = Nth column of per-atom array calculated by a compute with ID
      f_ID = per-atom vector calculated by a fix with ID
      f_ID[N] = Nth column of per-atom array calculated by a fix with ID
      v_name = per-atom vector calculated by an atom-style variable with name
      d_name = per-atom floating point vector with name, managed by fix property/atom
      i_name = per-atom integer vector with name, managed by fix property/atom
```

Examples:

```
dump myDump all atom 100 dump.atom
dump myDump all atom/mpiio 100 dump.atom.mpiio
dump myDump all atom/gz 100 dump.atom.gz
dump 2 subgroup atom 50 dump.run.bin
dump 2 subgroup atom 50 dump.run.mpiio.bin
dump 4a all custom 100 dump.myforce.* id type x y vx fx
dump 4b flow custom 100 dump.%.myforce id type c_myF[3] v_ke
dump 2 inner cfg 10 dump.snap.*.cfg mass type xs ys zs vx vy vz
dump snap all cfg 100 dump.config.*.cfg mass type xs ys zs id type c_Stress[2]
dump 1 all xtc 1000 file.xtc
```

Description:

Dump a snapshot of atom quantities to one or more files every N timesteps in one of several styles. The *image* and *movie* styles are the exception: the *image* style renders a JPG, PNG, or PPM image file of the atom configuration every N timesteps while the *movie* style combines and compresses them into a movie file; both are discussed in detail on the dump image doc page. The timesteps on which dump output is written can also be controlled by a variable. See the dump_modify every command.

Only information for atoms in the specified group is dumped. The dump_modify thresh and region commands can also alter what atoms are included. Not all styles support all these options; see details below.

As described below, the filename determines the kind of output (text or binary or gzipped, one big file or one per timestep, one big file or multiple smaller files).

NOTE: Because periodic boundary conditions are enforced only on timesteps when neighbor lists are rebuilt, the coordinates of an atom written to a dump file may be slightly outside the simulation box.

NOTE: Unless the dump_modify sort option is invoked, the lines of atom information written to dump files (typically one line per atom) will be in an indeterminate order for each snapshot. This is even true when running on a single processor, if the atom_modify sort option is on, which it is by default. In this case atoms are re-ordered periodically during a simulation, due to spatial sorting. It is also true when running in parallel, because data for a single snapshot is collected from multiple processors, each of which owns a subset of the atoms.

For the *atom*, *custom*, *cfg*, and *local* styles, sorting is off by default. For the *dcd*, *xtc*, *xyz*, and *molfile* styles, sorting by atom ID is on by default. See the dump_modify doc page for details.

The *atom/gz*, *cfg/gz*, *custom/gz*, and *xyz/gz* styles are identical in command syntax to the corresponding styles without "gz", however, they generate compressed files using the zlib library. Thus the filename suffix ".gz" is mandatory. This is an alternative approach to writing compressed files via a pipe, as done by the regular dump styles, which may be required on clusters where the interface to the high-speed network disallows using the fork() library call (which is needed for a pipe). For the remainder of this doc page, you should thus consider the *atom* and *atom/gz* styles (etc) to be inter-changeable, with the exception of the required filename suffix.

As explained below, the *atom/mpiio*, *cfg/mpiio*, *custom/mpiio*, and *xyz/mpiio* styles are identical in command syntax and in the format of the dump files they create, to the corresponding styles without "mpiio", except the single dump file they produce is written in parallel via the MPI-IO library. For the remainder of this doc page, you should thus consider the *atom* and *atom/mpiio* styles (etc) to be inter-changeable. The one exception is how the filename is specified for the MPI-IO styles, as explained below.

The *style* keyword determines what atom quantities are written to the file and in what format. Settings made via the dump_modify command can also alter the format of individual values and the file itself.

The *atom*, *local*, and *custom* styles create files in a simple text format that is self-explanatory when viewing a dump file. Many of the LAMMPS post-processing tools, including Pizza.py, work with this format, as does the rerun command.

For post-processing purposes the *atom*, *local*, and *custom* text files are self-describing in the following sense.

The dimensions of the simulation box are included in each snapshot. For an orthogonal simulation box this information is is formatted as:

```
ITEM: BOX BOUNDS xx yy zz
xlo xhi
ylo yhi
zlo zhi
```

where xlo,xhi are the maximum extents of the simulation box in the x-dimension, and similarly for y and z. The "xx yy zz" represent 6 characters that encode the style of boundary for each of the 6 simulation box boundaries (xlo,xhi and ylo,yhi and zlo,zhi). Each of the 6 characters is either p = periodic, f = fixed, s = shrink wrap, or m = shrink wrapped with a minimum value. See the boundary command for details.

For triclinic simulation boxes (non-orthogonal), an orthogonal bounding box which encloses the triclinic simulation box is output, along with the 3 tilt factors (xy, xz, yz) of the triclinic box, formatted as follows:

```
ITEM: BOX BOUNDS xy xz yz xx yy zz
xlo_bound xhi_bound xy
ylo_bound yhi_bound xz
zlo_bound zhi_bound yz
```

The presence of the text "xy xz yz" in the ITEM line indicates that the 3 tilt factors will be included on each of the 3 following lines. This bounding box is convenient for many visualization programs. The meaning of the 6 character flags for "xx yy zz" is the same as above.

Note that the first two numbers on each line are now xlo_bound instead of xlo, etc, since they repesent a bounding box. See this section of the doc pages for a geometric description of triclinic boxes, as defined by LAMMPS, simple formulas for how the 6 bounding box extents (xlo_bound,xhi_bound,etc) are calculated from the triclinic parameters, and how to transform those parameters to and from other commonly used triclinic representations.

The "ITEM: ATOMS" line in each snapshot lists column descriptors for the per-atom lines that follow. For example, the descriptors would be "id type xs ys zs" for the default *atom* style, and would be the atom attributes you specify in the dump command for the *custom* style.

For style *atom*, atom coordinates are written to the file, along with the atom ID and atom type. By default, atom coords are written in a scaled format (from 0 to 1). I.e. an x value of 0.25 means the atom is at a location 1/4 of the distance from xlo to xhi of the box boundaries. The format can be changed to unscaled coords via the dump_modify settings. Image flags can also be added for each atom via dump_modify.

Style *custom* allows you to specify a list of atom attributes to be written to the dump file for each atom. Possible attributes are listed above and will appear in the order specified. You cannot specify a quantity that is not defined for a particular simulation - such as *q* for atom style *bond*, since that atom style doesn't assign charges. Dumps occur at the very end of a timestep, so atom attributes will include effects due to fixes that are applied during the timestep. An explanation of the possible dump custom attributes is given below.

For style *local*, local output generated by computes and fixes is used to generate lines of output that is written to the dump file. This local data is typically calculated by each processor based on the atoms it owns, but there may be zero or more entities per atom, e.g. a list of bond distances. An explanation of the possible dump local attributes is given below. Note that by using input from the compute property/local command with dump local, it is possible to generate information on bonds, angles, etc that can be cut and pasted directly into a data file read by the read_data command.

Style *cfg* has the same command syntax as style *custom* and writes extended CFG format files, as used by the AtomEye visualization package. Since the extended CFG format uses a single snapshot of the system per file, a wildcard "*" must be included in the filename, as discussed below. The list of atom attributes for style *cfg* must begin with either "mass type xs ys zs" or "mass type xsu ysu zsu" since these quantities are needed to write the CFG files in the appropriate format (though the "mass" and "type" fields do not appear explicitly in the file). Any remaining attributes will be stored as "auxiliary properties" in the CFG files. Note that you will typically want to use the dump_modify element command with CFG-formatted files, to associate element names with atom types, so that AtomEye can render atoms appropriately. When unwrapped coordinates *xsu*, *ysu*, and *zsu* are requested, the nominal AtomEye periodic cell dimensions are expanded by a large factor UNWRAPEXPAND = 10.0, which ensures atoms that are displayed correctly for up to UNWRAPEXPAND/2 periodic boundary crossings in any direction. Beyond this, AtomEye will rewrap the unwrapped coordinates. The expansion causes the atoms to be drawn farther away from the viewer, but it is easy to zoom the atoms closer, and the interatomic distances are unaffected.

The *dcd* style writes DCD files, a standard atomic trajectory format used by the CHARMM, NAMD, and XPlor molecular dynamics packages. DCD files are binary and thus may not be portable to different machines. The number of atoms per snapshot cannot change with the *dcd* style. The *unwrap* option of the dump_modify

command allows DCD coordinates to be written "unwrapped" by the image flags for each atom. Unwrapped means that if the atom has passed through a periodic boundary one or more times, the value is printed for what the coordinate would be if it had not been wrapped back into the periodic box. Note that these coordinates may thus be far outside the box size stored with the snapshot.

The *xtc* style writes XTC files, a compressed trajectory format used by the GROMACS molecular dynamics package, and described here. The precision used in XTC files can be adjusted via the dump_modify command. The default value of 1000 means that coordinates are stored to 1/1000 nanometer accuracy. XTC files are portable binary files written in the NFS XDR data format, so that any machine which supports XDR should be able to read them. The number of atoms per snapshot cannot change with the *xtc* style. The *unwrap* option of the dump_modify command allows XTC coordinates to be written "unwrapped" by the image flags for each atom. Unwrapped means that if the atom has passed thru a periodic boundary one or more times, the value is printed for what the coordinate would be if it had not been wrapped back into the periodic box. Note that these coordinates may thus be far outside the box size stored with the snapshot.

The *xyz* style writes XYZ files, which is a simple text-based coordinate format that many codes can read. Specifically it has a line with the number of atoms, then a comment line that is usually ignored followed by one line per atom with the atom type and the x-, y-, and z-coordinate of that atom. You can use the dump_modify element option to change the output from using the (numerical) atom type to an element name (or some other label). This will help many visualization programs to guess bonds and colors.

Note that *atom*, *custom*, *dcd*, *xtc*, and *xyz* style dump files can be read directly by VMD, a popular molecular viewing program. See Section tools of the manual and the tools/lmp2vmd/README.txt file for more information about support in VMD for reading and visualizing LAMMPS dump files.

Dumps are performed on timesteps that are a multiple of N (including timestep 0) and on the last timestep of a minimization if the minimization converges. Note that this means a dump will not be performed on the initial timestep after the dump command is invoked, if the current timestep is not a multiple of N. This behavior can be changed via the dump_modify first command, which can also be useful if the dump command is invoked after a minimization ended on an arbitrary timestep. N can be changed between runs by using the dump_modify every command (not allowed for *dcd* style). The dump_modify every command also allows a variable to be used to determine the sequence of timesteps on which dump files are written. In this mode a dump on the first timestep of a run will also not be written unless the dump_modify first command is used.

The specified filename determines how the dump file(s) is written. The default is to write one large text file, which is opened when the dump command is invoked and closed when an undump command is used or when LAMMPS exits. For the *dcd* and *xtc* styles, this is a single large binary file.

Dump filenames can contain two wildcard characters. If a "*" character appears in the filename, then one file per snapshot is written and the "*" character is replaced with the timestep value. For example, tmp.dump.* becomes tmp.dump.0, tmp.dump.10000, tmp.dump.20000, etc. This option is not available for the *dcd* and *xtc* styles. Note that the dump_modify pad command can be used to insure all timestep numbers are the same length (e.g. 00010), which can make it easier to read a series of dump files in order with some post-processing tools.

If a "%" character appears in the filename, then each of P processors writes a portion of the dump file, and the "%" character is replaced with the processor ID from 0 to P-1. For example, tmp.dump.% becomes tmp.dump.0, tmp.dump.1, ... tmp.dump.P-1, etc. This creates smaller files and can be a fast mode of output on parallel machines that support parallel I/O for output. This option is not available for the *dcd*, *xtc*, and *xyz* styles.

By default, P = the number of processors meaning one file per processor, but P can be set to a smaller value via the *nfile* or *fileper* keywords of the dump_modify command. These options can be the most efficient way of writing out dump files when running on large numbers of processors.

Note that using the "*" and "%" characters together can produce a large number of small dump files!

For the *atom/mpiio*, *cfg/mpiio*, *custom/mpiio*, and *xyz/mpiio* styles, a single dump file is written in parallel via the MPI-IO library, which is part of the MPI standard for versions 2.0 and above. Using MPI-IO requires two steps. First, build LAMMPS with its MPIIO package installed, e.g.

```
make yes-mpiio    # installs the MPIIO package
make g++          # build LAMMPS for your platform
```

Second, use a dump filename which contains ".mpiio". Note that it does not have to end in ".mpiio", just contain those characters. Unlike MPI-IO restart files, which must be both written and read using MPI-IO, the dump files produced by these MPI-IO styles are identical in format to the files produced by their non-MPI-IO style counterparts. This means you can write a dump file using MPI-IO and use the read_dump command or perform other post-processing, just as if the dump file was not written using MPI-IO.

Note that MPI-IO dump files are one large file which all processors write to. You thus cannot use the "%" wildcard character described above in the filename since that specifies generation of multiple files. You can use the ".bin" suffix described below in an MPI-IO dump file; again this file will be written in parallel and have the same binary format as if it were written without MPI-IO.

If the filename ends with ".bin", the dump file (or files, if "*" or "%" is also used) is written in binary format. A binary dump file will be about the same size as a text version, but will typically write out much faster. Of course, when post-processing, you will need to convert it back to text format (see the binary2txt tool) or write your own code to read the binary file. The format of the binary file can be understood by looking at the tools/binary2txt.cpp file. This option is only available for the *atom* and *custom* styles.

If the filename ends with ".gz", the dump file (or files, if "*" or "%" is also used) is written in gzipped format. A gzipped dump file will be about 3x smaller than the text version, but will also take longer to write. This option is not available for the *dcd* and *xtc* styles.

This section explains the local attributes that can be specified as part of the *local* style.

The *index* attribute can be used to generate an index number from 1 to N for each line written into the dump file, where N is the total number of local datums from all processors, or lines of output that will appear in the snapshot. Note that because data from different processors depend on what atoms they currently own, and atoms migrate between processor, there is no guarantee that the same index will be used for the same info (e.g. a particular bond) in successive snapshots.

The *c_ID* and *c_ID[N]* attributes allow local vectors or arrays calculated by a compute to be output. The ID in the attribute should be replaced by the actual ID of the compute that has been defined previously in the input script. See the compute command for details. There are computes for calculating local information such as indices, types, and energies for bonds and angles.

Note that computes which calculate global or per-atom quantities, as opposed to local quantities, cannot be output in a dump local command. Instead, global quantities can be output by the thermo_style custom command, and per-atom quantities can be output by the dump custom command.

If *c_ID* is used as a attribute, then the local vector calculated by the compute is printed. If *c_ID[N]* is used, then N must be in the range from 1-M, which will print the Nth column of the M-length local array calculated by the compute.

The *f_ID* and *f_ID[N]* attributes allow local vectors or arrays calculated by a fix to be output. The ID in the attribute should be replaced by the actual ID of the fix that has been defined previously in the input script.

If *f_ID* is used as a attribute, then the local vector calculated by the fix is printed. If *f_ID[N]* is used, then N must be in the range from 1-M, which will print the Nth column of the M-length local array calculated by the fix.

Here is an example of how to dump bond info for a system, including the distance and energy of each bond:

```
compute 1 all property/local batom1 batom2 btype
compute 2 all bond/local dist eng
dump 1 all local 1000 tmp.dump index c_1[1] c_1[2] c_1[3] c_2[1] c_2[2]
```

This section explains the atom attributes that can be specified as part of the *custom* and *cfg* styles.

The *id*, *mol*, *proc*, *procp1*, *type*, *element*, *mass*, *vx*, *vy*, *vz*, *fx*, *fy*, *fz*, *q* attributes are self-explanatory.

Id is the atom ID. *Mol* is the molecule ID, included in the data file for molecular systems. *Proc* is the ID of the processor (0 to Nprocs-1) that currently owns the atom. *Procp1* is the proc ID+1, which can be convenient in place of a *type* attribute (1 to Ntypes) for coloring atoms in a visualization program. *Type* is the atom type (1 to Ntypes). *Element* is typically the chemical name of an element, which you must assign to each type via the dump_modify element command. More generally, it can be any string you wish to associated with an atom type. *Mass* is the atom mass. *Vx*, *vy*, *vz*, *fx*, *fy*, *fz*, and *q* are components of atom velocity and force and atomic charge.

There are several options for outputting atom coordinates. The *x*, *y*, *z* attributes write atom coordinates "unscaled", in the appropriate distance units (Angstroms, sigma, etc). Use *xs*, *ys*, *zs* if you want the coordinates "scaled" to the box size, so that each value is 0.0 to 1.0. If the simulation box is triclinic (tilted), then all atom coords will still be between 0.0 and 1.0. Use *xu*, *yu*, *zu* if you want the coordinates "unwrapped" by the image flags for each atom. Unwrapped means that if the atom has passed thru a periodic boundary one or more times, the value is printed for what the coordinate would be if it had not been wrapped back into the periodic box. Note that using *xu*, *yu*, *zu* means that the coordinate values may be far outside the box bounds printed with the snapshot. Using *xsu*, *ysu*, *zsu* is similar to using *xu*, *yu*, *zu*, except that the unwrapped coordinates are scaled by the box size. Atoms that have passed through a periodic boundary will have the corresponding cooordinate increased or decreased by 1.0.

The image flags can be printed directly using the *ix*, *iy*, *iz* attributes. For periodic dimensions, they specify which image of the simulation box the atom is considered to be in. An image of 0 means it is inside the box as defined. A value of 2 means add 2 box lengths to get the true value. A value of -1 means subtract 1 box length to get the true value. LAMMPS updates these flags as atoms cross periodic boundaries during the simulation.

The *mux*, *muy*, *muz* attributes are specific to dipolar systems defined with an atom style of *dipole*. They give the orientation of the atom's point dipole moment. The *mu* attribute gives the magnitude of the atom's dipole moment.

The *radius* and *diameter* attributes are specific to spherical particles that have a finite size, such as those defined with an atom style of *sphere*.

The *omegax*, *omegay*, and *omegaz* attributes are specific to finite-size spherical particles that have an angular velocity. Only certain atom styles, such as *sphere* define this quantity.

The *angmomx*, *angmomy*, and *angmomz* attributes are specific to finite-size aspherical particles that have an angular momentum. Only the *ellipsoid* atom style defines this quantity.

The *tqx*, *tqy*, *tqz* attributes are for finite-size particles that can sustain a rotational torque due to interactions with other particles.

The *c_ID* and *c_ID[N]* attributes allow per-atom vectors or arrays calculated by a compute to be output. The ID in the attribute should be replaced by the actual ID of the compute that has been defined previously in the input script. See the compute command for details. There are computes for calculating the per-atom energy, stress,

centro-symmetry parameter, and coordination number of individual atoms.

Note that computes which calculate global or local quantities, as opposed to per-atom quantities, cannot be output in a dump custom command. Instead, global quantities can be output by the thermo_style custom command, and local quantities can be output by the dump local command.

If *c_ID* is used as a attribute, then the per-atom vector calculated by the compute is printed. If *c_ID[N]* is used, then N must be in the range from 1-M, which will print the Nth column of the M-length per-atom array calculated by the compute.

The *f_ID* and *f_ID[N]* attributes allow vector or array per-atom quantities calculated by a fix to be output. The ID in the attribute should be replaced by the actual ID of the fix that has been defined previously in the input script. The fix ave/atom command is one that calculates per-atom quantities. Since it can time-average per-atom quantities produced by any compute, fix, or atom-style variable, this allows those time-averaged results to be written to a dump file.

If *f_ID* is used as a attribute, then the per-atom vector calculated by the fix is printed. If *f_ID[N]* is used, then N must be in the range from 1-M, which will print the Nth column of the M-length per-atom array calculated by the fix.

The *v_name* attribute allows per-atom vectors calculated by a variable to be output. The name in the attribute should be replaced by the actual name of the variable that has been defined previously in the input script. Only an atom-style variable can be referenced, since it is the only style that generates per-atom values. Variables of style *atom* can reference individual atom attributes, per-atom atom attributes, thermodynamic keywords, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of creating quantities to output to a dump file.

The *d_name* and *i_name* attributes allow to output custom per atom floating point or integer properties that are managed by fix property/atom.

See Section_modify of the manual for information on how to add new compute and fix styles to LAMMPS to calculate per-atom quantities which could then be output into dump files.

Restrictions:

To write gzipped dump files, you must either compile LAMMPS with the -DLAMMPS_GZIP option or use the styles from the COMPRESS package - see the Making LAMMPS section of the documentation.

The *atom/gz*, *cfg/gz*, *custom/gz*, and *xyz/gz* styles are part of the COMPRESS package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The *atom/mpiio*, *cfg/mpiio*, *custom/mpiio*, and *xyz/mpiio* styles are part of the MPIIO package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The *xtc* style is part of the XTC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info. This is because some machines may not support the low-level XDR data format that XTC files are written with, which will result in a compile-time error when a low-level include file is not found. Putting this style in a package makes it easy to exclude from a LAMMPS build for those machines. However, the XTC package also includes two compatibility header files and associated functions, which should be a suitable substitute on machines that do not have the appropriate native header files. This option can be invoked at build time by adding -DLAMMPS_XDR to the CCFLAGS variable in the appropriate low-level Makefile, e.g. src/MAKE/Makefile.foo. This compatibility mode has been tested successfully on Cray

XT3/XT4/XT5 and IBM BlueGene/L machines and should also work on IBM BG/P, and Windows XP/Vista/7 machines.

Related commands:

dump h5md, dump image, dump molfile, dump_modify, undump

Default:

The defaults for the *image* and *movie* styles are listed on the dump image doc page.

dump h5md command

Syntax:

```
dump ID group-ID h5md N file.h5 args
```

- ID = user-assigned name for the dump
- group-ID = ID of the group of atoms to be imaged
- h5md = style of dump command (other styles *atom* or *cfg* or *dcd* or *xtc* or *xyz* or *local* or *custom* are discussed on the dump doc page)
- N = dump every this many timesteps
- file.h5 = name of file to write to
- args = list of data elements to dump, with their dump "subintervals". At least one element must be given and image may only be present if position is specified first.

```
position options
image
velocity options
force options
species options
file_from ID: do not open a new file, re-use the already opened file from dump ID
box value = yes or no
create_group value = yes or no
author value = quoted string
```

For the elements *position*, *velocity*, *force* and *species*, one may specify a sub-interval to write the data only every N_element iterations of the dump (i.e. every N*N_element time steps). This is specified by the option

```
every N_element
```

that follows directly the element declaration.

Examples:

```
dump h5md1 all h5md 100 dump_h5md.h5 position image
dump h5md1 all h5md 100 dump_h5md.h5 position velocity every 10
dump h5md1 all h5md 100 dump_h5md.h5 velocity author "John Doe"
```

Description:

Dump a snapshot of atom coordinates every N timesteps in the HDF5 based H5MD file format (de Buyl). HDF5 files are binary, portable and self-describing. This dump style will write only one file, on the root node.

Several dumps may write to the same file, by using file_from and referring to a previously defined dump. Several groups may also be stored within the same file by defining several dumps. A dump that refers (via *file_from*) to an already open dump ID and that concerns another particle group must specify *create_group yes*.

Each data element is written every N*N_element steps. For *image*, no subinterval is needed as it must be present at the same interval as *position*. *image* must be given after *position* in any case. The box information (edges in each dimension) is stored at the same interval than the *position* element, if present. Else it is stored every N steps.

NOTE: Because periodic boundary conditions are enforced only on timesteps when neighbor lists are rebuilt, the coordinates of an atom written to a dump file may be slightly outside the simulation box.

Use from write_dump:

It is possible to use this dump style with the write_dump command. In this case, the subintervals must not be set at all. The write_dump command can be used either to create a new file or to add current data to an existing dump file by using the *file_from* keyword.

Typically, the *species* data is fixed. The following two commands store the position data every 100 timesteps, with the image data, and store once the species data in the same file.

```
dump h5md1 all h5md 100 dump.h5 position image
write_dump all h5md dump.h5 file_from h5md1 species
```

Restrictions:

The number of atoms per snapshot cannot change with the h5md style. The position data is stored wrapped (box boundaries not enforced, see note above). Only orthogonal domains are currently supported. This is a limitation of the present dump h5md command and not of H5MD itself.

The *h5md* dump style is part of the USER-H5MD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info. It also requires (i) building the ch5md library provided with LAMMPS (See the Making LAMMPS section for more info.) and (ii) having the HDF5 library installed (C bindings are sufficient) on your system. The library ch5md is compiled with the h5cc wrapper provided by the HDF5 library.

Related commands:

dump, dump_modify, undump

(de Buyl) de Buyl, Colberg and Hofling, H5MD: A structured, efficient, and portable file format for molecular data, Comp. Phys. Comm. 185(6), 1546-1553 (2014) - [arXiv:1308.6382].

dump image command

dump movie command

Syntax:

```
dump ID group-ID style N file color diameter keyword value ...
```

- ID = user-assigned name for the dump
- group-ID = ID of the group of atoms to be imaged
- style = *image* or *movie* = style of dump command (other styles *atom* or *cfg* or *dcd* or *xtc* or *xyz* or *local* or *custom* are discussed on the dump doc page)
- N = dump every this many timesteps
- file = name of file to write image to
- color = atom attribute that determines color of each atom
- diameter = atom attribute that determines size of each atom
- zero or more keyword/value pairs may be appended
- keyword = *atom* or *adiam* or *bond* or *line* or *tri* or *body* or *size* or *view* or *center* or *up* or *zoom* or *persp* or *box* or *axes* or *subbox* or *shiny* or *ssao*

```
atom = yes/no = do or do not draw atoms
  adiam size = numeric value for atom diameter (distance units)
  bond values = color width = color and width of bonds
    color = atom or type or none
    width = number or atom or type or none
      number = numeric value for bond width (distance units)
  line = color width
    color = type
    width = numeric value for line width (distance units)
  tri = color tflag width
    color = type
    tflag = 1 for just triangle, 2 for just tri edges, 3 for both
    width = numeric value for tringle edge width (distance units)
  body = color bflag1 bflag2
    color = type
    bflag1,bflag2 = 2 numeric flags to affect how bodies are drawn
  size values = width height = size of images
    width = width of image in # of pixels
    height = height of image in # of pixels
  view values = theta phi = view of simulation box
    theta = view angle from +z axis (degrees)
    phi = azimuthal view angle (degrees)
    theta or phi can be a variable (see below)
  center values = flag Cx Cy Cz = center point of image
    flag = "s" for static, "d" for dynamic
    Cx,Cy,Cz = center point of image as fraction of box dimension (0.5 = center of box)
    Cx,Cy,Cz can be variables (see below)
  up values = Ux Uy Uz = direction that is "up" in image
    Ux,Uy,Uz = components of up vector
    Ux,Uy,Uz can be variables (see below)
  zoom value = zfactor = size that simulation box appears in image
    zfactor = scale image size by factor > 1 to enlarge, factor <1 to shrink
    zfactor can be a variable (see below)
  persp value = pfactor = amount of "perspective" in image
    pfactor = amount of perspective (0 = none,  <1 = some, > 1 = highly skewed)
    pfactor can be a variable (see below)
  box values = yes/no diam = draw outline of simulation box
```

```
    yes/no = do or do not draw simulation box lines
    diam = diameter of box lines as fraction of shortest box length
  axes values = yes/no length diam = draw xyz axes
    yes/no = do or do not draw xyz axes lines next to simulation box
    length = length of axes lines as fraction of respective box lengths
    diam = diameter of axes lines as fraction of shortest box length
  subbox values = yes/no diam = draw outline of processor sub-domains
    yes/no = do or do not draw sub-domain lines
    diam = diameter of sub-domain lines as fraction of shortest box length
  shiny value = sfactor = shinyness of spheres and cylinders
    sfactor = shinyness of spheres and cylinders from 0.0 to 1.0
  ssao value = yes/no seed dfactor = SSAO depth shading
    yes/no = turn depth shading on/off
    seed = random # seed (positive integer)
    dfactor = strength of shading from 0.0 to 1.0
```

Examples:

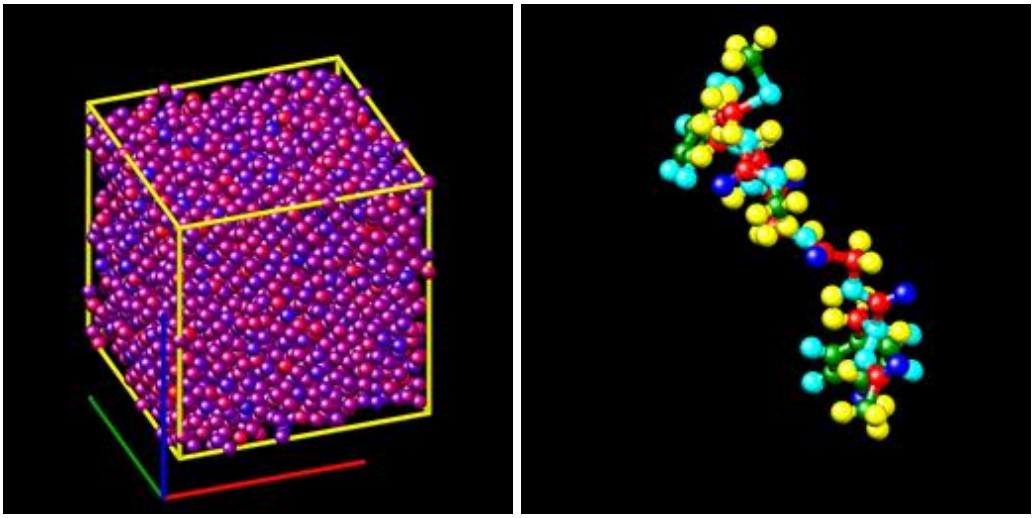
```
dump d0 all image 100 dump.*.jpg type type
dump d1 mobile image 500 snap.*.png element element ssao yes 4539 0.6
dump d2 all image 200 img-*.ppm type type zoom 2.5 adiam 1.5 size 1280 720
dump m0 all movie 1000 movie.mpg type type size 640 480
dump m1 all movie 1000 movie.avi type type size 640 480
dump m2 all movie 100 movie.m4v type type zoom 1.8 adiam v_value size 1280 720
```

Description:

Dump a high-quality rendered image of the atom configuration every N timesteps and save the images either as a sequence of JPEG or PNG or PPM files, or as a single movie file. The options for this command as well as the dump_modify command control what is included in the image or movie and how it appears. A series of such images can easily be manually converted into an animated movie of your simulation or the process can be automated without writing the intermediate files using the dump movie style; see further details below. Other dump styles store snapshots of numerical data asociated with atoms in various formats, as discussed on the dump doc page.

Note that a set of images or a movie can be made after a simulation has been run, using the rerun command to read snapshots from an existing dump file, and using these dump commands in the rerun script to generate the images/movie.

Here are two sample images, rendered as 1024x1024 JPEG files. Click to see the full-size images:



Only atoms in the specified group are rendered in the image. The dump_modify region and thresh commands can also alter what atoms are included in the image.

The filename suffix determines whether a JPEG, PNG, or PPM file is created with the *image* dump style. If the suffix is ".jpg" or ".jpeg", then a JPEG format file is created, if the suffix is ".png", then a PNG format is created, else a PPM (aka NETPBM) format file is created. The JPEG and PNG files are binary; PPM has a text mode header followed by binary data. JPEG images have lossy compression; PNG has lossless compression; and PPM files are uncompressed but can be compressed with gzip, if LAMMPS has been compiled with -DLAMMPS_GZIP and a ".gz" suffix is used.

Similarly, the format of the resulting movie is chosen with the *movie* dump style. This is handled by the underlying FFmpeg converter and thus details have to be looked up in the FFmpeg documentation. Typical examples are: .avi, .mpg, .m4v, .mp4, .mkv, .flv, .mov, .gif Additional settings of the movie compression like bitrate and framerate can be set using the dump_modify command.

To write out JPEG and PNG format files, you must build LAMMPS with support for the corresponding JPEG or PNG library. To convert images into movies, LAMMPS has to be compiled with the -DLAMMPS_FFMPEG flag. See this section of the manual for instructions on how to do this.

NOTE: Because periodic boundary conditions are enforced only on timesteps when neighbor lists are rebuilt, the coordinates of an atom in the image may be slightly outside the simulation box.

Dumps are performed on timesteps that are a multiple of N (including timestep 0) and on the last timestep of a minimization if the minimization converges. Note that this means a dump will not be performed on the initial timestep after the dump command is invoked, if the current timestep is not a multiple of N. This behavior can be changed via the dump_modify first command, which can be useful if the dump command is invoked after a minimization ended on an arbitrary timestep. N can be changed between runs by using the dump_modify every command.

Dump *image* filenames must contain a wildcard character "*", so that one image file per snapshot is written. The "*" character is replaced with the timestep value. For example, tmp.dump.*.jpg becomes tmp.dump.0.jpg, tmp.dump.10000.jpg, tmp.dump.20000.jpg, etc. Note that the dump_modify pad command can be used to insure all timestep numbers are the same length (e.g. 00010), which can make it easier to convert a series of images into a movie in the correct ordering.

Dump *movie* filenames on the other hand, must not have any wildcard character since only one file combining all images into a single movie will be written by the movie encoder.

The *color* and *diameter* settings determine the color and size of atoms rendered in the image. They can be any atom attribute defined for the dump custom command, including *type* and *element*. This includes per-atom quantities calculated by a compute, fix, or variable, which are prefixed by "c_", "f_", or "v_" respectively. Note that the *diameter* setting can be overridden with a numeric value applied to all atoms by the optional *adiam* keyword.

If *type* is specified for the *color* setting, then the color of each atom is determined by its atom type. By default the mapping of types to colors is as follows:

- type 1 = red
- type 2 = green
- type 3 = blue
- type 4 = yellow
- type 5 = aqua

- type 6 = cyan

and repeats itself for types > 6. This mapping can be changed by the dump_modify acolor command.

If *type* is specified for the *diameter* setting then the diameter of each atom is determined by its atom type. By default all types have diameter 1.0. This mapping can be changed by the dump_modify adiam command.

If *element* is specified for the *color* and/or *diameter* setting, then the color and/or diameter of each atom is determined by which element it is, which in turn is specified by the element-to-type mapping specified by the "dump_modify element" command. By default every atom type is C (carbon). Every element has a color and diameter associated with it, which is the same as the colors and sizes used by the AtomEye visualization package.

If other atom attributes are used for the *color* or *diameter* settings, they are interpreted in the following way.

If "vx", for example, is used as the *color* setting, then the color of the atom will depend on the x-component of its velocity. The association of a per-atom value with a specific color is determined by a "color map", which can be specified via the dump_modify command. The basic idea is that the atom-attribute will be within a range of values, and every value within the range is mapped to a specific color. Depending on how the color map is defined, that mapping can take place via interpolation so that a value of -3.2 is halfway between "red" and "blue", or discretely so that the value of -3.2 is "orange".

If "vx", for example, is used as the *diameter* setting, then the atom will be rendered using the x-component of its velocity as the diameter. If the per-atom value <= 0.0, them the atom will not be drawn. Note that finite-size spherical particles, as defined by atom_style sphere define a per-particle radius or diameter, which can be used as the *diameter* setting.

The various kewords listed above control how the image is rendered. As listed below, all of the keywords have defaults, most of which you will likely not need to change. The dump modify also has options specific to the dump image style, particularly for assigning colors to atoms, bonds, and other image features.

The *atom* keyword allow you to turn off the drawing of all atoms, if the specified value is *no*. Note that this will not turn off the drawing of particles that are represented as lines, triangles, or bodies, as discussed below. These particles can be drawn separately if the *line*, *tri*, or *body* keywords are used.

The *adiam* keyword allows you to override the *diameter* setting to set a single numeric *size*. All atoms will be drawn with that diameter, e.g. 1.5, which is in whatever distance units the input script defines, e.g. Angstroms.

The *bond* keyword allows to you to alter how bonds are drawn. A bond is only drawn if both atoms in the bond are being drawn due to being in the specified group and due to other selection criteria (e.g. region, threshhold settings of the dump_modify command). By default, bonds are drawn if they are defined in the input data file as read by the read_data command. Using *none* for both the bond *color* and *width* value will turn off the drawing of all bonds.

If *atom* is specified for the bond *color* value, then each bond is drawn in 2 halves, with the color of each half being the color of the atom at that end of the bond.

If *type* is specified for the *color* value, then the color of each bond is determined by its bond type. By default the mapping of bond types to colors is as follows:

- type 1 = red
- type 2 = green
- type 3 = blue

- type 4 = yellow
- type 5 = aqua
- type 6 = cyan

and repeats itself for bond types > 6. This mapping can be changed by the dump_modify bcolor command.

The bond *width* value can be a numeric value or *atom* or *type* (or *none* as indicated above).

If a numeric value is specified, then all bonds will be drawn as cylinders with that diameter, e.g. 1.0, which is in whatever distance units the input script defines, e.g. Angstroms.

If *atom* is specified for the *width* value, then each bond will be drawn with a width corresponding to the minimum diameter of the 2 atoms in the bond.

If *type* is specified for the *width* value then the diameter of each bond is determined by its bond type. By default all types have diameter 0.5. This mapping can be changed by the dump_modify bdiam command.

The *line* keyword can be used when atom_style line is used to define particles as line segments, and will draw them as lines. If this keyword is not used, such particles will be drawn as spheres, the same as if they were regular atoms. The only setting currently allowed for the *color* value is *type*, which will color the lines according to the atom type of the particle. By default the mapping of types to colors is as follows:

- type 1 = red
- type 2 = green
- type 3 = blue
- type 4 = yellow
- type 5 = aqua
- type 6 = cyan

and repeats itself for types > 6. There is not yet an option to change this via the dump_modify command.

The line *width* can only be a numeric value, which specifies that all lines will be drawn as cylinders with that diameter, e.g. 1.0, which is in whatever distance units the input script defines, e.g. Angstroms.

The *tri* keyword can be used when atom_style tri is used to define particles as triangles, and will draw them as triangles or edges (3 lines) or both, depending on the setting for *tflag*. If edges are drawn, the *width* setting determines the diameters of the line segments. If this keyword is not used, triangle particles will be drawn as spheres, the same as if they were regular atoms. The only setting currently allowed for the *color* value is *type*, which will color the triangles according to the atom type of the particle. By default the mapping of types to colors is as follows:

- type 1 = red
- type 2 = green
- type 3 = blue
- type 4 = yellow
- type 5 = aqua
- type 6 = cyan

and repeats itself for types > 6. There is not yet an option to change this via the dump_modify command.

The *body* keyword can be used when atom_style body is used to define body particles with internal state (e.g. sub-particles), and will drawn them in a manner specific to the body style. If this keyword is not used, such

particles will be drawn as spheres, the same as if they were regular atoms.

The body doc page descibes the body styles LAMMPS currently supports, and provides more details as to the kind of body particles they represent and how they are drawn by this dump image command. For all the body styles, individual atoms can be either a body particle or a usual point (non-body) particle. Non-body particles will be drawn the same way they would be as a regular atom. The *bflag1* and *bflag2* settings are numerical values which are passed to the body style to affect how the drawing of a body particle is done. See the body doc page for a description of what these parameters mean for each body style.

The *size* keyword sets the width and height of the created images, i.e. the number of pixels in each direction.

The *view*, *center*, *up*, *zoom*, and *persp* values determine how 3d simulation space is mapped to the 2d plane of the image. Basically they control how the simulation box appears in the image.

All of the *view*, *center*, *up*, *zoom*, and *persp* values can be specified as numeric quantities, whose meaning is explained below. Any of them can also be specified as an equal-style variable, by using v_name as the value, where "name" is the variable name. In this case the variable will be evaluated on the timestep each image is created to create a new value. If the equal-style variable is time-dependent, this is a means of changing the way the simulation box appears from image to image, effectively doing a pan or fly-by view of your simulation.

The *view* keyword determines the viewpoint from which the simulation box is viewed, looking towards the *center* point. The *theta* value is the vertical angle from the +z axis, and must be an angle from 0 to 180 degrees. The *phi* value is an azimuthal angle around the z axis and can be positive or negative. A value of 0.0 is a view along the +x axis, towards the *center* point. If *theta* or *phi* are specified via variables, then the variable values should be in degrees.

The *center* keyword determines the point in simulation space that will be at the center of the image. *Cx*, *Cy*, and *Cz* are speficied as fractions of the box dimensions, so that (0.5,0.5,0.5) is the center of the simulation box. These values do not have to be between 0.0 and 1.0, if you want the simulation box to be offset from the center of the image. Note, however, that if you choose strange values for *Cx*, *Cy*, or *Cz* you may get a blank image. Internally, *Cx*, *Cy*, and *Cz* are converted into a point in simulation space. If *flag* is set to "s" for static, then this conversion is done once, at the time the dump command is issued. If *flag* is set to "d" for dynamic then the conversion is performed every time a new image is created. If the box size or shape is changing, this will adjust the center point in simulation space.

The *up* keyword determines what direction in simulation space will be "up" in the image. Internally it is stored as a vector that is in the plane perpendicular to the view vector implied by the *theta* and *pni* values, and which is also in the plane defined by the view vector and user-specified up vector. Thus this internal vector is computed from the user-specified *up* vector as

```
up_internal = view cross (up cross view)
```

This means the only restriction on the specified *up* vector is that it cannot be parallel to the *view* vector, implied by the *theta* and *phi* values.

The *zoom* keyword scales the size of the simulation box as it appears in the image. The default *zfactor* value of 1 should display an image mostly filled by the atoms in the simulation box. A *zfactor* > 1 will make the simulation box larger; a *zfactor* < 1 will make it smaller. *Zfactor* must be a value > 0.0.

The *persp* keyword determines how much depth perspective is present in the image. Depth perspective makes lines that are parallel in simulation space appear non-parallel in the image. A *pfactor* value of 0.0 means that parallel lines will meet at infininty (1.0/pfactor), which is an orthographic rendering with no persepctive. A

pfactor value between 0.0 and 1.0 will introduce more perspective. A *pfactor* value > 1 will create a highly skewed image with a large amount of perspective.

NOTE: The *persp* keyword is not yet supported as an option.

The *box* keyword determines if and how the simulation box boundaries are rendered as thin cylinders in the image. If *no* is set, then the box boundaries are not drawn and the *diam* setting is ignored. If *yes* is set, the 12 edges of the box are drawn, with a diameter that is a fraction of the shortest box length in x,y,z (for 3d) or x,y (for 2d). The color of the box boundaries can be set with the dump_modify boxcolor command.

The *axes* keyword determines if and how the coordinate axes are rendered as thin cylinders in the image. If *no* is set, then the axes are not drawn and the *length* and *diam* settings are ignored. If *yes* is set, 3 thin cylinders are drawn to represent the x,y,z axes in colors red,green,blue. The origin of these cylinders will be offset from the lower left corner of the box by 10%. The *length* setting determines how long the cylinders will be as a fraction of the respective box lengths. The *diam* setting determines their thickness as a fraction of the shortest box length in x,y,z (for 3d) or x,y (for 2d).

The *subbox* keyword determines if and how processor sub-domain boundaries are rendered as thin cylinders in the image. If *no* is set (default), then the sub-domain boundaries are not drawn and the *diam* setting is ignored. If *yes* is set, the 12 edges of each processor sub-domain are drawn, with a diameter that is a fraction of the shortest box length in x,y,z (for 3d) or x,y (for 2d). The color of the sub-domain boundaries can be set with the dump_modify boxcolor command.

The *shiny* keyword determines how shiny the objects rendered in the image will appear. The *sfactor* value must be a value 0.0 <= *sfactor* <= 1.0, where *sfactor* = 1 is a highly reflective surface and *sfactor* = 0 is a rough non-shiny surface.

The *ssao* keyword turns on/off a screen space ambient occlusion (SSAO) model for depth shading. If *yes* is set, then atoms further away from the viewer are darkened via a randomized process, which is perceived as depth. The calculation of this effect can increase the cost of computing the image by roughly 2x. The strength of the effect can be scaled by the *dfactor* parameter. If *no* is set, no depth shading is performed.

A series of JPEG, PNG, or PPM images can be converted into a movie file and then played as a movie using commonly available tools. Using dump style *movie* automates this step and avoids the intermediate step of writing (many) image snapshot file. But LAMMPS has to be compiled with -DLAMMPS_FFMPEG and an FFmpeg executable have to be installed.

To manually convert JPEG, PNG or PPM files into an animated GIF or MPEG or other movie file you can use:

- a) Use the ImageMagick convert program.

  ```
  % convert *.jpg foo.gif
  % convert -loop 1 *.ppm foo.mpg
  ```

  Animated GIF files from ImageMagick are unoptimized. You can use a program like gifsicle to optimize and massively shrink them. MPEG files created by ImageMagick are in MPEG-1 format with rather inefficient compression and low quality.
- b) Use QuickTime.

  Select "Open Image Sequence" under the File menu Load the images into QuickTime to animate them Select "Export" under the File menu Save the movie as a QuickTime movie (*.mov) or in another format. QuickTime can generate very high quality and efficiently compressed movie files. Some of the supported

formats require to buy a license and some are not readable on all platforms until specific runtime libraries are installed.

- c) Use FFmpeg

  FFmpeg is a command line tool that is available on many platforms and allows extremely flexible encoding and decoding of movies.

```
cat snap.*.jpg | ffmpeg -y -f image2pipe -c:v mjpeg -i - -b:v 2000k movie.m4v
cat snap.*.ppm | ffmpeg -y -f image2pipe -c:v ppm -i - -b:v 2400k movie.avi
```

  Frontends for FFmpeg exist for multiple platforms. For more information see the FFmpeg homepage

---

Play the movie:

- a) Use your browser to view an animated GIF movie.

  Select "Open File" under the File menu Load the animated GIF file
- b) Use the freely available mplayer or ffplay tool to view a movie. Both are available for multiple OSes and support a large variety of file formats and decoders.

```
% mplayer foo.mpg
% ffplay bar.avi
```
- c) Use the Pizza.py animate tool, which works directly on a series of image files.

```
a = animate("foo*.jpg")
```
- d) QuickTime and other Windows- or MacOS-based media players can obviously play movie files directly. Similarly for corresponding tools bundled with Linux desktop environments. However, due to licensing issues with some file formats, the formats may require installing additional libraries, purchasing a license, or may not be supported.

See Section_modify of the manual for information on how to add new compute and fix styles to LAMMPS to calculate per-atom quantities which could then be output into dump files.

Restrictions:

To write JPEG images, you must use the -DLAMMPS_JPEG switch when building LAMMPS and link with a JPEG library. To write PNG images, you must use the -DLAMMPS_PNG switch when building LAMMPS and link with a PNG library.

To write *movie* dumps, you must use the -DLAMMPS_FFMPEG switch when building LAMMPS and have the FFmpeg executable available on the machine where LAMMPS is being run. Typically it's name is lowercase, i.e. ffmpeg.

See the Making LAMMPS section of the documentation for details on how to compile with optional switches.

Note that since FFmpeg is run as an external program via a pipe, LAMMPS has limited control over its execution and no knowledge about errors and warnings printed by it. Those warnings and error messages will be printed to the screen only. Due to the way image data is communicated to FFmpeg, it will often print the message

```
pipe:: Input/output error
```

which can be safely ignored. Other warnings and errors have to be addressed according to the FFmpeg documentation. One known issue is that certain movie file formats (e.g. MPEG level 1 and 2 format streams) have

video bandwith limits that can be crossed when rendering too large of image sizes. Typical warnings look like this:

```
[mpeg @ 0x98b5e0] packet too large, ignoring buffer limits to mux it
[mpeg @ 0x98b5e0] buffer underflow st=0 bufi=281407 size=285018
[mpeg @ 0x98b5e0] buffer underflow st=0 bufi=283448 size=285018
```

In this case it is recommended to either reduce the size of the image or encode in a different format that is also supported by your copy of FFmpeg, and which does not have this limitation (e.g. .avi, .mkv, mp4).

Related commands:

dump, dump_modify, undump

Default:

The defaults for the keywords are as follows:

- adiam = not specified (use diameter setting)
- atom = yes
- bond = none none (if no bonds in system)
- bond = atom 0.5 (if bonds in system)
- size = 512 512
- view = 60 30 (for 3d)
- view = 0 0 (for 2d)
- center = s 0.5 0.5 0.5
- up = 0 0 1 (for 3d)
- up = 0 1 0 (for 2d)
- zoom = 1.0
- persp = 0.0
- box = yes 0.02
- axes = no 0.0 0.0
- subbox no 0.0
- shiny = 1.0
- ssao = no

dump_modify command

Syntax:

```
dump_modify dump-ID keyword values ...
```

- dump-ID = ID of dump to modify
- one or more keyword/value pairs may be appended
- these keywords apply to various dump styles
- keyword = *append* or *buffer* or *element* or *every* or *fileper* or *first* or *flush* or *format* or *image* or *label* or *nfile* or *pad* or *precision* or *region* or *scale* or *sort* or *thresh* or *unwrap*

```
  append arg = yes or no
    buffer arg = yes or no
    element args = E1 E2 ... EN, where N = # of atom types
      E1,...,EN = element name, e.g. C or Fe or Ga
    every arg = N
      N = dump every this many timesteps
      N can be a variable (see below)
    fileper arg = Np
      Np = write one file for every this many processors
    first arg = yes or no
    format arg = C-style format string for one line of output
    flush arg = yes or no
    image arg = yes or no
    label arg = string
      string = character string (e.g. BONDS) to use in header of dump local file
    nfile arg = Nf
      Nf = write this many files, one from each of Nf processors
    pad arg = Nchar = # of characters to convert timestep to
    precision arg = power-of-10 value from 10 to 1000000
    region arg = region-ID or "none"
    scale arg = yes or no
    sfactor arg = coordinate scaling factor (> 0.0)
    tfactor arg = time scaling factor (> 0.0)
    sort arg = off or id or N or -N
       off = no sorting of per-atom lines within a snapshot
       id = sort per-atom lines by atom ID
       N = sort per-atom lines in ascending order by the Nth column
       -N = sort per-atom lines in descending order by the Nth column
    thresh args = attribute operation value
      attribute = same attributes (x,fy,etotal,sxx,etc) used by dump custom style
      operation = "" or ">=" or "==" or "!="
      value = numeric value to compare to
      these 3 args can be replaced by the word "none" to turn off thresholding
    unwrap arg = yes or no
```

- these keywords apply only to the *image* and *movie* styles
- keyword = *acolor* or *adiam* or *amap* or *backcolor* or *bcolor* or *bdiam* or *boxcolor* or *color* or *bitrate* or *framerate*

```
  acolor args = type color
      type = atom type or range of types (see below)
      color = name of color or color1/color2/...
    adiam args = type diam
      type = atom type or range of types (see below)
      diam = diameter of atoms of that type (distance units)
    amap args = lo hi style delta N entry1 entry2 ... entryN
      lo = number or min = lower bound of range of color map
```

```
    hi = number or max = upper bound of range of color map
    style = 2 letters = "c" or "d" or "s" plus "a" or "f"
      "c" for continuous
      "d" for discrete
      "s" for sequential
      "a" for absolute
      "f" for fractional
    delta = binsize (only used for style "s", otherwise ignored)
      binsize = range is divided into bins of this width
    N = # of subsequent entries
    entry = value color (for continuous style)
      value = number or min or max = single value within range
      color = name of color used for that value
    entry = lo hi color (for discrete style)
      lo/hi = number or min or max = lower/upper bound of subset of range
      color = name of color used for that subset of values
    entry = color (for sequential style)
      color = name of color used for a bin of values
  backcolor arg = color
    color = name of color for background
  bcolor args = type color
    type = bond type or range of types (see below)
    color = name of color or color1/color2/...
  bdiam args = type diam
    type = bond type or range of types (see below)
    diam = diameter of bonds of that type (distance units)
  boxcolor arg = color
    color = name of color for simulation box lines and processor sub-domain lines
  color args = name R G B
    name = name of color
    R,G,B = red/green/blue numeric values from 0.0 to 1.0
  bitrate arg = rate
    rate = target bitrate for movie in kbps
  framerate arg = fps
    fps = frames per second for movie
```

Examples:

```
dump_modify 1 format "%d %d %20.15g %g %g" scale yes
dump_modify myDump image yes scale no flush yes
dump_modify 1 region mySphere thresh x <0.0 thresh epair >= 3.2
dump_modify xtcdump precision 10000 sfactor 0.1
dump_modify 1 every 1000 nfile 20
dump_modify 1 every v_myVar
dump_modify 1 amap min max cf 0.0 3 min green 0.5 yellow max blue boxcolor red
```

Description:

Modify the parameters of a previously defined dump command. Not all parameters are relevant to all dump styles.

As explained on the dump doc page, the *atom/mpiio*, *custom/mpiio*, and *xyz/mpiio* dump styles are identical in command syntax and in the format of the dump files they create, to the corresponding styles without "mpiio", except the single dump file they produce is written in parallel via the MPI-IO library. Thus if a dump_modify option below is valid for the *atom* style, it is also valid for the *atom/mpiio* style, and similarly for the other styles which allow for use of MPI-IO.

These keywords apply to various dump styles, including the dump image and dump movie styles. The description gives details.

The *append* keyword applies to all dump styles except *cfg* and *xtc* and *dcd*. It also applies only to text output files, not to binary or gzipped or image/movie files. If specified as *yes*, then dump snapshots are appended to the end of an existing dump file. If specified as *no*, then a new dump file will be created which will overwrite an existing file with the same name. This keyword can only take effect if the dump_modify command is used after the dump command, but before the first command that causes dump snapshots to be output, e.g. a run or minimize command. Once the dump file has been opened, this keyword has no further effect.

The *buffer* keyword applies only to dump styles *atom*, *cfg*, *custom*, *local*, and *xyz*. It also applies only to text output files, not to binary or gzipped files. If specified as *yes*, which is the default, then each processor writes its output into an internal text buffer, which is then sent to the processor(s) which perform file writes, and written by those processors(s) as one large chunk of text. If specified as *no*, each processor sends its per-atom data in binary format to the processor(s) which perform file wirtes, and those processor(s) format and write it line by line into the output file.

The buffering mode is typically faster since each processor does the relatively expensive task of formatting the output for its own atoms. However it requires about twice the memory (per processor) for the extra buffering.

The *element* keyword applies only to the the dump *cfg*, *xyz*, and *image* styles. It associates element names (e.g. H, C, Fe) with LAMMPS atom types. See the list of element names at the bottom of this page.

In the case of dump *cfg*, this allows the AtomEye visualization package to read the dump file and render atoms with the appropriate size and color.

In the case of dump *image*, the output images will follow the same AtomEye convention. An element name is specified for each atom type (1 to Ntype) in the simulation. The same element name can be given to multiple atom types.

In the case of *xyz* format dumps, there are no restrictions to what label can be used as an element name. Any whitespace separated text will be accepted.

The *every* keyword changes the dump frequency originally specified by the dump command to a new value. The every keyword can be specified in one of two ways. It can be a numeric value in which case it must be > 0. Or it can be an equal-style variable, which should be specified as v_name, where name is the variable name.

In this case, the variable is evaluated at the beginning of a run to determine the next timestep at which a dump snapshot will be written out. On that timestep the variable will be evaluated again to determine the next timestep, etc. Thus the variable should return timestep values. See the stagger() and logfreq() and stride() math functions for equal-style variables, as examples of useful functions to use in this context. Other similar math functions could easily be added as options for equal-style variables. Also see the next() function, which allows use of a file-style variable which reads successive values from a file, each time the variable is evaluated. Used with the *every* keyword, if the file contains a list of ascending timesteps, you can output snapshots whenever you wish.

Note that when using the variable option with the *every* keyword, you need to use the *first* option if you want an initial snapshot written to the dump file. The *every* keyword cannot be used with the dump *dcd* style.

For example, the following commands will write snapshots at timesteps 0,10,20,30,100,200,300,1000,2000,etc:

```
variable        s equal logfreq(10,3,10)
dump            1 all atom 100 tmp.dump
dump_modify     1 every v_s first yes
```

The following commands would write snapshots at the timesteps listed in file tmp.times:

```
variable        f file tmp.times
variable        s equal next(f)
dump            1 all atom 100 tmp.dump
dump_modify     1 every v_s
```

NOTE: When using a file-style variable with the *every* keyword, the file of timesteps must list a first timestep that is beyond the current timestep (e.g. it cannot be 0). And it must list one or more timesteps beyond the length of the run you perform. This is because the dump command will generate an error if the next timestep it reads from the file is not a value greater than the current timestep. Thus if you wanted output on steps 0,15,100 of a 100-timestep run, the file should contain the values 15,100,101 and you should also use the dump_modify first command. Any final value > 100 could be used in place of 101.

The *first* keyword determines whether a dump snapshot is written on the very first timestep after the dump command is invoked. This will always occur if the current timestep is a multiple of N, the frequency specified in the dump command, including timestep 0. But if this is not the case, a dump snapshot will only be written if the setting of this keyword is *yes*. If it is *no*, which is the default, then it will not be written.

The *flush* keyword determines whether a flush operation is invoked after a dump snapshot is written to the dump file. A flush insures the output in that file is current (no buffering by the OS), even if LAMMPS halts before the simulation completes. Flushes cannot be performed with dump style *xtc*.

The text-based dump styles have a default C-style format string which simply specifies %d for integers and %g for floating-point values. The *format* keyword can be used to override the default with a new C-style format string. Do not include a trailing "\\n" newline character in the format string. This option has no effect on the *dcd* and *xtc* dump styles since they write binary files. Note that for the *cfg* style, the first two fields (atom id and type) are not actually written into the CFG file, though you must include formats for them in the format string.

NOTE: Any value written to a text-based dump file that is a per-atom quantity calculated by a compute or fix is stored internally as a floating-point value. If the value is actually an integer and you wish it to appear in the text dump file as a (large) integer, then you need to use an appropriate format. For example, these commands:

```
compute     1 all property/local batom1 batom2
dump        1 all local 100 tmp.bonds index c_1[1] c_1[2]
dump_modify 1 format "%d %0.0f %0.0f"
```

will output the two atom IDs for atoms in each bond as integers. If the dump_modify command were omitted, they would appear as floating-point values, assuming they were large integers (more than 6 digits). The "index" keyword should use the "%d" format since it is not generated by a compute or fix, and is stored internally as an integer.

The *fileper* keyword is documented below with the *nfile* keyword.

The *image* keyword applies only to the dump *atom* style. If the image value is *yes*, 3 flags are appended to each atom's coords which are the absolute box image of the atom in each dimension. For example, an x image flag of -2 with a normalized coord of 0.5 means the atom is in the center of the box, but has passed thru the box boundary 2 times and is really 2 box lengths to the left of its current coordinate. Note that for dump style *custom* these various values can be printed in the dump file by using the appropriate atom attributes in the dump command itself.

The *label* keyword applies only to the dump *local* style. When it writes local information, such as bond or angle topology to a dump file, it will use the specified *label* to format the header. By default this includes 2 lines:

```
ITEM: NUMBER OF ENTRIES
```

```
ITEM: ENTRIES ...
```

The word "ENTRIES" will be replaced with the string specified, e.g. BONDS or ANGLES.

The *nfile* or *fileper* keywords can be used in conjunction with the "%" wildcard character in the specified dump file name, for all dump styles except the *dcd*, *image*, *movie*, *xtc*, and *xyz* styles (for which "%" is not allowed). As explained on the dump command doc page, the "%" character causes the dump file to be written in pieces, one piece for each of P processors. By default P = the number of processors the simulation is running on. The *nfile* or *fileper* keyword can be used to set P to a smaller value, which can be more efficient when running on a large number of processors.

The *nfile* keyword sets P to the specified Nf value. For example, if Nf = 4, and the simulation is running on 100 processors, 4 files will be written, by processors 0,25,50,75. Each will collect information from itself and the next 24 processors and write it to a dump file.

For the *fileper* keyword, the specified value of Np means write one file for every Np processors. For example, if Np = 4, every 4th processor (0,4,8,12,etc) will collect information from itself and the next 3 processors and write it to a dump file.

The *pad* keyword only applies when the dump filename is specified with a wildcard "*" character which becomes the timestep. If *pad* is 0, which is the default, the timestep is converted into a string of unpadded length, e.g. 100 or 12000 or 2000000. When *pad* is specified with *Nchar* > 0, the string is padded with leading zeroes so they are all the same length = *Nchar*. For example, pad 7 would yield 0000100, 0012000, 2000000. This can be useful so that post-processing programs can easily read the files in ascending timestep order.

The *precision* keyword only applies to the dump *xtc* style. A specified value of N means that coordinates are stored to 1/N nanometer accuracy, e.g. for N = 1000, the coordinates are written to 1/1000 nanometer accuracy.

The *sfactor* and *tfactor* keywords only apply to the dump *xtc* style. They allow customization of the unit conversion factors used when writing to XTC files. By default they are initialized for whatever units style is being used, to write out coordinates in nanometers and time in picoseconds. I.e. for *real* units, LAMMPS defines *sfactor* = 0.1 and *tfactor* = 0.001, since the Angstroms and fmsec used by *real* units are 0.1 nm and 0.001 psec respectively. If you are using a units system with distance and time units far from nm and psec, you may wish to write XTC files with different units, since the compression algorithm used in XTC files is most effective when the typical magnitude of position data is between 10.0 and 0.1.

The *region* keyword only applies to the dump *custom*, *cfg*, *image*, and *movie* styles. If specified, only atoms in the region will be written to the dump file or included in the image/movie. Only one region can be applied as a filter (the last one specified). See the region command for more details. Note that a region can be defined as the "inside" or "outside" of a geometric shape, and it can be the "union" or "intersection" of a series of simpler regions.

The *scale* keyword applies only to the dump *atom* style. A scale value of *yes* means atom coords are written in normalized units from 0.0 to 1.0 in each box dimension. If the simluation box is triclinic (tilted), then all atom coords will still be between 0.0 and 1.0. A value of *no* means they are written in absolute distance units (e.g. Angstroms or sigma).

The *sort* keyword determines whether lines of per-atom output in a snapshot are sorted or not. A sort value of *off* means they will typically be written in indeterminate order, either in serial or parallel. This is the case even in serial if the atom_modify sort option is turned on, which it is by default, to improve performance. A sort value of *id* means sort the output by atom ID. A sort value of N or -N means sort the output by the value in the Nth column

of per-atom info in either ascending or descending order.

The dump *local* style cannot be sorted by atom ID, since there are typically multiple lines of output per atom. Some dump styles, such as *dcd* and *xtc*, require sorting by atom ID to format the output file correctly. If multiple processors are writing the dump file, via the "%" wildcard in the dump filename, then sorting cannot be performed.

NOTE: Unless it is required by the dump style, sorting dump file output requires extra overhead in terms of CPU and communication cost, as well as memory, versus unsorted output.

The *thresh* keyword only applies to the dump *custom*, *cfg*, *image*, and *movie* styles. Multiple thresholds can be specified. Specifying "none" turns off all threshold criteria. If thresholds are specified, only atoms whose attributes meet all the threshold criteria are written to the dump file or included in the image. The possible attributes that can be tested for are the same as those that can be specified in the dump custom command, with the exception of the *element* attribute, since it is not a numeric value. Note that different attributes can be output by the dump custom command than are used as threshold criteria by the dump_modify command. E.g. you can output the coordinates and stress of atoms whose energy is above some threshold.

The *unwrap* keyword only applies to the dump *dcd* and *xtc* styles. If set to *yes*, coordinates will be written "unwrapped" by the image flags for each atom. Unwrapped means that if the atom has passed thru a periodic boundary one or more times, the value is printed for what the coordinate would be if it had not been wrapped back into the periodic box. Note that these coordinates may thus be far outside the box size stored with the snapshot.

These keywords apply only to the dump image and dump movie styles. Any keyword that affects an image, also affects a movie, since the movie is simply a collection of images. Some of the keywords only affect the dump movie style. The descriptions give details.

The *acolor* keyword can be used with the dump image command, when its atom color setting is *type*, to set the color that atoms of each type will be drawn in the image.

The specified *type* should be an integer from 1 to Ntypes = the number of atom types. A wildcard asterisk can be used in place of or in conjunction with the *type* argument to specify a range of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

The specified *color* can be a single color which is any of the 140 pre-defined colors (see below) or a color name defined by the dump_modify color option. Or it can be two or more colors separated by a "/" character, e.g. red/green/blue. In the former case, that color is assigned to all the specified atom types. In the latter case, the list of colors are assigned in a round-robin fashion to each of the specified atom types.

The *adiam* keyword can be used with the dump image command, when its atom diameter setting is *type*, to set the size that atoms of each type will be drawn in the image. The specified *type* should be an integer from 1 to Ntypes. As with the *acolor* keyword, a wildcard asterisk can be used as part of the *type* argument to specify a range of atomt types. The specified *diam* is the size in whatever distance units the input script is using, e.g. Angstroms.

The *amap* keyword can be used with the dump image command, with its *atom* keyword, when its atom setting is an atom-attribute, to setup a color map. The color map is used to assign a specific RGB (red/green/blue) color value to an individual atom when it is drawn, based on the atom's attribute, which is a numeric value, e.g. its x-component of velocity if the atom-attribute "vx" was specified.

The basic idea of a color map is that the atom-attribute will be within a range of values, and that range is associated with a a series of colors (e.g. red, blue, green). An atom's specific value (vx = -3.2) can then mapped to the series of colors (e.g. halfway between red and blue), and a specific color is determined via an interpolation procedure.

There are many possible options for the color map, enabled by the *amap* keyword. Here are the details.

The *lo* and *hi* settings determine the range of values allowed for the atom attribute. If numeric values are used for *lo* and/or *hi*, then values that are lower/higher than that value are set to the value. I.e. the range is static. If *lo* is specified as *min* or *hi* as *max* then the range is dynamic, and the lower and/or upper bound will be calculated each time an image is drawn, based on the set of atoms being visualized.

The *style* setting is two letters, such as "ca". The first letter is either "c" for continuous, "d" for discrete, or "s" for sequential. The second letter is either "a" for absolute, or "f" for fractional.

A continuous color map is one in which the color changes continuously from value to value within the range. A discrete color map is one in which discrete colors are assigned to sub-ranges of values within the range. A sequential color map is one in which discrete colors are assigned to a sequence of sub-ranges of values covering the entire range.

An absolute color map is one in which the values to which colors are assigned are specified explicitly as values within the range. A fractional color map is one in which the values to which colors are assigned are specified as a fractional portion of the range. For example if the range is from -10.0 to 10.0, and the color red is to be assigned to atoms with a value of 5.0, then for an absolute color map the number 5.0 would be used. But for a fractional map, the number 0.75 would be used since 5.0 is 3/4 of the way from -10.0 to 10.0.

The *delta* setting must be specified for all styles, but is only used for the sequential style; otherwise the value is ignored. It specifies the bin size to use within the range for assigning consecutive colors to. For example, if the range is from -10.0 to 10.0 and a *delta* of 1.0 is used, then 20 colors will be assigned to the range. The first will be from -10.0 <= color1 < -9.0, then 2nd from -9.0 <= color2 < -8.0, etc.

The *N* setting is how many entries follow. The format of the entries depends on whether the color map style is continuous, discrete or sequential. In all cases the *color* setting can be any of the 140 pre-defined colors (see below) or a color name defined by the dump_modify color option.

For continuous color maps, each entry has a *value* and a *color*. The *value* is either a number within the range of values or *min* or *max*. The *value* of the first entry must be *min* and the *value* of the last entry must be *max*. Any entries in between must have increasing values. Note that numeric values can be specified either as absolute numbers or as fractions (0.0 to 1.0) of the range, depending on the "a" or "f" in the style setting for the color map.

Here is how the entries are used to determine the color of an individual atom, given the value X of its atom attribute. X will fall between 2 of the entry values. The color of the atom is linearly interpolated (in each of the RGB values) between the 2 colors associated with those entries. For example, if X = -5.0 and the 2 surrounding entries are "red" at -10.0 and "blue" at 0.0, then the atom's color will be halfway between "red" and "blue", which happens to be "purple".

For discrete color maps, each entry has a *lo* and *hi* value and a *color*. The *lo* and *hi* settings are either numbers within the range of values or *lo* can be *min* or *hi* can be *max*. The *lo* and *hi* settings of the last entry must be *min* and *max*. Other entries can have any *lo* and *hi* values and the sub-ranges of different values can overlap. Note that numeric *lo* and *hi* values can be specified either as absolute numbers or as fractions (0.0 to 1.0) of the range, depending on the "a" or "f" in the style setting for the color map.

Here is how the entries are used to determine the color of an individual atom, given the value X of its atom attribute. The entries are scanned from first to last. The first time that *lo* <= X <= *hi*, X is assigned the color associated with that entry. You can think of the last entry as assigning a default color (since it will always be matched by X), and the earlier entries as colors that override the default. Also note that no interpolation of a color RGB is done. All atoms will be drawn with one of the colors in the list of entries.

For sequential color maps, each entry has only a *color*. Here is how the entries are used to determine the color of an individual atom, given the value X of its atom attribute. The range is partitioned into N bins of width *binsize*. Thus X will fall in a specific bin from 1 to N, say the Mth bin. If it falls on a boundary between 2 bins, it is considered to be in the higher of the 2 bins. Each bin is assigned a color from the E entries. If E < N, then the colors are repeated. For example if 2 entries with colors red and green are specified, then the odd numbered bins will be red and the even bins green. The color of the atom is the color of its bin. Note that the sequential color map is really a shorthand way of defining a discrete color map without having to specify where all the bin boundaries are.

Here is an example of using a sequential color map to color all the atoms in individual molecules with a different color. See the examples/pour/in.pour.2d.molecule input script for an example of how this is used.

```
variable        colors string &
                "red green blue yellow white &
                purple pink orange lime gray"
variable        mol atom mol%10
dump            1 all image 250 image.*.jpg v_mol type &
                zoom 1.6 adiam 1.5
dump_modify     1 pad 5 amap 0 10 sa 1 10 ${colors}
```

In this case, 10 colors are defined, and molecule IDs are mapped to one of the colors, even if there are 1000s of molecules.

The *backcolor* sets the background color of the images. The color name can be any of the 140 pre-defined colors (see below) or a color name defined by the dump_modify color option.

The *bcolor* keyword can be used with the dump image command, with its *bond* keyword, when its color setting is *type*, to set the color that bonds of each type will be drawn in the image.

The specified *type* should be an integer from 1 to Nbondtypes = the number of bond types. A wildcard asterisk can be used in place of or in conjunction with the *type* argument to specify a range of bond types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of bond types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

The specified *color* can be a single color which is any of the 140 pre-defined colors (see below) or a color name defined by the dump_modify color option. Or it can be two or more colors separated by a "/" character, e.g. red/green/blue. In the former case, that color is assigned to all the specified bond types. In the latter case, the list of colors are assigned in a round-robin fashion to each of the specified bond types.

The *bdiam* keyword can be used with the dump image command, with its *bond* keyword, when its diam setting is *type*, to set the diameter that bonds of each type will be drawn in the image. The specified *type* should be an integer from 1 to Nbondtypes. As with the *bcolor* keyword, a wildcard asterisk can be used as part of the *type* argument to specify a range of bond types. The specified *diam* is the size in whatever distance units you are using, e.g. Angstroms.

The *bitrate* keyword can be used with the dump movie command to define the size of the resulting movie file and its quality via setting how many kbits per second are to be used for the movie file. Higher bitrates require less compression and will result in higher quality movies. The quality is also determined by the compression format and encoder. The default setting is 2000 kbit/s, which will result in average quality with older compression formats.

NOTE: Not all movie file formats supported by dump movie allow the bitrate to be set. If not, the setting is silently ignored.

The *boxcolor* keyword sets the color of the simulation box drawn around the atoms in each image as well as the color of processor sub-domain boundaries. See the "dump image box" command for how to specify that a box be drawn via the *box* keyword, and the sub-domain boundaries via the *subbox* keyword. The color name can be any of the 140 pre-defined colors (see below) or a color name defined by the dump_modify color option.

The *color* keyword allows definition of a new color name, in addition to the 140-predefined colors (see below), and associates 3 red/green/blue RGB values with that color name. The color name can then be used with any other dump_modify keyword that takes a color name as a value. The RGB values should each be floating point values between 0.0 and 1.0 inclusive.

When a color name is converted to RGB values, the user-defined color names are searched first, then the 140 pre-defined color names. This means you can also use the *color* keyword to overwrite one of the pre-defined color names with new RBG values.

The *framerate* keyword can be used with the dump movie command to define the duration of the resulting movie file. Movie files written by the dump *movie* command have a default frame rate of 24 frames per second and the images generated will be converted at that rate. Thus a sequence of 1000 dump images will result in a movie of about 42 seconds. To make a movie run longer you can either generate images more frequently or lower the frame rate. To speed a movie up, you can do the inverse. Using a frame rate higher than 24 is not recommended, as it will result in simply dropping the rendered images. It is more efficient to dump images less frequently.

Restrictions: none

Related commands:

dump, dump image, undump

Default:

The option defaults are

- append = no
- buffer = yes for dump styles *atom*, *custom*, *loca*, and *xyz*
- element = "C" for every atom type
- every = whatever it was set to via the dump command
- fileper = # of processors
- first = no
- flush = yes
- format = %d and %g for each integer or floating point value
- image = no
- label = ENTRIES
- nfile = 1

- pad = 0
- precision = 1000
- region = none
- scale = yes
- sort = off for dump styles *atom*, *custom*, *cfg*, and *local*
- sort = id for dump styles *dcd*, *xtc*, and *xyz*
- thresh = none
- unwrap = no

- acolor = * red/green/blue/yellow/aqua/cyan
- adiam = * 1.0
- amap = min max cf 0.0 2 min blue max red
- backcolor = black
- bcolor = * red/green/blue/yellow/aqua/cyan
- bdiam = * 0.5
- bitrate = 2000
- boxcolor = yellow
- color = 140 color names are pre-defined as listed below
- framerate = 24

These are the standard 109 element names that LAMMPS pre-defines for use with the dump image and dump_modify commands.

- 1-10 = "H", "He", "Li", "Be", "B", "C", "N", "O", "F", "Ne"
- 11-20 = "Na", "Mg", "Al", "Si", "P", "S", "Cl", "Ar", "K", "Ca"
- 21-30 = "Sc", "Ti", "V", "Cr", "Mn", "Fe", "Co", "Ni", "Cu", "Zn"
- 31-40 = "Ga", "Ge", "As", "Se", "Br", "Kr", "Rb", "Sr", "Y", "Zr"
- 41-50 = "Nb", "Mo", "Tc", "Ru", "Rh", "Pd", "Ag", "Cd", "In", "Sn"
- 51-60 = "Sb", "Te", "I", "Xe", "Cs", "Ba", "La", "Ce", "Pr", "Nd"
- 61-70 = "Pm", "Sm", "Eu", "Gd", "Tb", "Dy", "Ho", "Er", "Tm", "Yb"
- 71-80 = "Lu", "Hf", "Ta", "W", "Re", "Os", "Ir", "Pt", "Au", "Hg"
- 81-90 = "Tl", "Pb", "Bi", "Po", "At", "Rn", "Fr", "Ra", "Ac", "Th"
- 91-100 = "Pa", "U", "Np", "Pu", "Am", "Cm", "Bk", "Cf", "Es", "Fm"
- 101-109 = "Md", "No", "Lr", "Rf", "Db", "Sg", "Bh", "Hs", "Mt"

These are the 140 colors that LAMMPS pre-defines for use with the dump image and dump_modify commands. Additional colors can be defined with the dump_modify color command. The 3 numbers listed for each name are the RGB (red/green/blue) values. Divide each value by 255 to get the equivalent 0.0 to 1.0 value.

aliceblue = 240, 248, 255	antiquewhite = 250, 235, 215	aqua = 0, 255, 255	aquamarine = 127, 255, 212	azure = 240, 255, 255
beige = 245, 245, 220	bisque = 255, 228, 196	black = 0, 0, 0	blanchedalmond = 255, 255, 205	blue = 0, 0, 255
blueviolet = 138, 43, 226	brown = 165, 42, 42	burlywood = 222, 184, 135	cadetblue = 95, 158, 160	chartreuse = 127, 255, 0
chocolate = 210, 105, 30	coral = 255, 127, 80	cornflowerblue = 100, 149, 237	cornsilk = 255, 248, 220	crimson = 220, 20, 60
cyan = 0, 255, 255	darkblue = 0, 0, 139	darkcyan = 0, 139, 139	darkgoldenrod = 184, 134, 11	darkgray = 169, 169, 169
darkgreen = 0, 100, 0	darkkhaki = 189, 183, 107	darkmagenta = 139, 0, 139	darkolivegreen = 85, 107, 47	darkorange = 255, 140, 0

darkorchid = 153, 50, 204	darkred = 139, 0, 0	darksalmon = 233, 150, 122	darkseagreen = 143, 188, 143	darkslateblue = 72, 61, 139
darkslategray = 47, 79, 79	darkturquoise = 0, 206, 209	darkviolet = 148, 0, 211	deeppink = 255, 20, 147	deepskyblue = 0, 191, 255
dimgray = 105, 105, 105	dodgerblue = 30, 144, 255	firebrick = 178, 34, 34	floralwhite = 255, 250, 240	forestgreen = 34, 139, 34
fuchsia = 255, 0, 255	gainsboro = 220, 220, 220	ghostwhite = 248, 248, 255	gold = 255, 215, 0	goldenrod = 218, 165, 32
gray = 128, 128, 128	green = 0, 128, 0	greenyellow = 173, 255, 47	honeydew = 240, 255, 240	hotpink = 255, 105, 180
indianred = 205, 92, 92	indigo = 75, 0, 130	ivory = 255, 240, 240	khaki = 240, 230, 140	lavender = 230, 230, 250
lavenderblush = 255, 240, 245	lawngreen = 124, 252, 0	lemonchiffon = 255, 250, 205	lightblue = 173, 216, 230	lightcoral = 240, 128, 128
lightcyan = 224, 255, 255	lightgoldenrodyellow = 250, 250, 210	lightgreen = 144, 238, 144	lightgrey = 211, 211, 211	lightpink = 255, 182, 193
lightsalmon = 255, 160, 122	lightseagreen = 32, 178, 170	lightskyblue = 135, 206, 250	lightslategray = 119, 136, 153	lightsteelblue = 176, 196, 222
lightyellow = 255, 255, 224	lime = 0, 255, 0	limegreen = 50, 205, 50	linen = 250, 240, 230	magenta = 255, 0, 255
maroon = 128, 0, 0	mediumaquamarine = 102, 205, 170	mediumblue = 0, 0, 205	mediumorchid = 186, 85, 211	mediumpurple = 147, 112, 219
mediumseagreen = 60, 179, 113	mediumslateblue = 123, 104, 238	mediumspringgreen = 0, 250, 154	mediumturquoise = 72, 209, 204	mediumvioletred = 199, 21, 133
midnightblue = 25, 25, 112	mintcream = 245, 255, 250	mistyrose = 255, 228, 225	moccasin = 255, 228, 181	navajowhite = 255, 222, 173
navy = 0, 0, 128	oldlace = 253, 245, 230	olive = 128, 128, 0	olivedrab = 107, 142, 35	orange = 255, 165, 0
orangered = 255, 69, 0	orchid = 218, 112, 214	palegoldenrod = 238, 232, 170	palegreen = 152, 251, 152	paleturquoise = 175, 238, 238
palevioletred = 219, 112, 147	papayawhip = 255, 239, 213	peachpuff = 255, 239, 213	peru = 205, 133, 63	pink = 255, 192, 203
plum = 221, 160, 221	powderblue = 176, 224, 230	purple = 128, 0, 128	red = 255, 0, 0	rosybrown = 188, 143, 143
royalblue = 65, 105, 225	saddlebrown = 139, 69, 19	salmon = 250, 128, 114	sandybrown = 244, 164, 96	seagreen = 46, 139, 87
seashell = 255, 245, 238	sienna = 160, 82, 45	silver = 192, 192, 192	skyblue = 135, 206, 235	slateblue = 106, 90, 205
slategray = 112, 128, 144	snow = 255, 250, 250	springgreen = 0, 255, 127	steelblue = 70, 130, 180	tan = 210, 180, 140
teal = 0, 128, 128	thistle = 216, 191, 216	tomato = 253, 99, 71	turquoise = 64, 224, 208	violet = 238, 130, 238
wheat = 245, 222, 179	white = 255, 255, 255	whitesmoke = 245, 245, 245	yellow = 255, 255, 0	yellowgreen = 154, 205, 50

dump molfile command

Syntax:

```
dump ID group-ID molfile N file format path
```

- ID = user-assigned name for the dump
- group-ID = ID of the group of atoms to be imaged
- molfile = style of dump command (other styles *atom* or *cfg* or *dcd* or *xtc* or *xyz* or *local* or *custom* are discussed on the dump doc page)
- N = dump every this many timesteps
- file = name of file to write to
- format = file format to be used
- path = file path with plugins (optional)

Examples:

```
dump mf1 all molfile 10 melt1.xml hoomd
dump mf2 all molfile 10 melt2-*.pdb pdb .
dump mf3 all molfile 50 melt3.xyz xyz .:/home/akohlmey/vmd/plugins/LINUX/molfile
```

Description:

Dump a snapshot of atom coordinates and selected additional quantities to one or more files every N timesteps in one of several formats. Only information for atoms in the specified group is dumped. This specific dump style uses molfile plugins that are bundled with the VMD molecular visualization and analysis program. See Section tools of the manual and the tools/lmp2vmd/README.txt file for more information about support in VMD for reading and visualizing native LAMMPS dump files.

Unless the filename contains a * character, the output will be written to one single file with the specified format. Otherwise there will be one file per snapshot and the * will be replaced by the time step number when the snapshot is written.

NOTE: Because periodic boundary conditions are enforced only on timesteps when neighbor lists are rebuilt, the coordinates of an atom written to a dump file may be slightly outside the simulation box.

The molfile plugin API has a few restrictions that have to be honored by this dump style: the number of atoms must not change, the atoms must be sorted, outside of the coordinates no change in atom properties (like type, mass, charge) will be recorded.

The *format* keyword determines what format is used to write out the dump. For this to work, LAMMPS must be able to find and load a compatible molfile plugin that supports this format. Settings made via the dump_modify command can alter per atom properties like element names.

The *path* keyword determines which in directories. This is a "path" like other search paths, i.e. it can contain multiple directories separated by a colon (or semi-colon on windows). This keyword is optional and default to ".", the current directory.

The *unwrap* option of the dump_modify command allows coordinates to be written "unwrapped" by the image flags for each atom. Unwrapped means that if the atom has passed through a periodic boundary one or more times, the value is printed for what the coordinate would be if it had not been wrapped back into the periodic box.

Note that these coordinates may thus be far outside the box size stored with the snapshot.

Dumps are performed on timesteps that are a multiple of N (including timestep 0) and on the last timestep of a minimization if the minimization converges. Note that this means a dump will not be performed on the initial timestep after the dump command is invoked, if the current timestep is not a multiple of N. This behavior can be changed via the dump_modify first command, which can be useful if the dump command is invoked after a minimization ended on an arbitrary timestep. N can be changed between runs by using the dump_modify every command. The dump_modify every command also allows a variable to be used to determine the sequence of timesteps on which dump files are written.

Restrictions:

The *molfile* dump style is part of the USER-MOLFILE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Molfile plugins provide a consistent programming interface to read and write file formats commonly used in molecular simulations. The USER-MOLFILE package only provides the interface code, not the plugins. These can be obtained from a VMD installation which has to match the platform that you are using to compile LAMMPS for. By adding plugins to VMD, support for new file formats can be added to LAMMPS (or VMD or other programs that use them) without having to recompile the application itself. The plugins are installed in the directory: /plugins//molfile

NOTE: while the programming interface (API) to the plugins is backward compatible, the binary interface (ABI) has been changing over time, so it is necessary to compile this package with the plugin header files from VMD that match the binary plugins. These header files in the directory: /plugins/include For convenience, the package ships with a set of header files that are compatible with VMD 1.9 and 1.9.1 (June 2012)

Related commands:

dump, dump_modify, undump

Default:

The default path is ".". All other properties have to be specified.

echo command

Syntax:

```
echo style
```

- style = *none* or *screen* or *log* or *both*

Examples:

```
echo both
echo log
```

Description:

This command determines whether LAMMPS echoes each input script command to the screen and/or log file as it is read and processed. If an input script has errors, it can be useful to look at echoed output to see the last command processed.

The command-line switch -echo can be used in place of this command.

Restrictions: none

Related commands: none

Default:

```
echo log
```

fix command

Syntax:

```
fix ID group-ID style args
```

- ID = user-assigned name for the fix
- group-ID = ID of the group of atoms to apply the fix to
- style = one of a long list of possible style names (see below)
- args = arguments used by a particular style

Examples:

```
fix 1 all nve
fix 3 all nvt temp 300.0 300.0 0.01
fix mine top setforce 0.0 NULL 0.0
```

Description:

Set a fix that will be applied to a group of atoms. In LAMMPS, a "fix" is any operation that is applied to the system during timestepping or minimization. Examples include updating of atom positions and velocities due to time integration, controlling temperature, applying constraint forces to atoms, enforcing boundary conditions, computing diagnostics, etc. There are dozens of fixes defined in LAMMPS and new ones can be added; see this section for a discussion.

Fixes perform their operations at different stages of the timestep. If 2 or more fixes operate at the same stage of the timestep, they are invoked in the order they were specified in the input script.

The ID of a fix can only contain alphanumeric characters and underscores.

Fixes can be deleted with the unfix command.

NOTE: The unfix command is the only way to turn off a fix; simply specifying a new fix with a similar style will not turn off the first one. This is especially important to realize for integration fixes. For example, using a fix nve command for a second run after using a fix nvt command for the first run, will not cancel out the NVT time integration invoked by the "fix nvt" command. Thus two time integrators would be in place!

If you specify a new fix with the same ID and style as an existing fix, the old fix is deleted and the new one is created (presumably with new settings). This is the same as if an "unfix" command were first performed on the old fix, except that the new fix is kept in the same order relative to the existing fixes as the old one originally was. Note that this operation also wipes out any additional changes made to the old fix via the fix_modify command.

The fix modify command allows settings for some fixes to be reset. See the doc page for individual fixes for details.

Some fixes store an internal "state" which is written to binary restart files via the restart or write_restart commands. This allows the fix to continue on with its calculations in a restarted simulation. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file. See the doc pages for individual fixes for info on which ones can be restarted.

Some fixes calculate one of three styles of quantities: global, per-atom, or local, which can be used by other commands or output as described below. A global quantity is one or more system-wide values, e.g. the energy of a wall interacting with particles. A per-atom quantity is one or more values per atom, e.g. the displacement vector for each atom since time 0. Per-atom values are set to 0.0 for atoms not in the specified fix group. Local quantities are calculated by each processor based on the atoms it owns, but there may be zero or more per atoms.

Note that a single fix may produces either global or per-atom or local quantities (or none at all), but never more than one of these.

Global, per-atom, and local quantities each come in three kinds: a single scalar value, a vector of values, or a 2d array of values. The doc page for each fix describes the style and kind of values it produces, e.g. a per-atom vector. Some fixes produce more than one kind of a single style, e.g. a global scalar and a global vector.

When a fix quantity is accessed, as in many of the output commands discussed below, it can be referenced via the following bracket notation, where ID is the ID of the fix:

f_ID	entire scalar, vector, or array
f_ID[I]	one element of vector, one column of array
f_ID[I][J]	one element of array

In other words, using one bracket reduces the dimension of the quantity once (vector -> scalar, array -> vector). Using two brackets reduces the dimension twice (array -> scalar). Thus a command that uses scalar fix values as input can also process elements of a vector or array.

Note that commands and variables which use fix quantities typically do not allow for all kinds, e.g. a command may require a vector of values, not a scalar. This means there is no ambiguity about referring to a fix quantity as f_ID even if it produces, for example, both a scalar and vector. The doc pages for various commands explain the details.

In LAMMPS, the values generated by a fix can be used in several ways:

- Global values can be output via the thermo_style custom or fix ave/time command. Or the values can be referenced in a variable equal or variable atom command.
- Per-atom values can be output via the dump custom command or the fix ave/spatial command. Or they can be time-averaged via the fix ave/atom command or reduced by the compute reduce command. Or the per-atom values can be referenced in an atom-style variable.
- Local values can be reduced by the compute reduce command, or histogrammed by the fix ave/histo command.

See this howto section for a summary of various LAMMPS output options, many of which involve fixes.

The results of fixes that calculate global quantities can be either "intensive" or "extensive" values. Intensive means the value is independent of the number of atoms in the simulation, e.g. temperature. Extensive means the value scales with the number of atoms in the simulation, e.g. total rotational kinetic energy. Thermodynamic output will normalize extensive values by the number of atoms in the system, depending on the "thermo_modify norm" setting. It will not normalize intensive values. If a fix value is accessed in another way, e.g. by a variable, you may want to know whether it is an intensive or extensive value. See the doc page for individual fixes for further info.

Each fix style has its own documentation page which describes its arguments and what it does, as listed below. Here is an alphabetic list of fix styles available in LAMMPS. They are also given in more compact form in the Fix section of this page.

There are also additional fix styles (not listed here) submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the fix section of this page.

- adapt - change a simulation parameter over time
- addforce - add a force to each atom
- append/atoms - append atoms to a running simulation
- atom/swap - Monte Carlo atom type swapping
- aveforce - add an averaged force to each atom
- ave/atom - compute per-atom time-averaged quantities
- ave/chunk - compute per-chunk time-averaged quantities
- ave/correlate - compute/output time correlations
- ave/histo - compute/output time-averaged histograms
- ave/spatial - compute/output time-averaged per-atom quantities by layer
- ave/time - compute/output global time-averaged quantities
- balance - perform dynamic load-balancing
- bond/break - break bonds on the fly
- bond/create - create bonds on the fly
- bond/swap - Monte Carlo bond swapping
- box/relax - relax box size during energy minimization
- deform - change the simulation box size/shape
- deposit - add new atoms above a surface
- drag - drag atoms towards a defined coordinate
- dt/reset - reset the timestep based on velocity, forces
- efield - impose electric field on system
- enforce2d - zero out z-dimension velocity and force
- evaporate - remove atoms from simulation periodically
- external - callback to an external driver program
- freeze - freeze atoms in a granular simulation
- gcmc - grand canonical insertions/deletions
- gld - generalized Langevin dynamics integrator
- gravity - add gravity to atoms in a granular simulation
- heat - add/subtract momentum-conserving heat
- indent - impose force due to an indenter
- langevin - Langevin temperature control
- lineforce - constrain atoms to move in a line
- momentum - zero the linear and/or angular momentum of a group of atoms
- move - move atoms in a prescribed fashion
- msst - multi-scale shock technique (MSST) integration
- neb - nudged elastic band (NEB) spring forces
- nph - constant NPH time integration via Nose/Hoover
- nphug - constant-stress Hugoniostat integration
- nph/asphere - NPH for aspherical particles
- nph/sphere - NPH for spherical particles
- npt - constant NPT time integration via Nose/Hoover
- npt/asphere - NPT for aspherical particles
- npt/sphere - NPT for spherical particles
- nve - constant NVE time integration
- nve/asphere - NVE for aspherical particles
- nve/asphere/noforce - NVE for aspherical particles without forces"
- nve/body - NVE for body particles
- nve/limit - NVE with limited step length
- nve/line - NVE for line segments

- nve/noforce - NVE without forces (v only)
- nve/sphere - NVE for spherical particles
- nve/tri - NVE for triangles
- nvt - constant NVT time integration via Nose/Hoover
- nvt/asphere - NVT for aspherical particles
- nvt/sllod - NVT for NEMD with SLLOD equations
- nvt/sphere - NVT for spherical particles
- oneway - constrain particles on move in one direction
- orient/fcc - add grain boundary migration force
- planeforce - constrain atoms to move in a plane
- poems - constrain clusters of atoms to move as coupled rigid bodies
- pour - pour new atoms/molecules into a granular simulation domain
- press/berendsen - pressure control by Berendsen barostat
- print - print text and variables during a simulation
- property/atom - add customized per-atom values
- qeq/comb - charge equilibration for COMB potential qeq/dynamic - charge equilibration via dynamic method qeq/fire - charge equilibration via FIRE minimizer qeq/point - charge equilibration via point method qeq/shielded - charge equilibration via shielded method qeq/slater - charge equilibration via Slater method rattle - RATTLE constraints on bonds and/or angles
- reax/bonds - write out ReaxFF bond information recenter - constrain the center-of-mass position of a group of atoms
- restrain - constrain a bond, angle, dihedral
- rigid - constrain one or more clusters of atoms to move as a rigid body with NVE integration
- rigid/nph - constrain one or more clusters of atoms to move as a rigid body with NPH integration
- rigid/npt - constrain one or more clusters of atoms to move as a rigid body with NPT integration
- rigid/nve - constrain one or more clusters of atoms to move as a rigid body with alternate NVE integration
- rigid/nvt - constrain one or more clusters of atoms to move as a rigid body with NVT integration
- rigid/small - constrain many small clusters of atoms to move as a rigid body with NVE integration
- rigid/small/nph - constrain many small clusters of atoms to move as a rigid body with NPH integration
- rigid/small/npt - constrain many small clusters of atoms to move as a rigid body with NPT integration
- rigid/small/nve - constrain many small clusters of atoms to move as a rigid body with alternate NVE integration
- rigid/small/nvt - constrain many small clusters of atoms to move as a rigid body with NVT integration
- setforce - set the force on each atom
- shake - SHAKE constraints on bonds and/or angles
- spring - apply harmonic spring force to group of atoms
- spring/rg - spring on radius of gyration of group of atoms
- spring/self - spring from each atom to its origin
- srd - stochastic rotation dynamics (SRD)
- store/force - store force on each atom
- store/state - store attributes for each atom
- temp/berendsen - temperature control by Berendsen thermostat
- temp/csld - canonical sampling thermostat with Langevin dynamics
- temp/csvr - canonical sampling thermostat with Hamiltonian dynamics
- temp/rescale - temperature control by velocity rescaling
- tfmc - perform force-bias Monte Carlo with time-stamped method
- thermal/conductivity - Muller-Plathe kinetic energy exchange for thermal conductivity calculation
- tmd - guide a group of atoms to a new configuration
- ttm - two-temperature model for electronic/atomic coupling
- tune/kspace - auto-tune KSpace parameters
- vector - accumulate a global vector every N timesteps
- viscosity - Muller-Plathe momentum exchange for viscosity calculation

- viscous - viscous damping for granular simulations
- wall/colloid - Lennard-Jones wall interacting with finite-size particles
- wall/gran - frictional wall(s) for granular simulations
- wall/harmonic - harmonic spring wall
- wall/lj1043 - Lennard-Jones 10-4-3 wall
- wall/lj126 - Lennard-Jones 12-6 wall
- wall/lj93 - Lennard-Jones 9-3 wall
- wall/piston - moving reflective piston wall
- wall/reflect - reflecting wall(s)
- wall/region - use region surface as wall
- wall/srd - slip/no-slip wall for SRD particles

Restrictions:

Some fix styles are part of specific packages. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info on packages. The doc pages for individual fixes tell if it is part of a package.

Related commands:

unfix, fix_modify

Default: none

fix adapt command

Syntax:

```
fix ID group-ID adapt N attribute args ... keyword value ...
```

- ID, group-ID are documented in fix command
- adapt = style name of this fix command
- N = adapt simulation settings every this many timesteps
- one or more attribute/arg pairs may be appended
- attribute = *pair* or *kspace* or *atom*

```
  pair args = pstyle pparam I J v_name
      pstyle = pair style name, e.g. lj/cut
      pparam = parameter to adapt over time
      I,J = type pair(s) to set parameter for
      v_name = variable with name that calculates value of pparam
    kspace arg = v_name
      v_name = variable with name that calculates scale factor on K-space terms
    atom args = aparam v_name
      aparam = parameter to adapt over time
      v_name = variable with name that calculates value of aparam
```

- zero or more keyword/value pairs may be appended
- keyword = *scale* or *reset*

```
  scale value = no or yes
      no = the variable value is the new setting
      yes = the variable value multiplies the original setting
    reset value = no or yes
      no = values will remain altered at the end of a run
      yes = reset altered values to their original values at the end of a run
```

Examples:

```
fix 1 all adapt 1 pair soft a 1 1 v_prefactor
fix 1 all adapt 1 pair soft a 2* 3 v_prefactor
fix 1 all adapt 1 pair lj/cut epsilon * * v_scale1 coul/cut scale 3 3 v_scale2 scale yes reset yes
fix 1 all adapt 10 atom diameter v_size
```

Description:

Change or adapt one or more specific simulation attributes or settings over time as a simulation runs. Pair potential and K-space and atom attributes which can be varied by this fix are discussed below. Many other fixes can also be used to time-vary simulation parameters, e.g. the "fix deform" command will change the simulation box size/shape and the "fix move" command will change atom positions and velocities in a prescribed manner. Also note that many commands allow variables as arguments for specific parameters, if described in that manner on their doc pages. An equal-style variable can calculate a time-dependent quantity, so this is another way to vary a simulation parameter over time.

If N is specified as 0, the specified attributes are only changed once, before the simulation begins. This is all that is needed if the associated variables are not time-dependent. If $N > 0$, then changes are made every N steps during the simulation, presumably with a variable that is time-dependent.

Depending on the value of the *reset* keyword, attributes changed by this fix will or will not be reset back to their original values at the end of a simulation. Even if *reset* is specified as *yes*, a restart file written during a simulation will contain the modified settings.

If the *scale* keyword is set to *no*, then the value the parameter is set to will be whatever the variable generates. If the *scale* keyword is set to *yes*, then the value of the altered parameter will be the initial value of that parameter multiplied by whatever the variable generates. I.e. the variable is now a "scale factor" applied in (presumably) a time-varying fashion to the parameter.

Note that whether scale is *no* or *yes*, internally, the parameters themselves are actually altered by this fix. Make sure you use the *reset yes* option if you want the parameters to be restored to their initial values after the run.

The *pair* keyword enables various parameters of potentials defined by the pair_style command to be changed, if the pair style supports it. Note that the pair_style and pair_coeff commands must be used in the usual manner to specify these parameters initially; the fix adapt command simply overrides the parameters.

The *pstyle* argument is the name of the pair style. If pair_style hybrid or hybrid/overlay is used, *pstyle* should be a sub-style name. If there are multiple sub-styles using the same pair style, then *pstyle* should be specified as "style:N" where N is which instance of the pair style you wish to adapt, e.g. the first, second, etc. For example, *pstyle* could be specified as "soft" or "lubricate" or "lj/cut:1" or "lj/cut:2". The *pparam* argument is the name of the parameter to change. This is the current list of pair styles and parameters that can be varied by this fix. See the doc pages for individual pair styles and their energy formulas for the meaning of these parameters:

born	a,b,c	type pairs
buck	a,c	type pairs
coul/cut	scale	type pairs
coul/debye	scale	type pairs
coul/long	scale	type pairs
lj/cut	epsilon,sigma	type pairs
lj/expand	epsilon,sigma,delta	type pairs
lubricate	mu	global
gauss	a	type pairs
morse	d0,r0,alpha	type pairs
soft	a	type pairs

NOTE: It is easy to add new potentials and their parameters to this list. All it typically takes is adding an extract() method to the pair_*.cpp file associated with the potential.

Some parameters are global settings for the pair style, e.g. the viscosity setting "mu" for pair_style lubricate. Other parameters apply to atom type pairs within the pair style, e.g. the prefactor "a" for pair_style soft.

Note that for many of the potentials, the parameter that can be varied is effectively a prefactor on the entire energy expression for the potential, e.g. the lj/cut epsilon. The parameters listed as "scale" are exactly that, since the energy expression for the coul/cut potential (for example) has no labeled prefactor in its formula. To apply an effective prefactor to some potentials, multiple parameters need to be altered. For example, the Buckingham potential needs both the A and C terms altered together. To scale the Buckingham potential, you should thus list the pair style twice, once for A and once for C.

If a type pair parameter is specified, the *I* and *J* settings should be specified to indicate which type pairs to apply it to. If a global parameter is specified, the *I* and *J* settings still need to be specified, but are ignored.

Similar to the pair_coeff command, I and J can be specified in one of two ways. Explicit numeric values can be used for each, as in the 1st example above. I <= J is required. LAMMPS sets the coefficients for the symmetric J,I interaction to the same values.

A wild-card asterisk can be used in place of or in conjunction with the I,J arguments to set the coefficients for multiple pairs of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that only type pairs with I <= J are considered; if asterisks imply type pairs where J < I, they are ignored.

IMPROTANT NOTE: If pair_style hybrid or hybrid/overlay is being used, then the *pstyle* will be a sub-style name. You must specify I,J arguments that correspond to type pair values defined (via the pair_coeff command) for that sub-style.

The *v_name* argument for keyword *pair* is the name of an equal-style variable which will be evaluated each time this fix is invoked to set the parameter to a new value. It should be specified as v_name, where name is the variable name. Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify parameters that change as a function of time or span consecutive runs in a continuous fashion. For the latter, see the *start* and *stop* keywords of the run command and the *elaplong* keyword of thermo_style custom for details.

For example, these commands would change the prefactor coefficient of the pair_style soft potential from 10.0 to 30.0 in a linear fashion over the course of a simulation:

```
variable prefactor equal ramp(10,30)
fix 1 all adapt 1 pair soft a * * v_prefactor
```

The *kspace* keyword used the specified variable as a scale factor on the energy, forces, virial calculated by whatever K-Space solver is defined by the kspace_style command. If the variable has a value of 1.0, then the solver is unaltered.

The *kspace* keyword works this way whether the *scale* keyword is set to *no* or *yes*.

The *atom* keyword enables various atom properties to be changed. The *aparam* argument is the name of the parameter to change. This is the current list of atom parameters that can be varied by this fix:

- charge = charge on particle
- diameter = diameter of particle

The *v_name* argument of the *atom* keyword is the name of an equal-style variable which will be evaluated each time this fix is invoked to set the parameter to a new value. It should be specified as v_name, where name is the variable name. See the discussion above describing the formulas associated with equal-style variables. The new value is assigned to the corresponding attribute for all atoms in the fix group.

NOTE: The *atom* keyword works this way whether the *scale* keyword is set to *no* or *yes*. I.e. the use of scale yes is not yet supported by the *atom* keyword.

If the atom parameter is *diameter* and per-atom density and per-atom mass are defined for particles (e.g. atom_style granular), then the mass of each particle is also changed when the diameter changes (density is assumed to stay constant).

For example, these commands would shrink the diameter of all granular particles in the "center" group from 1.0 to 0.1 in a linear fashion over the course of a 1000-step simulation:

```
variable size equal ramp(1.0,0.1)
fix 1 center adapt 10 atom diameter v_size
```

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

For rRESPA time integration, this fix changes parameters on the outermost rRESPA level.

Restrictions: none

Related commands:

compute ti

Default:

The option defaults are scale = no, reset = no.

fix adapt/fep command

Syntax:

```
fix ID group-ID adapt/fep N attribute args ... keyword value ...
```

- ID, group-ID are documented in fix command
- adapt/fep = style name of this fix command
- N = adapt simulation settings every this many timesteps
- one or more attribute/arg pairs may be appended
- attribute = *pair* or *kspace* or *atom*

```
  pair args = pstyle pparam I J v_name
      pstyle = pair style name, e.g. lj/cut
      pparam = parameter to adapt over time
      I,J = type pair(s) to set parameter for
      v_name = variable with name that calculates value of pparam
    kspace arg = v_name
      v_name = variable with name that calculates scale factor on K-space terms
    atom args = aparam v_name
      aparam = parameter to adapt over time
      I = type(s) to set parameter for
      v_name = variable with name that calculates value of aparam
```

- zero or more keyword/value pairs may be appended
- keyword = *scale* or *reset* or *after*

```
  scale value = no or yes
      no = the variable value is the new setting
      yes = the variable value multiplies the original setting
    reset value = no or yes
      no = values will remain altered at the end of a run
      yes = reset altered values to their original values at the end
      of a run
    after value = no or yes
      no = parameters are adapted at timestep N
      yes = parameters are adapted one timestep after N
```

Examples:

```
fix 1 all adapt/fep 1 pair soft a 1 1 v_prefactor
fix 1 all adapt/fep 1 pair soft a 2* 3 v_prefactor
fix 1 all adapt/fep 1 pair lj/cut epsilon * * v_scale1 coul/cut scale 3 3 v_scale2 scale yes reset y
fix 1 all adapt/fep 10 atom diameter 1 v_size
```

Description:

Change or adapt one or more specific simulation attributes or settings over time as a simulation runs.

This is an enhanced version of the fix_adapt command with two differences,

- It is possible to modify the charges of chosen atom types only, instead of scaling all the charges in the system.
- There is a new option *after* for better compatibility with "fix ave/time".

This version is suited for free energy calculations using compute_ti or compute_fep.

If *N* is specified as 0, the specified attributes are only changed once, before the simulation begins. This is all that is needed if the associated variables are not time-dependent. If $N > 0$, then changes are made every *N* steps during the simulation, presumably with a variable that is time-dependent.

Depending on the value of the *reset* keyword, attributes changed by this fix will or will not be reset back to their original values at the end of a simulation. Even if *reset* is specified as *yes*, a restart file written during a simulation will contain the modified settings.

If the *scale* keyword is set to *no*, then the value the parameter is set to will be whatever the variable generates. If the *scale* keyword is set to *yes*, then the value of the altered parameter will be the initial value of that parameter multiplied by whatever the variable generates. I.e. the variable is now a "scale factor" applied in (presumably) a time-varying fashion to the parameter. Internally, the parameters themselves are actually altered; make sure you use the *reset yes* option if you want the parameters to be restored to their initial values after the run.

If the *after* keyword is set to *yes*, then the parameters are changed one timestep after the multiple of N. In this manner, if a fix such as "fix ave/time" is used to calculate averages at every N timesteps, all the contributions to the average will be obtained with the same values of the parameters.

The *pair* keyword enables various parameters of potentials defined by the pair_style command to be changed, if the pair style supports it. Note that the pair_style and pair_coeff commands must be used in the usual manner to specify these parameters initially; the fix adapt command simply overrides the parameters.

The *pstyle* argument is the name of the pair style. If pair_style hybrid or hybrid/overlay is used, *pstyle* should be a sub-style name. For example, *pstyle* could be specified as "soft" or "lubricate". The *pparam* argument is the name of the parameter to change. This is the current list of pair styles and parameters that can be varied by this fix. See the doc pages for individual pair styles and their energy formulas for the meaning of these parameters:

born	a,b,c	type pairs
buck	a,c	type pairs
coul/cut	scale	type pairs
coul/debye	scale	type pairs
coul/long	scale	type pairs
lj/cut	epsilon,sigma	type pairs
lj/expand	epsilon,sigma,delta	type pairs
lubricate	mu	global
gauss	a	type pairs
soft	a	type pairs

NOTE: It is easy to add new potentials and their parameters to this list. All it typically takes is adding an extract() method to the pair_*.cpp file associated with the potential.

Some parameters are global settings for the pair style, e.g. the viscosity setting "mu" for pair_style lubricate. Other parameters apply to atom type pairs within the pair style, e.g. the prefactor "a" for pair_style soft.

Note that for many of the potentials, the parameter that can be varied is effectively a prefactor on the entire energy expression for the potential, e.g. the lj/cut epsilon. The parameters listed as "scale" are exactly that, since the energy expression for the coul/cut potential (for example) has no labeled prefactor in its formula. To apply an effective prefactor to some potentials, multiple parameters need to be altered. For example, the Buckingham potential needs both the A and C terms altered together. To scale the Buckingham potential, you should thus list the pair style twice, once for A and once for C.

If a type pair parameter is specified, the *I* and *J* settings should be specified to indicate which type pairs to apply it to. If a global parameter is specified, the *I* and *J* settings still need to be specified, but are ignored.

Similar to the pair_coeff command, I and J can be specified in one of two ways. Explicit numeric values can be used for each, as in the 1st example above. I <= J is required. LAMMPS sets the coefficients for the symmetric J,I interaction to the same values.

A wild-card asterisk can be used in place of or in conjunction with the I,J arguments to set the coefficients for multiple pairs of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that only type pairs with I <= J are considered; if asterisks imply type pairs where J < I, they are ignored.

IMPROTANT NOTE: If pair_style hybrid or hybrid/overlay is being used, then the *pstyle* will be a sub-style name. You must specify I,J arguments that correspond to type pair values defined (via the pair_coeff command) for that sub-style.

The *v_name* argument for keyword *pair* is the name of an equal-style variable which will be evaluated each time this fix is invoked to set the parameter to a new value. It should be specified as v_name, where name is the variable name. Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify parameters that change as a function of time or span consecutive runs in a continuous fashion. For the latter, see the *start* and *stop* keywords of the run command and the *elaplong* keyword of thermo_style custom for details.

For example, these commands would change the prefactor coefficient of the pair_style soft potential from 10.0 to 30.0 in a linear fashion over the course of a simulation:

```
variable prefactor equal ramp(10,30)
fix 1 all adapt 1 pair soft a * * v_prefactor
```

The *kspace* keyword used the specified variable as a scale factor on the energy, forces, virial calculated by whatever K-Space solver is defined by the kspace_style command. If the variable has a value of 1.0, then the solver is unaltered.

The *kspace* keyword works this way whether the *scale* keyword is set to *no* or *yes*.

The *atom* keyword enables various atom properties to be changed. The *aparam* argument is the name of the parameter to change. This is the current list of atom parameters that can be varied by this fix:

- charge = charge on particle
- diameter = diameter of particle

The *I* argument indicates which atom types are affected. A wild-card asterisk can be used in place of or in conjunction with the I argument to set the coefficients for multiple atom types.

The *v_name* argument of the *atom* keyword is the name of an equal-style variable which will be evaluated each time this fix is invoked to set the parameter to a new value. It should be specified as v_name, where name is the variable name. See the discussion above describing the formulas associated with equal-style variables. The new value is assigned to the corresponding attribute for all atoms in the fix group.

If the atom parameter is *diameter* and per-atom density and per-atom mass are defined for particles (e.g. atom_style granular), then the mass of each particle is also changed when the diameter changes (density is assumed to stay constant).

For example, these commands would shrink the diameter of all granular particles in the "center" group from 1.0 to 0.1 in a linear fashion over the course of a 1000-step simulation:

```
variable size equal ramp(1.0,0.1)
fix 1 center adapt 10 atom diameter * v_size
```

For rRESPA time integration, this fix changes parameters on the outermost rRESPA level.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

compute fep, fix_adapt, compute ti

Default:

The option defaults are scale = no, reset = no, after = no.

fix addforce command

fix addforce/cuda command

Syntax:

```
fix ID group-ID addforce fx fy fz keyword value ...
```

- ID, group-ID are documented in fix command
- addforce = style name of this fix command
- fx,fy,fz = force component values (force units)

```
  any of fx,fy,fz can be a variable (see below)
```

- zero or more keyword/value pairs may be appended to args
- keyword = *every* or *region* or *energy*

```
every value = Nevery
    Nevery = add force every this many timesteps
  region value = region-ID
    region-ID = ID of region atoms must be in to have added force
  energy value = v_name
    v_name = variable with name that calculates the potential energy of each atom in the added
```

Examples:

```
fix kick flow addforce 1.0 0.0 0.0
fix kick flow addforce 1.0 0.0 v_oscillate
fix ff boundary addforce 0.0 0.0 v_push energy v_espace
```

Description:

Add fx,fy,fz to the corresponding component of force for each atom in the group. This command can be used to give an additional push to atoms in a simulation, such as for a simulation of Poiseuille flow in a channel.

Any of the 3 quantities defining the force components can be specified as an equal-style or atom-style variable, namely *fx*, *fy*, *fz*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value(s) used to determine the force component.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent force field.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent force field with optional time-dependence as well.

If the *every* keyword is used, the *Nevery* setting determines how often the forces are applied. The default value is 1, for every timestep.

If the *region* keyword is used, the atom must also be in the specified geometric region in order to have force added to it.

Adding a force to atoms implies a change in their potential energy as they move due to the applied force field. For dynamics via the "run" command, this energy can be optionally added to the system's potential energy for thermodynamic output (see below). For energy minimization via the "minimize" command, this energy must be added to the system's potential energy to formulate a self-consistent minimization problem (see below).

The *energy* keyword is not allowed if the added force is a constant vector F = (fx,fy,fz), with all components defined as numeric constants and not as variables. This is because LAMMPS can compute the energy for each atom directly as E = -x dot F = -(x*fx + y*fy + z*fz), so that -Grad(E) = F.

The *energy* keyword is optional if the added force is defined with one or more variables, and if you are performing dynamics via the run command. If the keyword is not used, LAMMPS will set the energy to 0.0, which is typically fine for dynamics.

The *energy* keyword is required if the added force is defined with one or more variables, and you are performing energy minimization via the "minimize" command. The keyword specifies the name of an atom-style variable which is used to compute the energy of each atom as function of its position. Like variables used for *fx*, *fy*, *fz*, the energy variable is specified as v_name, where name is the variable name.

Note that when the *energy* keyword is used during an energy minimization, you must insure that the formula defined for the atom-style variable is consistent with the force variable formulas, i.e. that -Grad(E) = F. For example, if the force were a spring-like F = kx, then the energy formula should be E = -0.5kx^2. If you don't do this correctly, the minimization will not converge properly.

Styles with a *cuda* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *energy* option is supported by this fix to add the potential "energy" inferred by the added force to the system's potential energy as part of thermodynamic output. This is a fictitious quantity but is needed so that the minimize command can include the forces added by this fix in a consistent manner. I.e. there is a decrease in potential energy when atoms move in the direction of the added force.

This fix computes a global scalar and a global 3-vector of forces, which can be accessed by various output commands. The scalar is the potential energy discussed above. The vector is the total force on the group of atoms before the forces on individual atoms are changed by the fix. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command. You should not specify force components with a variable that has time-dependence for use with a minimizer, since the minimizer increments the timestep as the iteration count during the minimization.

NOTE: If you want the fictitious potential energy associated with the added forces to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the fix_modify *energy* option for this fix.

Restrictions: none

Related commands:

fix setforce, fix aveforce

Default:

The option default for the every keyword is every = 1.

fix addtorque command

Syntax:

```
fix ID group-ID addtorque Tx Ty Tz
```

- ID, group-ID are documented in fix command
- addtorque = style name of this fix command
- Tx,Ty,Tz = torque component values (torque units)
- any of Tx,Ty,Tz can be a variable (see below)

Examples:

```
fix kick bead addtorque 2.0 3.0 5.0
fix kick bead addtorque 0.0 0.0 v_oscillate
```

Description:

Add a set of forces to each atom in the group such that:

- the components of the total torque applied on the group (around its center of mass) are Tx,Ty,Tz
- the group would move as a rigid body in the absence of other forces.

This command can be used to drive a group of atoms into rotation.

Any of the 3 quantities defining the torque components can be specified as an equal-style variable, namely *Tx*, *Ty*, *Tz*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the torque component.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent torque.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *energy* option is supported by this fix to add the potential "energy" inferred by the added forces to the system's potential energy as part of thermodynamic output. This is a fictitious quantity but is needed so that the minimize command can include the forces added by this fix in a consistent manner. I.e. there is a decrease in potential energy when atoms move in the direction of the added forces.

This fix computes a global scalar and a global 3-vector, which can be accessed by various output commands. The scalar is the potential energy discussed above. The vector is the total torque on the group of atoms before the forces on individual atoms are changed by the fix. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command. You

should not specify force components with a variable that has time-dependence for use with a minimizer, since the minimizer increments the timestep as the iteration count during the minimization.

Restrictions:

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix addforce

Default: none

fix append/atoms command

Syntax:

```
fix ID group-ID append/atoms face ... keyword value ...
```

- ID, group-ID are documented in fix command
- append/atoms = style name of this fix command
- face = *zhi*
- zero or more keyword/value pairs may be appended
- keyword = *basis* or *size* or *freq* or *temp* or *random* or *units*

```
  basis values = M itype
      M = which basis atom
      itype = atom type (1-N) to assign to this basis atom
    size args = Lz
      Lz = z size of lattice region appended in a single event(distance units)
    freq args = freq
      freq = the number of timesteps between append events
    temp args = target damp seed extent
      target = target temperature for the region between zhi-extent and zhi (temperature units)
      damp = damping parameter (time units)
      seed = random number seed for langevin kicks
      extent = extent of thermostated region (distance units)
    random args = xmax ymax zmax seed
      xmax, ymax, zmax = maximum displacement in particular direction (distance units)
      seed = random number seed for random displacement
    units value = lattice or box
      lattice = the wall position is defined in lattice units
      box = the wall position is defined in simulation box units
```

Examples:

```
fix 1 all append/atoms zhi size 5.0 freq 295 units lattice
fix 4 all append/atoms zhi size 15.0 freq 5 units box
fix A all append/atoms zhi size 1.0 freq 1000 units lattice
```

Description:

This fix creates atoms on a lattice, appended on the zhi edge of the system box. This can be useful when a shock or wave is propagating from zlo. This allows the system to grow with time to accommodate an expanding wave. A simulation box must already exist, which is typically created via the create_box command. Before using this command, a lattice must also be defined using the lattice command.

This fix will automatically freeze atoms on the zhi edge of the system, so that overlaps are avoided when new atoms are appended.

The *basis* keyword specifies an atom type that will be assigned to specific basis atoms as they are created. See the lattice command for specifics on how basis atoms are defined for the unit cell of the lattice. By default, all created atoms are assigned type = 1 unless this keyword specifies differently.

The *size* keyword defines the size in z of the chunk of material to be added.

The *random* keyword will give the atoms random displacements around their lattice points to simulate some initial temperature.

The *temp* keyword will cause a region to be thermostated with a Langevin thermostat on the zhi boundary. The size of the region is measured from zhi and is set with the *extent* argument.

The *units* keyword determines the meaning of the distance units used to define a wall position, but only when a numeric constant is used. A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacings.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix style is part of the SHOCK package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The boundary on which atoms are added with append/atoms must be shrink/minimum. The opposite boundary may be any boundary type other than periodic.

Related commands:

fix wall/piston command

Default:

The keyword defaults are size = 0.0, freq = 0, units = lattice. All added atoms are of type 1 unless the basis keyword is used.

fix atc command

Syntax:

```
fix   atc
```

- fixID = name of fix
- group = name of group fix is to be applied
- type = *thermal* or *two_temperature* or *hardy* or *field*

```
thermal = thermal coupling with fields: temperature
 two_temperature = electron-phonon coupling with field: temperature and electron_temperature
 hardy = on-the-fly post-processing using kernel localization functions (see "related" section for
 field = on-the-fly post-processing using mesh-based localization functions (see "related" section
```

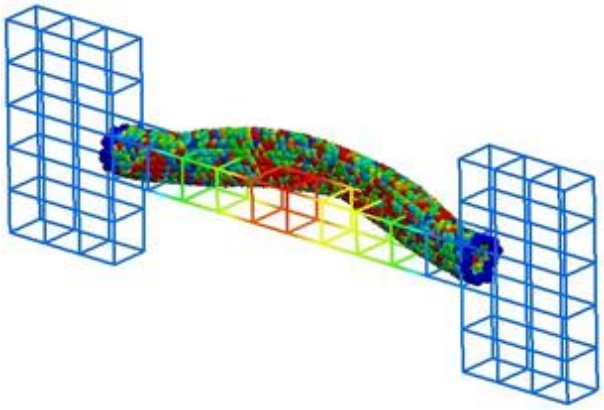
- parameter_file = name of the file with material parameters. Note: Neither hardy nor field requires a parameter file

Examples:

```
fix AtC internal atc thermal Ar_thermal.dat
fix AtC internal atc two_temperature Ar_ttm.mat
fix AtC internal atc hardy
fix AtC internal atc field
```

Description:

This fix is the beginning to creating a coupled FE/MD simulation and/or an on-the-fly estimation of continuum fields. The coupled versions of this fix do Verlet integration and the post-processing does not. After instantiating this fix, several other fix_modify commands will be needed to set up the problem, e.g. define the finite element mesh and prescribe initial and boundary conditions.



```
The following coupling example is typical, but non-exhaustive:
 # ... commands to create and initialize the MD system

 # initial fix to designate coupling type and group to apply it to
 # tag group physics material_file
 fix AtC internal atc thermal Ar_thermal.mat

 # create a uniform 12 x 2 x 2 mesh that covers region contain the group
 # nx ny nz region periodicity
 fix_modify AtC mesh create 12 2 2 mdRegion f p p
```

```
# specify the control method for the type of coupling
# physics control_type
fix_modify AtC thermal control flux

# specify the initial values for the empirical field "temperature"
# field node_group value
fix_modify AtC initial temperature all 30

# create an output stream for nodal fields
# filename output_frequency
fix_modify AtC output atc_fe_output 100

run 1000
```

likewise for this post-processing example:

```
# ... commands to create and initialize the MD system

# initial fix to designate post-processing and the group to apply it to
# no material file is allowed nor required
fix AtC internal atc hardy

# for hardy fix, specific kernel function (function type and range) to # be used as a localizatio
fix AtC kernel quartic_sphere 10.0

# create a uniform 1 x 1 x 1 mesh that covers region contain the group
# with periodicity this effectively creats a system average
fix_modify AtC mesh create 1 1 1 box p p p

# change from default lagrangian map to eulerian
# refreshed every 100 steps
fix_modify AtC atom_element_map eulerian 100

# start with no field defined
# add mass density, potential energy density, stress and temperature
fix_modify AtC fields add density energy stress temperature

# create an output stream for nodal fields
# filename output_frequency
fix_modify AtC output nvtFE 100 text

run 1000
```

the mesh's linear interpolation functions can be used as the localization function by using the field option:

fix AtC internal atc field

fix_modify AtC mesh create 1 1 1 box p p p

...

Note coupling and post-processing can be combined in the same simulations using separate fixes.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. The fix_modify options relevant to this fix are listed below. No global scalar or vector or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is

not invoked during energy minimization.

Restrictions:

Thermal and two_temperature (coupling) types use a Verlet time-integration algorithm. The hardy type does not contain its own time-integrator and must be used with a separate fix that does contain one, e.g. nve, nvt, etc.

- Currently,
- - the coupling is restricted to thermal physics
- - the FE computations are done in serial on each processor.

Related commands:

After specifying this fix in your input script, several other fix_modify commands are used to setup the problem, e.g. define the finite element mesh and prescribe initial and boundary conditions.

fix_modify commands for setup:

- fix_modify AtC mesh create
- fix_modify AtC mesh quadrature
- fix_modify AtC mesh read
- fix_modify AtC mesh write
- fix_modify AtC mesh create_nodeset
- fix_modify AtC mesh add_to_nodeset
- fix_modify AtC mesh create_faceset box
- fix_modify AtC mesh create_faceset plane
- fix_modify AtC mesh create_elementset
- fix_modify AtC mesh delete_elements
- fix_modify AtC mesh nodeset_to_elementset
- fix_modify AtC boundary
- fix_modify AtC internal_quadrature
- fix_modify AtC time_integration (thermal)
- fix_modify AtC time_integration (momentum)
- fix_modify AtC extrinsic electron_integration
- fix_modify AtC internal_element_set
- fix_modify AtC decomposition

fix_modify commands for boundary and initial conditions:

- fix_modify AtC initial
- fix_modify AtC fix
- fix_modify AtC unfix
- fix_modify AtC fix_flux
- fix_modify AtC unfix_flux
- fix_modify AtC source
- fix_modify AtC remove_source

fix_modify commands for control and filtering:

- fix_modify AtC control
- fix_modify AtC control thermal
- fix_modify AtC control thermal correction_max_iterations

- fix_modify AtC control momentum
- fix_modify AtC control localized_lambda
- fix_modify AtC control lumped_lambda_solve
- fix_modify AtC control mask_direction control
- fix_modify AtC filter
- fix_modify AtC filter scale
- fix_modify AtC filter type
- fix_modify AtC equilibrium_start
- fix_modify AtC extrinsic exchange
- fix_modify AtC poisson_solver

fix_modify commands for output:

- fix_modify AtC output
- fix_modify AtC output nodeset
- fix_modify AtC output elementset
- fix_modify AtC output boundary_integral
- fix_modify AtC output contour_integral
- fix_modify AtC mesh output
- fix_modify AtC write_restart
- fix_modify AtC read_restart

fix_modify commands for post-processing:

- fix_modify AtC kernel
- fix_modify AtC fields
- fix_modify AtC grdients
- fix_modify AtC rates
- fix_modify AtC computes
- fix_modify AtC on_the_fly
- fix_modify AtC pair_interactions/bond_interactions
- fix_modify AtC sample_frequency
- fix_modify AtC set

miscellaneous fix_modify commands:

- fix_modify AtC atom_element_map
- fix_modify AtC atom_weight
- fix_modify AtC write_atom_weights
- fix_modify AtC reset_time
- fix_modify AtC reset_atomic_reference_positions
- fix_modify AtC fe_md_boundary
- fix_modify AtC boundary_faceset
- fix_modify AtC consistent_fe_initialization
- fix_modify AtC mass_matrix
- fix_modify AtC material
- fix_modify AtC atomic_charge
- fix_modify AtC source_integration
- fix_modify AtC temperature_definition
- fix_modify AtC track_displacement
- fix_modify AtC boundary_dynamics
- fix_modify AtC add_species

- fix_modify AtC add_molecule
- fix_modify AtC remove_species
- fix_modify AtC remove_molecule

Note: a set of example input files with the attendant material files are included with this package

Default: None

For detailed exposition of the theory and algorithms please see:

(Wagner) Wagner, GJ; Jones, RE; Templeton, JA; Parks, MA, "An atomistic-to-continuum coupling method for heat transfer in solids." Special Issue of Computer Methods and Applied Mechanics (2008) 197:3351.

(Zimmerman2004) Zimmerman, JA; Webb, EB; Hoyt, JJ;. Jones, RE; Klein, PA; Bammann, DJ, "Calculation of stress in atomistic simulation." Special Issue of Modelling and Simulation in Materials Science and Engineering (2004), 12:S319.

(Zimmerman2010) Zimmerman, JA; Jones, RE; Templeton, JA, "A material frame approach for evaluating continuum variables in atomistic simulations." Journal of Computational Physics (2010), 229:2364.

(Templeton2010) Templeton, JA; Jones, RE; Wagner, GJ, "Application of a field-based method to spatially varying thermal transport problems in molecular dynamics." Modelling and Simulation in Materials Science and Engineering (2010), 18:085007.

(Jones) Jones, RE; Templeton, JA; Wagner, GJ; Olmsted, D; Modine, JA, "Electron transport enhanced molecular dynamics for metals and semi-metals." International Journal for Numerical Methods in Engineering (2010), 83:940.

(Templeton2011) Templeton, JA; Jones, RE; Lee, JW; Zimmerman, JA; Wong, BM, "A long-range electric field solver for molecular dynamics based on atomistic-to-continuum modeling." Journal of Chemical Theory and Computation (2011), 7:1736.

(Mandadapu) Mandadapu, KK; Templeton, JA; Lee, JW, "Polarization as a field variable from molecular dynamics simulations." Journal of Chemical Physics (2013), 139:054115.

Please refer to the standard finite element (FE) texts, e.g. T.J.R Hughes " The finite element method ", Dover 2003, for the basics of FE simulation.

fix atom/swap command

Syntax:

```
fix ID group-ID atom/swap N X seed T keyword values ...
```

- ID, group-ID are documented in fix command
- atom/swap = style name of this fix command
- N = invoke this fix every N steps
- X = number of swaps to attempt every N steps
- seed = random # seed (positive integer)
- T = scaling temperature of the MC swaps (temperature units)
- one or more keyword/value pairs may be appended to args
- keyword = *types* or *mu* or *ke* or *semi-grand* or *region*

```
  types values = two or more atom types
    mu values = chemical potential of swap types (energy units)
    ke value = no or yes
      no = no conservation of kinetic energy after atom swaps
      yes = kinetic energy is conserved after atom swaps
    semi-grand value = no or yes
      no = particle type counts and fractions conserved
      yes = semi-grand canonical ensemble, particle fractions not conserved
    region value = region-ID
      region-ID = ID of region to use as an exchange/move volume
```

Examples:

```
fix 2 all atom/swap 1 1 29494 300.0 ke no types 1 2
fix myFix all atom/swap 100 1 12345 298.0 region my_swap_region types 5 6
fix SGMC all atom/swap 1 100 345 1.0 semi-grand yes types 1 2 3 mu 0.0 4.3 -5.0
```

Description:

This fix performs Monte Carlo swaps of atoms of one given atom type with atoms of the other given atom types. The specified T is used in the Metropolis criterion dictating swap probabilities.

Perform X swaps of atoms of one type with atoms of another type according to a Monte Carlo probability. Swap candidates must be in the fix group, must be in the region (if specified), and must be of one of the listed types. Swaps are attempted between candidates that are chosen randomly with equal probability among the candidate atoms. Swaps are not attempted between atoms of the same type since nothing would happen.

All atoms in the simulation domain can be moved using regular time integration displacements, e.g. via fix_nvt, resulting in a hybrid MC+MD simulation. A smaller-than-usual timestep size may be needed when running such a hybrid simulation, especially if the swapped atoms are not well equilibrated.

The *types* keyword is required. At least two atom types must be specified.

The *ke* keyword can be set to *no* to turn off kinetic energy conservation for swaps. The default is *yes*, which means that swapped atoms have their velocities scaled by the ratio of the masses of the swapped atom types. This ensures that the kinetic energy of each atom is the same after the swap as it was before the swap, even though the atom masses have changed.

The *semi-grand* keyword can be set to *yes* to switch to the semi-grand canonical ensemble as discussed in (Sadigh). This means that the total number of each particle type does not need to be conserved. The default is *no*, which means that the only kind of swap allowed exchanges an atom of one type with an atom of a different given type. In other words, the relative mole fractions of the swapped atoms remains constant. Whereas in the semi-grand canonical ensemble, the composition of the system can change. Note that when using *semi-grand*, atoms in the fix group whose type is not listed in the *types* keyword are ineligible for attempted conversion. An attempt is made to switch the selected atom (if eligible) to one of the other listed types with equal probability. Acceptance of each attempt depends upon the Metropolis criterion.

The *mu* keyword allows users to specify chemical potentials. This is required and allowed only when using *semi-grand*. All chemical potentials are absolute, so there is one for each swap type listed following the *types* keyword. In semi-grand canonical ensemble simulations the chemical composition of the system is controlled by the difference in these values. So shifting all values by a constant amount will have no effect on the simulation.

This command may optionally use the *region* keyword to define swap volume. The specified region must have been previously defined with a region command. It must be defined with side = *in*. Swap attempts occur only between atoms that are both within the specified region. Swaps are not otherwise attempted.

You should ensure you do not swap atoms belonging to a molecule, or LAMMPS will soon generate an error when it tries to find those atoms. LAMMPS will warn you if any of the atoms eligible for swapping have a non-zero molecule ID, but does not check for this at the time of swapping.

If not using *semi-grand* this fix checks to ensure all atoms of the given types have the same atomic charge. LAMMPS doesn't enforce this in general, but it is needed for this fix to simplify the swapping procedure. Successful swaps will swap the atom type and charge of the swapped atoms. Conversely, when using *semi-grand*, it is assumed that all the atom types involved in switches have the same charge. Otherwise, charge would not be conserved. As a consequence, no checks on atomic charges are performed, and successful switches update the atom type but not the atom charge. While it is possible to use *semi-grand* with groups of atoms that have different charges, these charges will not be changed when the atom types change.

Since this fix computes total potential energies before and after proposed swaps, so even complicated potential energy calculations are OK, including the following:

- long-range electrostatics (kspace)
- many body pair styles
- hybrid pair styles
- eam pair styles
- triclinic systems
- need to include potential energy contributions from other fixes

Some fixes have an associated potential energy. Examples of such fixes include: efield, gravity, addforce, langevin, restrain, temp/berendsen, temp/rescale, and wall fixes. For that energy to be included in the total potential energy of the system (the quantity used when performing GCMC moves), you MUST enable the fix_modify *energy* option for that fix. The doc pages for individual fix commands specify if this should be done.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the fix to binary restart files. This includes information about the random number generator seed, the next timestep for MC exchanges, etc. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

None of the fix_modify options are relevant to this fix.

This fix computes a global vector of length 2, which can be accessed by various output commands. The vector values are the following global cumulative quantities:

- 1 = swap attempts
- 2 = swap successes

The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the MC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix_nvt, neighbor, fix_deposit, fix_evaporate, delete_atoms, fix_gcmc

Default:

The option defaults are ke = yes, semi-grand = no, mu = 0.0 for all atom types.

(Sadigh) B Sadigh, P Erhart, A Stukowski, A Caro, E Martinez, and L Zepeda-Ruiz, Phys. Rev. B, 85, 184203 (2012).

fix ave/atom command

Syntax:

```
fix ID group-ID ave/atom Nevery Nrepeat Nfreq value1 value2 ...
```

- ID, group-ID are documented in fix command
- ave/atom = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of times to use input values for calculating averages
- Nfreq = calculate averages every this many timesteps one or more input values can be listed
- value = x, y, z, vx, vy, vz, fx, fy, fz, c_ID, c_ID[i], f_ID, f_ID[i], v_name

```
x,y,z,vx,vy,vz,fx,fy,fz = atom attribute (position, velocity, force component)
c_ID = per-atom vector calculated by a compute with ID
c_ID[I] = Ith column of per-atom array calculated by a compute with ID
f_ID = per-atom vector calculated by a fix with ID
f_ID[I] = Ith column of per-atom array calculated by a fix with ID
v_name = per-atom vector calculated by an atom-style variable with name
```

Examples:

```
fix 1 all ave/atom 1 100 100 vx vy vz
fix 1 all ave/atom 10 20 1000 c_my_stress[1]
```

Description:

Use one or more per-atom vectors as inputs every few timesteps, and average them atom by atom over longer timescales. The resulting per-atom averages can be used by other output commands such as the fix ave/spatial or dump custom commands.

The group specified with the command means only atoms within the group have their averages computed. Results are set to 0.0 for atoms not in the group.

Each input value can be an atom attribute (position, velocity, force component) or can be the result of a compute or fix or the evaluation of an atom-style variable. In the latter cases, the compute, fix, or variable must produce a per-atom vector, not a global quantity or local quantity. If you wish to time-average global quantities from a compute, fix, or variable, then see the fix ave/time command.

Computes that produce per-atom vectors or arrays are those which have the word *atom* in their style name. See the doc pages for individual fixes to determine which ones produce per-atom vectors or arrays. Variables of style *atom* are the only ones that can be used with this fix since they produce per-atom vectors.

Each per-atom value of each input vector is averaged independently.

The *Nevery*, *Nrepeat*, and *Nfreq* arguments specify on what timesteps the input values will be used in order to contribute to the average. The final averaged quantities are generated on timesteps that are a multiple of *Nfreq*. The average is over *Nrepeat* quantities, computed in the preceding portion of the simulation every *Nevery* timesteps. *Nfreq* must be a multiple of *Nevery* and *Nevery* must be non-zero even if *Nrepeat* is 1. Also, the timesteps contributing to the average value cannot overlap, i.e. Nrepeat*Nevery can not exceed Nfreq.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then values on timesteps 90,92,94,96,98,100 will be used to compute the final average on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc.

The atom attribute values (x,y,z,vx,vy,vz,fx,fy,fz) are self-explanatory. Note that other atom attributes can be used as inputs to this fix by using the compute property/atom command and then specifying an input value from that compute.

NOTE: The x,y,z attributes are values that are re-wrapped inside the periodic box whenever an atom crosses a periodic boundary. Thus if you time average an atom that spends half its time on either side of the periodic box, you will get a value in the middle of the box. If this is not what you want, consider averaging unwrapped coordinates, which can be provided by the compute property/atom command via its xu,yu,zu attributes.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If no bracketed term is appended, the per-atom vector calculated by the compute is used. If a bracketed term containing an index I is appended, the Ith column of the per-atom array calculated by the compute is used. Users can also write code for their own compute styles and add them to LAMMPS.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If no bracketed term is appended, the per-atom vector calculated by the fix is used. If a bracketed term containing an index I is appended, the Ith column of the per-atom array calculated by the fix is used. Note that some fixes only produce their values on certain timesteps, which must be compatible with *Nevery*, else an error will result. Users can also write code for their own fix styles and add them to LAMMPS.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script as an atom-style variable Variables of style *atom* can reference thermodynamic keywords, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of generating per-atom quantities to time average.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global scalar or vector quantities are stored by this fix for access by various output commands.

This fix produces a per-atom vector or array which can be accessed by various output commands. A vector is produced if only a single quantity is averaged by this fix. If two or more quantities are averaged, then an array of values is produced. The per-atom values can only be accessed on timesteps that are multiples of *Nfreq* since that is when averaging is performed.

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

compute, fix ave/histo, fix ave/spatial, fix ave/time, variable,

Default: none

fix ave/chunk command

Syntax:

```
fix ID group-ID ave/chunk Nevery Nrepeat Nfreq chunkID value1 value2 ... keyword args ...
```

- ID, group-ID are documented in fix command
- ave/chunk = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of times to use input values for calculating averages
- Nfreq = calculate averages every this many timesteps
- chunkID = ID of compute chunk/atom command
- one or more input values can be listed
- value = vx, vy, vz, fx, fy, fz, density/mass, density/number, temp, c_ID, c_ID[I], f_ID, f_ID[I], v_name

```
vx,vy,vz,fx,fy,fz = atom attribute (velocity, force component)
density/number, density/mass = number or mass density
temp = temperature
c_ID = per-atom vector calculated by a compute with ID
c_ID[I] = Ith column of per-atom array calculated by a compute with ID
f_ID = per-atom vector calculated by a fix with ID
f_ID[I] = Ith column of per-atom array calculated by a fix with ID
v_name = per-atom vector calculated by an atom-style variable with name
```

- zero or more keyword/arg pairs may be appended
- keyword = *norm* or *ave* or *bias* or *adof* or *cdof* or *file* or *overwrite* or *title1* or *title2* or *title3*

```
norm arg = all or sample or none = how output on Nfreq steps is normalized
    all = output is sum of atoms across all Nrepeat samples, divided by atom count
    sample = output is sum of Nrepeat sample averages, divided by Nrepeat
    none = output is sum of Nrepeat sample sums, divided by Nrepeat
  ave args = one or running or window M
    one = output new average value every Nfreq steps
    running = output cumulative average of all previous Nfreq steps
    window M = output average of M most recent Nfreq steps
  bias arg = bias-ID
    bias-ID = ID of a temperature compute that removes a velocity bias for temperature calcula
  adof value = dof_per_atom
    dof_per_atom = define this many degrees-of-freedom per atom for temperature calculation
  cdof value = dof_per_chunk
    dof_per_chunk = define this many degrees-of-freedom per chunk for temperature calculation
  file arg = filename
    filename = file to write results to
  overwrite arg = none = overwrite output file with only latest output
  format arg = string
    string = C-style format string
  title1 arg = string
    string = text to print as 1st line of output file
  title2 arg = string
    string = text to print as 2nd line of output file
  title3 arg = string
    string = text to print as 3rd line of output file
```

Examples:

```
fix 1 all ave/chunk 10000 1 10000 binchunk c_myCentro title1 "My output values"
fix 1 flow ave/chunk 100 10 1000 molchunk vx vz norm sample file vel.profile
fix 1 flow ave/chunk 100 5 1000 binchunk density/mass ave running
```

```
fix 1 flow ave/chunk 100 5 1000 binchunk density/mass ave running
```

NOTE:

If you are trying to replace an older fix ave/spatial command with the newer, more flexible fix ave/chunk and compute chunk/atom commands, you simply need to split the fix ave/spatial arguments across the two new commands. For example, this command:

```
fix 1 flow ave/spatial 100 10 1000 y 0.0 1.0 vx vz norm sample file vel.profile
```

could be replaced by:

```
compute cc1 flow chunk/atom bin/1d y 0.0 1.0
fix 1 flow ave/chunk 100 10 1000 cc1 vx vz norm sample file vel.profile
```

Description:

Use one or more per-atom vectors as inputs every few timesteps, sum the values over the atoms in each chunk at each timestep, then average the per-chunk values over longer timescales. The resulting chunk averages can be used by other output commands such as thermo_style custom, and can also be written to a file.

In LAMMPS, chunks are collections of atoms defined by a compute chunk/atom command, which assigns each atom to a single chunk (or no chunk). The ID for this command is specified as chunkID. For example, a single chunk could be the atoms in a molecule or atoms in a spatial bin. See the compute chunk/atom doc page and "Section_howto 23 for details of how chunks can be defined and examples of how they can be used to measure properties of a system.

Note that only atoms in the specified group contribute to the summing and averaging calculations. The compute chunk/atom command defines its own group as well as an optional region. Atoms will have a chunk ID = 0, meaning they belong to no chunk, if they are not in that group or region. Thus you can specify the "all" group for this command if you simply want to use the chunk definitions provided by chunkID.

Each specified per-atom value can be an atom attribute (position, velocity, force component), a mass or number density, or the result of a compute or fix or the evaluation of an atom-style variable. In the latter cases, the compute, fix, or variable must produce a per-atom quantity, not a global quantity. Note that the compute property/atom command provides access to any attribute defined and stored by atoms. If you wish to time-average global quantities from a compute, fix, or variable, then see the fix ave/time command.

Computes that produce per-atom quantities are those which have the word *atom* in their style name. See the doc pages for individual fixes to determine which ones produce per-atom quantities. Variables of style *atom* are the only ones that can be used with this fix since all other styles of variable produce global quantities.

The per-atom values of each input vector are summed and averaged independently of the per-atom values in other input vectors.

NOTE: This fix works by creating an array of size *Nchunk* by Nvalues on each processor. *Nchunk* is the number of chunks which is defined by the compute chunk/atom command. Nvalues is the number of input values specified. Each processor loops over its atoms, tallying its values to the appropriate chunk. Then the entire array is summed across all processors. This means that using a large number of chunks will incur an overhead in memory and computational cost (summing across processors), so be careful to define a reasonable number of chunks.

The *Nevery*, *Nrepeat*, and *Nfreq* arguments specify on what timesteps the input values will be accessed and contribute to the average. The final averaged quantities are generated on timesteps that are a multiples of *Nfreq*.

The average is over *Nrepeat* quantities, computed in the preceding portion of the simulation every *Nevery* timesteps. *Nfreq* must be a multiple of *Nevery* and *Nevery* must be non-zero even if *Nrepeat* is 1. Also, the timesteps contributing to the average value cannot overlap, i.e. Nrepeat*Nevery can not exceed Nfreq.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then values on timesteps 90,92,94,96,98,100 will be used to compute the final average on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc. If Nrepeat=1 and Nfreq = 100, then no time averaging is done; values are simply generated on timesteps 100,200,etc.

Each input value can also be averaged over the atoms in each chunk. The way the averaging is done across the *Nrepeat* timesteps to produce output on the *Nfreq* timesteps, and across multiple *Nfreq* outputs, is determined by the *norm* and *ave* keyword settings, as discussed below.

NOTE: To perform per-chunk averaging within a *Nfreq* time window, the number of chunks *Nchunk* defined by the compute chunk/atom command must remain constant. If the *ave* keyword is set to *running* or *window* then *Nchunk* must remain constant for the duration of the simulation. This fix forces the chunk/atom compute specified by chunkID to hold *Nchunk* constant for the appropriate time windows, by not allowing it to re-calcualte *Nchunk*, which can also affect how it assigns chunk IDs to atoms. More details are given on the compute chunk/atom doc page.

The atom attribute values (vx,vy,vz,fx,fy,fz) are self-explanatory. As noted above, any other atom attributes can be used as input values to this fix by using the compute property/atom command and then specifying an input value from that compute.

The *density/number* value means the number density is computed for each chunk, i.e. number/volume. The *density/mass* value means the mass density is computed for each chunk, i.e. total-mass/volume. The output values are in units of 1/volume or density (mass/volume). See the units command doc page for the definition of density for each choice of units, e.g. gram/cm^3. If the chunks defined by the compute chunk/atom command are spatial bins, the volume is the bin volume. Otherwise it is the volume of the entire simulation box.

The *temp* value means the temperature is computed for each chunk, by the formula KE = DOF/2 k T, where KE = total kinetic energy of the chunk of atoms (sum of 1/2 m v^2), DOF = the total number of degrees of freedom for all atoms in the chunk, k = Boltzmann constant, and T = temperature.

The DOF is calculated as N*adof + cdof, where N = number of atoms in the chunk, adof = degrees of freedom per atom, and cdof = degrees of freedom per chunk. By default adof = 2 or 3 = dimensionality of system, as set via the dimension command, and cdof = 0.0. This gives the usual formula for temperature.

Note that currently this temperature only includes translational degrees of freedom for each atom. No rotational degrees of freedom are included for finite-size particles. Also no degrees of freedom are subtracted for any velocity bias or constraints that are applied, such as compute temp/partial, or fix shake or fix rigid. This is because those degrees of freedom (e.g. a constrained bond) could apply to sets of atoms that are both included and excluded from a specific chunk, and hence the concept is somewhat ill-defined. In some cases, you can use the *adof* and *cdof* keywords to adjust the calculated degress of freedom appropriately, as explained below.

Also note that a bias can be subtracted from atom velocities before they are used in the above formula for KE, by using the *bias* keyword. This allows, for example, a thermal temperature to be computed after removal of a flow velocity profile.

Note that the per-chunk temperature calculated by this fix and the compute temp/chunk command can be different. The compute calculates the temperature for each chunk for a single snapshot. This fix can do that but can also time average those values over many snapshots, or it can compute a temperature as if the atoms in the

chunk on different timesteps were collected together as one set of atoms to calculate their temperature. The compute allows the center-of-mass velocity of each chunk to be subtracted before calculating the temperature; this fix does not.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If no bracketed integer is appended, the per-atom vector calculated by the compute is used. If a bracketed integer is appended, the Ith column of the per-atom array calculated by the compute is used. Users can also write code for their own compute styles and add them to LAMMPS.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If no bracketed integer is appended, the per-atom vector calculated by the fix is used. If a bracketed integer is appended, the Ith column of the per-atom array calculated by the fix is used. Note that some fixes only produce their values on certain timesteps, which must be compatible with *Nevery*, else an error results. Users can also write code for their own fix styles and add them to LAMMPS.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. Variables of style *atom* can reference thermodynamic keywords and various per-atom attributes, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of generating per-atom quantities to average within chunks.

Additional optional keywords also affect the operation of this fix and its outputs.

The *norm* keyword affects how averaging is done for the per-chunk values that are output every *Nfreq* timesteps.

It the *norm* setting is *all*, which is the default, a chunk value is summed over all atoms in all *Nrepeat* samples, as is the count of atoms in the chunk. The averaged output value for the chunk on the *Nfreq* timesteps is Total-sum / Total-count. In other words it is an average over atoms across the entire *Nfreq* timescale.

If the *norm* setting is *sample*, the chunk value is summed over atoms for each sample, as is the count, and an "average sample value" is computed for each sample, i.e. Sample-sum / Sample-count. The output value for the chunk on the *Nfreq* timesteps is the average of the *Nrepeat* "average sample values", i.e. the sum of *Nrepeat* "average sample values" divided by *Nrepeat*. In other words it is an average of an average.

If the *norm* setting is *none*, a similar computation as for the *sample* seting is done, except the individual "average sample values" are "summed sample values". A summed sample value is simply the chunk value summed over atoms in the sample, without dividing by the number of atoms in the sample. The output value for the chunk on the *Nfreq* timesteps is the average of the *Nrepeat* "summed sample values", i.e. the sum of *Nrepeat* "summed sample values" divided by *Nrepeat*.

The *ave* keyword determines how the per-chunk values produced every *Nfreq* steps are averaged with values produced on previous steps that were multiples of *Nfreq*, before they are accessed by another output command or written to a file.

If the *ave* setting is *one*, which is the default, then the chunk values produced on timesteps that are multiples of *Nfreq* are independent of each other; they are output as-is without further averaging.

If the *ave* setting is *running*, then the chunk values produced on timesteps that are multiples of *Nfreq* are summed and averaged in a cumulative sense before being output. Each output chunk value is thus the average of the chunk value produced on that timestep with all preceding values for the same chunk. This running average begins when the fix is defined; it can only be restarted by deleting the fix via the unfix command, or re-defining the fix by re-specifying it.

If the *ave* setting is *window*, then the chunk values produced on timesteps that are multiples of *Nfreq* are summed and averaged within a moving "window" of time, so that the last M values for the same chunk are used to produce the output. E.g. if M = 3 and Nfreq = 1000, then the output on step 10000 will be the average of the individual chunk values on steps 8000,9000,10000. Outputs on early steps will average over less than M values if they are not available.

The *bias* keyword specifies the ID of a temperature compute that removes a "bias" velocity from each atom, specified as *bias-ID*. It is only used when the *temp* value is calculated, to compute the thermal temperature of each chunk after the translational kinetic energy components have been altered in a prescribed way, e.g. to remove a flow velocity profile. See the doc pages for individual computes that calculate a temperature to see which ones implement a bias.

The *adof* and *cdof* keywords define the values used in the degree of freedom (DOF) formula described above for for temperature calculation for each chunk. They are only used when the *temp* value is calculated. They can be used to calculate a more appropriate temperature for some kinds of chunks. Here are 3 examples:

If spatially binned chunks contain some number of water molecules and fix shake is used to make each molecule rigid, then you could calculate a temperature with 6 degrees of freedom (DOF) (3 translational, 3 rotational) per molecule by setting *adof* to 2.0.

If compute temp/partial is used with the *bias* keyword to only allow the x component of velocity to contribute to the temperature, then *adof* = 1.0 would be appropriate.

If each chunk consists of a large molecule, with some number of its bonds constrained by fix shake or the entire molecule by fix rigid/small, *adof* = 0.0 and *cdof* could be set to the remaining degrees of freedom for the entire molecule (entire chunk in this case), e.g. 6 for 3d, or 3 for 2d, for a rigid molecule.

The *file* keyword allows a filename to be specified. Every *Nfreq* timesteps, a section of chunk info will be written to a text file in the following format. A line with the timestep and number of chunks is written. Then one line per chunk is written, containing the chunk ID (1-Nchunk), an optional original ID value, optional coordinate values for chunks that represent spatial bins, the number of atoms in the chunk, and one or more calculated values. More explanation of the optional values is given below. The number of values in each line corresponds to the number of values specified in the fix ave/chunk command. The number of atoms and the value(s) are summed or average quantities, as explained above.

The *overwrite* keyword will continuously overwrite the output file with the latest output, so that it only contains one timestep worth of output. This option can only be used with the *ave running* setting.

The *format* keyword sets the numeric format of each value when it is printed to a file via the *file* keyword. Note that all values are floating point quantities. The default format is %g. You can specify a higher precision if desired, e.g. %20.16g.

The *title1* and *title2* and *title3* keywords allow specification of the strings that will be printed as the first 3 lines of the output file, assuming the *file* keyword was used. LAMMPS uses default values for each of these, so they do not need to be specified.

By default, these header lines are as follows:

```
# Chunk-averaged data for fix ID and group name
# Timestep Number-of-chunks
# Chunk (OrigID) (Coord1) (Coord2) (Coord3) Ncount value1 value2 ...
```

In the first line, ID and name are replaced with the fix-ID and group name. The second line describes the two values that are printed at the first of each section of output. In the third line the values are replaced with the appropriate value names, e.g. fx or c_myCompute**2**.

The words in parenthesis only appear with corresponding columns if the chunk style specified for the compute chunk/atom command supports them. The OrigID column is only used if the *compress* keyword was set to *yes* for the compute chunk/atom command. This means that the original chunk IDs (e.g. molecule IDs) will have been compressed to remove chunk IDs with no atoms assigned to them. Thus a compresed chunk ID of 3 may correspond to an original chunk ID or molecule ID of 415. The OrigID column will list 415 for the 3rd chunk.

The CoordN columns only appear if a *binning* style was used in the compute chunk/atom command. For *bin/1d*, *bin/2d*, and *bin/3d* styles the column values are the center point of the bin in the corresponding dimension. Just Coord1 is used for *bin/1d*, Coord2 is added for *bin/2d*, Coord3 is added for *bin/3d*. For *bin/sphere*, just Coord1 is used, and it is the radial coordinate. For *bin/cylinder*, Coord1 and Coord2 are used. Coord1 is the radial coordinate (away from the cylinder axis), and coord2 is the coordinate along the cylinder axis.

Note that if the value of the *units* keyword used in the compute chunk/atom command is *box* or *lattice*, the coordinate values will be in distance units. If the value of the *units* keyword is *reduced*, the coordinate values will be in unitless reduced units (0-1). This is not true for the Coord1 value of style *bin/sphere* or *bin/cylinder* which both represent radial dimensions. Those values are always in distance units.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global array of values which can be accessed by various output commands. The values can only be accessed on timesteps that are multiples of *Nfreq* since that is when averaging is performed. The global array has # of rows = the number of chunks *Nchunk* as calculated by the specified compute chunk/atom command. The # of columns = M+1+Nvalues, where M = 1 to 4, depending on whether the optional columns for OrigID and CoordN are used, as explained above. Following the optional columns, the next column contains the count of atoms in the chunk, and the remaining columns are the Nvalue quantities. When the array is accessed with a row I that exceeds the current number of chunks, than a 0.0 is returned by the fix instead of an error, since the number of chunks can vary as a simulation runs depending on how that value is computed by the compute chunk/atom command.

The array values calculated by this fix are treated as "intensive", since they are typically already normalized by the count of atoms in each chunk.

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

compute, fix ave/atom, fix ave/histo, fix ave/time, variable, fix ave/correlate

Default:

The option defaults are norm = all, ave = one, bias = none, no file output, and title 1,2,3 = strings as described above.

fix ave/correlate command

Syntax:

```
fix ID group-ID ave/correlate Nevery Nrepeat Nfreq value1 value2 ... keyword args ...
```

- ID, group-ID are documented in fix command
- ave/correlate = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of correlation time windows to accumulate
- Nfreq = calculate time window averages every this many timesteps
- one or more input values can be listed
- value = c_ID, c_ID[N], f_ID, f_ID[N], v_name

```
  c_ID = global scalar calculated by a compute with ID
  c_ID[I] = Ith component of global vector calculated by a compute with ID
  f_ID = global scalar calculated by a fix with ID
  f_ID[I] = Ith component of global vector calculated by a fix with ID
  v_name = global value calculated by an equal-style variable with name
```

- zero or more keyword/arg pairs may be appended
- keyword = *type* or *ave* or *start* or *prefactor* or *file* or *overwrite* or *title1* or *title2* or *title3*

```
type arg = auto or upper or lower or auto/upper or auto/lower or full
    auto = correlate each value with itself
    upper = correlate each value with each succeeding value
    lower = correlate each value with each preceding value
    auto/upper = auto + upper
    auto/lower = auto + lower
    full = correlate each value with every other value, including itself = auto + upper + lowe
  ave args = one or running
    one = zero the correlation accumulation every Nfreq steps
    running = accumulate correlations continuously
  start args = Nstart
    Nstart = start accumulating correlations on this timestep
  prefactor args = value
    value = prefactor to scale all the correlation data by
  file arg = filename
    filename = name of file to output correlation data to
  overwrite arg = none = overwrite output file with only latest output
  title1 arg = string
    string = text to print as 1st line of output file
  title2 arg = string
    string = text to print as 2nd line of output file
  title3 arg = string
    string = text to print as 3rd line of output file
```

Examples:

```
fix 1 all ave/correlate 5 100 1000 c_myTemp file temp.correlate
fix 1 all ave/correlate 1 50 10000 &
          c_thermo_press[1] c_thermo_press[2] c_thermo_press[3] &
          type upper ave running title1 "My correlation data"
```

Description:

Use one or more global scalar values as inputs every few timesteps, calculate time correlations bewteen them at varying time intervals, and average the correlation data over longer timescales. The resulting correlation values can be time integrated by variables or used by other output commands such as thermo_style custom, and can also be written to a file. See the fix ave/correlate/long command for an alternate method for computing correlation functions efficiently over very long time windows.

The group specified with this command is ignored. However, note that specified values may represent calculations performed by computes and fixes which store their own "group" definitions.

Each listed value can be the result of a compute or fix or the evaluation of an equal-style variable. In each case, the compute, fix, or variable must produce a global quantity, not a per-atom or local quantity. If you wish to spatial- or time-average or histogram per-atom quantities from a compute, fix, or variable, then see the fix ave/spatial, fix ave/atom, or fix ave/histo commands. If you wish to sum a per-atom quantity into a single global quantity, see the compute reduce command.

Computes that produce global quantities are those which do not have the word *atom* in their style name. Only a few fixes produce global quantities. See the doc pages for individual fixes for info on which ones produce such values. Variables of style *equal* are the only ones that can be used with this fix. Variables of style *atom* cannot be used, since they produce per-atom values.

The input values must either be all scalars. What kinds of correlations between input values are calculated is determined by the *type* keyword as discussed below.

The *Nevery*, *Nrepeat*, and *Nfreq* arguments specify on what timesteps the input values will be used to calculate correlation data. The input values are sampled every *Nevery* timesteps. The correlation data for the preceding samples is computed on timesteps that are a multiple of *Nfreq*. Consider a set of samples from some initial time up to an output timestep. The initial time could be the beginning of the simulation or the last output time; see the *ave* keyword for options. For the set of samples, the correlation value Cij is calculated as:

```
Cij(delta) = ave(Vi(t)*Vj(t+delta))
```

which is the correlation value between input values Vi and Vj, separated by time delta. Note that the second value Vj in the pair is always the one sampled at the later time. The ave() represents an average over every pair of samples in the set that are separated by time delta. The maximum delta used is of size (*Nrepeat*-1)**Nevery*. Thus the correlation between a pair of input values yields *Nrepeat* correlation datums:

```
Cij(0), Cij(Nevery), Cij(2*Nevery), ..., Cij((Nrepeat-1)*Nevery)
```

For example, if Nevery=5, Nrepeat=6, and Nfreq=100, then values on timesteps 0,5,10,15,...,100 will be used to compute the final averages on timestep 100. Six averages will be computed: Cij(0), Cij(5), Cij(10), Cij(15), Cij(20), and Cij(25). Cij(10) on timestep 100 will be the average of 19 samples, namely Vi(0)*Vj(10), Vi(5)*Vj(15), Vi(10)*V j20), Vi(15)*Vj(25), ..., Vi(85)*Vj(95), Vi(90)*Vj(100).

Nfreq must be a multiple of *Nevery*; *Nevery* and *Nrepeat* must be non-zero. Also, if the *ave* keyword is set to *one* which is the default, then *Nfreq* >= (*Nrepeat*-1)**Nevery* is required.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If no bracketed term is appended, the global scalar calculated by the compute is used. If a bracketed term is appended, the Ith element of the global vector calculated by the compute is used.

Note that there is a compute reduce command which can sum per-atom quantities into a global scalar or vector which can thus be accessed by fix ave/correlate. Or it can be a compute defined not in your input script, but by

thermodynamic output or other fixes such as fix nvt or fix temp/rescale. See the doc pages for these commands which give the IDs of these computes. Users can also write code for their own compute styles and add them to LAMMPS.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If no bracketed term is appended, the global scalar calculated by the fix is used. If a bracketed term is appended, the Ith element of the global vector calculated by the fix is used.

Note that some fixes only produce their values on certain timesteps, which must be compatible with *Nevery*, else an error will result. Users can also write code for their own fix styles and add them to LAMMPS.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. Only equal-style variables can be referenced. See the variable command for details. Note that variables of style *equal* define a formula which can reference individual atom properties or thermodynamic keywords, or they can invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of specifying quantities to time correlate.

Additional optional keywords also affect the operation of this fix.

The *type* keyword determines which pairs of input values are correlated with each other. For N input values Vi, for i = 1 to N, let the number of pairs = Npair. Note that the second value in the pair Vi(t)*Vj(t+delta) is always the one sampled at the later time.

- If *type* is set to *auto* then each input value is correlated with itself. I.e. Cii = Vi*Vi, for i = 1 to N, so Npair = N.
- If *type* is set to *upper* then each input value is correlated with every succeeding value. I.e. Cij = Vi*Vj, for i < j, so Npair = N*(N-1)/2.
- If *type* is set to *lower* then each input value is correlated with every preceeding value. I.e. Cij = Vi*Vj, for i > j, so Npair = N*(N-1)/2.
- If *type* is set to *auto/upper* then each input value is correlated with itself and every succeeding value. I.e. Cij = Vi*Vj, for i >= j, so Npair = N*(N+1)/2.
- If *type* is set to *auto/lower* then each input value is correlated with itself and every preceding value. I.e. Cij = Vi*Vj, for i <= j, so Npair = N*(N+1)/2.
- If *type* is set to *full* then each input value is correlated with itself and every other value. I.e. Cij = Vi*Vj, for i,j = 1,N so Npair = N^2.

The *ave* keyword determines what happens to the accumulation of correlation samples every *Nfreq* timesteps. If the *ave* setting is *one*, then the accumulation is restarted or zeroed every *Nfreq* timesteps. Thus the outputs on successive *Nfreq* timesteps are essentially independent of each other. The exception is that the Cij(0) = Vi(T)*Vj(T) value at a timestep T, where T is a multiple of *Nfreq*, contributes to the correlation output both at time T and at time T+Nfreq.

If the *ave* setting is *running*, then the accumulation is never zeroed. Thus the output of correlation data at any timestep is the average over samples accumulated every *Nevery* steps since the fix was defined. it can only be restarted by deleting the fix via the unfix command, or by re-defining the fix by re-specifying it.

The *start* keyword specifies what timestep the accumulation of correlation samples will begin on. The default is step 0. Setting it to a larger value can avoid adding non-equilibrated data to the correlation averages.

The *prefactor* keyword specifies a constant which will be used as a multiplier on the correlation data after it is averaged. It is effectively a scale factor on Vi*Vj, which can be used to account for the size of the time window or other unit conversions.

The *file* keyword allows a filename to be specified. Every *Nfreq* steps, an array of correlation data is written to the file. The number of rows is *Nrepeat*, as described above. The number of columns is the Npair+2, also as described above. Thus the file ends up to be a series of these array sections.

The *overwrite* keyword will continuously overwrite the output file with the latest output, so that it only contains one timestep worth of output. This option can only be used with the *ave running* setting.

The *title1* and *title2* and *title3* keywords allow specification of the strings that will be printed as the first 3 lines of the output file, assuming the *file* keyword was used. LAMMPS uses default values for each of these, so they do not need to be specified.

By default, these header lines are as follows:

```
# Time-correlated data for fix ID
# TimeStep Number-of-time-windows
# Index TimeDelta Ncount valueI*valueJ valueI*valueJ ...
```

In the first line, ID is replaced with the fix-ID. The second line describes the two values that are printed at the first of each section of output. In the third line the value pairs are replaced with the appropriate fields from the fix ave/correlate command.

Let Sij = a set of time correlation data for input values I and J, namely the *Nrepeat* values:

```
Sij = Cij(0), Cij(Nevery), Cij(2*Nevery), ..., Cij(*Nrepeat-1)*Nevery)
```

As explained below, these datums are output as one column of a global array, which is effectively the correlation matrix.

The *trap* function defined for equal-style variables can be used to perform a time integration of this vector of datums, using a trapezoidal rule. This is useful for calculating various quantities which can be derived from time correlation data. If a normalization factor is needed for the time integration, it can be included in the variable formula or via the *prefactor* keyword.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global array of values which can be accessed by various output commands. The values can only be accessed on timesteps that are multiples of *Nfreq* since that is when averaging is performed. The global array has # of rows = *Nrepeat* and # of columns = Npair+2. The first column has the time delta (in timesteps) between the pairs of input values used to calculate the correlation, as described above. The 2nd column has the number of samples contributing to the correlation average, as described above. The remaining Npair columns are for I,J pairs of the N input values, as determined by the *type* keyword, as described above.

- For *type* = *auto*, the Npair = N columns are ordered: C11, C22, ..., CNN.
- For *type* = *upper*, the Npair = N*(N-1)/2 columns are ordered: C12, C13, ..., C1N, C23, ..., C2N, C34, ..., CN-1N.
- For *type* = *lower*, the Npair = N*(N-1)/2 columns are ordered: C21, C31, C32, C41, C42, C43, ..., CN1, CN2, ..., CNN-1.
- For *type* = *auto/upper*, the Npair = N*(N+1)/2 columns are ordered: C11, C12, C13, ..., C1N, C22, C23, ..., C2N, C33, C34, ..., CN-1N, CNN.

- For *type* = *auto/lower*, the Npair = N*(N+1)/2 columns are ordered: C11, C21, C22, C31, C32, C33, C41, ..., C44, CN1, CN2, ..., CNN-1, CNN.
- For *type* = *full*, the Npair = N^2 columns are ordered: C11, C12, ..., C1N, C21, C22, ..., C2N, C31, ..., C3N, ..., CN1, ..., CNN-1, CNN.

The array values calculated by this fix are treated as "intensive". If you need to divide them by the number of atoms, you must do this in a later processing step, e.g. when using them in a variable.

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

fix ave/correlate/long, compute, fix ave/time, fix ave/atom, fix ave/spatial, fix ave/histo, variable

Default: none

The option defaults are ave = one, type = auto, start = 0, no file output, title 1,2,3 = strings as described above, and prefactor = 1.0.

fix ave/correlate/long command

Syntax:

```
fix ID group-ID ave/correlate/long Nevery Nfreq value1 value2 ... keyword args ...
```

- ID, group-ID are documented in fix command
- ave/correlate/long = style name of this fix command
- Nevery = use input values every this many timesteps
- Nfreq = save state of the time correlation functions every this many timesteps
- one or more input values can be listed
- value = c_ID, c_ID[N], f_ID, f_ID[N], v_name

```
c_ID = global scalar calculated by a compute with ID
c_ID[I] = Ith component of global vector calculated by a compute with ID
f_ID = global scalar calculated by a fix with ID
f_ID[I] = Ith component of global vector calculated by a fix with ID
v_name = global value calculated by an equal-style variable with name
```

- zero or more keyword/arg pairs may be appended
- keyword = *type* or *start* or *file* or *overwrite* or *title1* or *title2* or *ncorr* or *p* or *m*

```
type arg = auto or upper or lower or auto/upper or auto/lower or full
    auto = correlate each value with itself
    upper = correlate each value with each succeeding value
    lower = correlate each value with each preceding value
    auto/upper = auto + upper
    auto/lower = auto + lower
    full = correlate each value with every other value, including itself = auto + upper + lowe
  start args = Nstart
    Nstart = start accumulating correlations on this timestep
  file arg = filename
    filename = name of file to output correlation data to
  overwrite arg = none = overwrite output file with only latest output
  title1 arg = string
    string = text to print as 1st line of output file
  title2 arg = string
    string = text to print as 2nd line of output file
  ncorr arg = Ncorrelators
    Ncorrelators = number of correlators to store
  nlen args = Nlen
    Nlen = length of each correlator
  ncount args = Ncount
    Ncount = number of values over which succesive correlators are averaged
```

Examples:

```
fix 1 all ave/correlate/long 5 1000 c_myTemp file temp.correlate
fix 1 all ave/correlate/long 1 10000 &
          c_thermo_press[1] c_thermo_press[2] c_thermo_press[3] &
          type upper title1 "My correlation data" nlen 15 ncount 3
```

Description:

This fix is similar in spirit and syntax to the fix ave/correlate. However, this fix allows the efficient calculation of time correlation functions on the fly over extremely long time windows without too much CPU overhead, using a multiple-tau method (Ramirez) that decreases the resolution of the stored correlation function with time.

The group specified with this command is ignored. However, note that specified values may represent calculations performed by computes and fixes which store their own "group" definitions.

Each listed value can be the result of a compute or fix or the evaluation of an equal-style variable. See the fix ave/correlate doc page for details.

The *Nevery* and *Nfreq* arguments specify on what timesteps the input values will be used to calculate correlation data, and the frequency with which the time correlation functions will be output to a file. Note that there is no *Nrepeat* argument, unlike the fix ave/correlate command.

The optional keywords *ncorr*, *nlen*, and *ncount* are unique to this command and determine the number of correlation points calculated and the memory and CPU overhead used by this calculation. *Nlen* and *ncount* determine the amount of averaging done at longer correlation times. The default values *nlen=16*, *ncount=2* ensure that the systematic error of the multiple-tau correlator is always below the level of the statistical error of a typical simulation (which depends on the ensemble size and the simulation length).

The maximum correlation time (in time steps) that can be reached is given by the formula (nlen-1) * ncount^(ncorr-1). Longer correlation times are discarded and not calculated. With the default values of the parameters (ncorr=20, nlen=16 and ncount=2), this corresponds to 7864320 time steps. If longer correlation times are needed, the value of ncorr should be increased. Using nlen=16 and ncount=2, with ncorr=30, the maximum number of steps that can be correlated is 80530636808. If ncorr=40, correlation times in excess of 8e12 time steps can be calculated.

The total memory needed for each correlation pair is roughly 4*ncorr*nlen*8 bytes. With the default values of the parameters, this corresponds to about 10 KB.

For the meaning of the additional optional keywords, see the fix ave/correlate doc page.

Restart, fix_modify, output, run start/stop, minimize info:

Since this fix in intended for the calculation of time correlation functions over very long MD simulations, the information about this fix is written automatically to binary restart files, so that the time correlation calculation can continue in subsequent simulations. None of the fix_modify options are relevant to this fix.

No parameter of this fix can be used with the start/stop keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This compute is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix ave/correlate

Default: none

The option defaults for keywords that are also keywords for the fix ave/correlate command are as follows: type = auto, start = 0, no file output, title 1,2 = strings as described on the fix ave/correlate doc page.

The option defaults for keywords unique to this command are as follows: ncorr=20, nlen=16, ncount=2.

(Ramirez) J. Ramirez, S.K. Sukumaran, B. Vorselaars and A.E. Likhtman, J. Chem. Phys. 133, 154103 (2010).

fix ave/histo command

fix ave/histo/weight command

Syntax:

```
fix ID group-ID style Nevery Nrepeat Nfreq lo hi Nbin value1 value2 ... keyword args ...
```

- ID, group-ID are documented in fix command
- style = *ave/histo* or *ave/histo/weight* = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of times to use input values for calculating histogram
- Nfreq = calculate histogram every this many timesteps
- lo,hi = lo/hi bounds within which to histogram
- Nbin = # of histogram bins
- one or more input values can be listed
- value = x, y, z, vx, vy, vz, fx, fy, fz, c_ID, c_ID[N], f_ID, f_ID[N], v_name

```
x,y,z,vx,vy,vz,fx,fy,fz = atom attribute (position, velocity, force component)
c_ID = scalar or vector calculated by a compute with ID
c_ID[I] = Ith component of vector or Ith column of array calculated by a compute with ID
f_ID = scalar or vector calculated by a fix with ID
f_ID[I] = Ith component of vector or Ith column of array calculated by a fix with ID
v_name = value(s) calculated by an equal-style or atom-style variable with name
```

- zero or more keyword/arg pairs may be appended
- keyword = *mode* or *file* or *ave* or *start* or *beyond* or *overwrite* or *title1* or *title2* or *title3*

```
mode arg = scalar or vector
    scalar = all input values are scalars
    vector = all input values are vectors
  file arg = filename
    filename = name of file to output histogram(s) to
  ave args = one or running or window
    one = output a new average value every Nfreq steps
    running = output cumulative average of all previous Nfreq steps
    window M = output average of M most recent Nfreq steps
  start args = Nstart
    Nstart = start averaging on this timestep
  beyond arg = ignore or end or extra
    ignore = ignore values outside histogram lo/hi bounds
    end = count values outside histogram lo/hi bounds in end bins
    extra = create 2 extra bins for value outside histogram lo/hi bounds
  overwrite arg = none = overwrite output file with only latest output
  title1 arg = string
    string = text to print as 1st line of output file
  title2 arg = string
    string = text to print as 2nd line of output file
  title3 arg = string
    string = text to print as 3rd line of output file, only for vector mode
```

Examples:

```
fix 1 all ave/histo 100 5 1000 0.5 1.5 50 c_myTemp file temp.histo ave running
fix 1 all ave/histo 100 5 1000 -5 5 100 c_thermo_press[2] c_thermo_press[3] title1 "My output values
fix 1 all ave/histo 1 100 1000 -2.0 2.0 18 vx vy vz mode vector ave running beyond extra
fix 1 all ave/histo/weight 1 1 1 10 100 2000 c_XRD[1] c_XRD[2]
```

Description:

Use one or more values as inputs every few timesteps, histogram them, and average the histogram over longer timescales. The resulting histogram can be used by other output commands, and can also be written to a file. The fix ave/histo/weight command has identical syntax to fix ave/histo, except that exactly two values must be specified. See details below.

The group specified with this command is ignored for global and local input values. For per-atom input values, only atoms in the group contribute to the histogram. Note that regardless of the specified group, specified values may represent calculations performed by computes and fixes which store their own "group" definition.

A histogram is simply a count of the number of values that fall within a histogram bin. *Nbins* are defined, with even spacing between *lo* and *hi*. Values that fall outside the lo/hi bounds can be treated in different ways; see the discussion of the *beyond* keyword below.

Each input value can be an atom attribute (position, velocity, force component) or can be the result of a compute or fix or the evaluation of an equal-style or atom-style variable. The set of input values can be either all global, all per-atom, or all local quantities. Inputs of different kinds (e.g. global and per-atom) cannot be mixed. Atom attributes are per-atom vector values. See the doc page for individual "compute" and "fix" commands to see what kinds of quantities they generate.

The input values must either be all scalars or all vectors (or arrays), depending on the setting of the *mode* keyword.

Note that the output of this command is a single histogram for all input values combined together, not one histogram per input value. See below for details on the format of the output of this fix.

If *mode* = vector, then the input values may either be vectors or arrays. If a global array is listed, then it is the same as if the individual columns of the array had been listed one by one. E.g. these 2 fix ave/histo commands are equivalent, since the compute com/chunk command creates a global array with 3 columns:

```
compute myCOM all com/chunk
fix 1 all ave/histo 100 1 100 c_myCOM file tmp1.com mode vector
fix 2 all ave/histo 100 1 100 c_myCOM[1] c_myCOM[2] c_myCOM[3] file tmp2.com mode vector
```

If the fix ave/histo/weight command is used, exactly two values must be specified. If the values are vectors, they must be the same length. The first value (a scalar or vector) is what is histogrammed into bins, in the same manner the fix ave/histo command operates. The second value (a scalar or vector) is used as a "weight". This means that instead of each value tallying a "1" to its bin, the corresponding weight is tallied. E.g. the Nth entry in the first vector tallies the Nth entry (weight) in the second vector.

The *Nevery*, *Nrepeat*, and *Nfreq* arguments specify on what timesteps the input values will be used in order to contribute to the histogram. The final histogram is generated on timesteps that are multiple of *Nfreq*. It is averaged over *Nrepeat* histograms, computed in the preceding portion of the simulation every *Nevery* timesteps. *Nfreq* must be a multiple of *Nevery* and *Nevery* must be non-zero even if *Nrepeat* is 1. Also, the timesteps contributing to the histogram value cannot overlap, i.e. Nrepeat*Nevery can not exceed Nfreq.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then input values on timesteps 90,92,94,96,98,100 will be used to compute the final histogram on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc. If Nrepeat=1 and Nfreq = 100, then no time averaging of the histogram is done; a histogram is simply generated on timesteps 100,200,etc.

The atom attribute values (x,y,z,vx,vy,vz,fx,fy,fz) are self-explanatory. Note that other atom attributes can be used as inputs to this fix by using the compute property/atom command and then specifying an input value from that compute.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If *mode* = scalar, then if no bracketed term is appended, the global scalar calculated by the compute is used. If a bracketed term is appended, the Ith element of the global vector calculated by the compute is used. If *mode* = vector, then if no bracketed term is appended, the global or per-atom or local vector calculated by the compute is used. Or if the compute calculates an array, all of the columns of the array are used as if they had been specified as individual vectors (see description above). If a bracketed term is appended, the Ith column of the global or per-atom or local array calculated by the compute is used.

Note that there is a compute reduce command which can sum per-atom quantities into a global scalar or vector which can thus be accessed by fix ave/histo. Or it can be a compute defined not in your input script, but by thermodynamic output or other fixes such as fix nvt or fix temp/rescale. See the doc pages for these commands which give the IDs of these computes. Users can also write code for their own compute styles and add them to LAMMPS.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If *mode* = scalar, then if no bracketed term is appended, the global scalar calculated by the fix is used. If a bracketed term is appended, the Ith element of the global vector calculated by the fix is used. If *mode* = vector, then if no bracketed term is appended, the global or per-atom or local vector calculated by the fix is used. Or if the fix calculates an array, all of the columns of the array are used as if they had been specified as individual vectors (see description above). If a bracketed term is appended, the Ith column of the global or per-atom or local array calculated by the fix is used.

Note that some fixes only produce their values on certain timesteps, which must be compatible with *Nevery*, else an error will result. Users can also write code for their own fix styles and add them to LAMMPS.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. If *mode* = scalar, then only equal-style variables can be used, which produce a global value. If *mode* = vector, then only atom-style variables can be used, which produce a per-atom vector. See the variable command for details. Note that variables of style *equal* and *atom* define a formula which can reference individual atom properties or thermodynamic keywords, or they can invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of specifying quantities to histogram.

Additional optional keywords also affect the operation of this fix.

If the *mode* keyword is set to *scalar*, then all input values must be global scalars, or elements of global vectors. If the *mode* keyword is set to *vector*, then all input values must be global or per-atom or local vectors, or columns of global or per-atom or local arrays.

The *beyond* keyword determines how input values that fall outside the *lo* to *hi* bounds are treated. Values such that *lo* <= value <= *hi* are assigned to one bin. Values on a bin boundary are assigned to the lower of the 2 bins. If *beyond* is set to *ignore* then values < *lo* and values > *hi* are ignored, i.e. they are not binned. If *beyond* is set to *end* then values < *lo* are counted in the first bin and values > *hi* are counted in the last bin. If *beyond* is set to *extend* then two extra bins are created, so that there are Nbins+2 total bins. Values < *lo* are counted in the first bin and values > *hi* are counted in the last bin (Nbins+1). Values between *lo* and *hi* (inclusive) are counted in bins 2 thru Nbins+1. The "coordinate" stored and printed for these two extra bins is *lo* and *hi*.

The *ave* keyword determines how the histogram produced every *Nfreq* steps are averaged with histograms produced on previous steps that were multiples of *Nfreq*, before they are accessed by another output command or

written to a file.

If the *ave* setting is *one*, then the histograms produced on timesteps that are multiples of *Nfreq* are independent of each other; they are output as-is without further averaging.

If the *ave* setting is *running*, then the histograms produced on timesteps that are multiples of *Nfreq* are summed and averaged in a cumulative sense before being output. Each bin value in the histogram is thus the average of the bin value produced on that timestep with all preceding values for the same bin. This running average begins when the fix is defined; it can only be restarted by deleting the fix via the unfix command, or by re-defining the fix by re-specifying it.

If the *ave* setting is *window*, then the histograms produced on timesteps that are multiples of *Nfreq* are summed within a moving "window" of time, so that the last M histograms are used to produce the output. E.g. if M = 3 and Nfreq = 1000, then the output on step 10000 will be the combined histogram of the individual histograms on steps 8000,9000,10000. Outputs on early steps will be sums over less than M histograms if they are not available.

The *start* keyword specifies what timestep histogramming will begin on. The default is step 0. Often input values can be 0.0 at time 0, so setting *start* to a larger value can avoid including a 0.0 in a running or windowed histogram.

The *file* keyword allows a filename to be specified. Every *Nfreq* steps, one histogram is written to the file. This includes a leading line that contains the timestep, number of bins, the total count of values contributing to the histogram, the count of values that were not histogrammed (see the *beyond* keyword), the minimum value encountered, and the maximum value encountered. The min/max values include values that were not histogrammed. Following the leading line, one line per bin is written into the file. Each line contains the bin #, the coordinate for the center of the bin (between *lo* and *hi*), the count of values in the bin, and the normalized count. The normalized count is the bin count divided by the total count (not including values not histogrammed), so that the normalized values sum to 1.0 across all bins.

The *overwrite* keyword will continuously overwrite the output file with the latest output, so that it only contains one timestep worth of output. This option can only be used with the *ave running* setting.

The *title1* and *title2* and *title3* keywords allow specification of the strings that will be printed as the first 3 lines of the output file, assuming the *file* keyword was used. LAMMPS uses default values for each of these, so they do not need to be specified.

By default, these header lines are as follows:

```
# Histogram for fix ID
# TimeStep Number-of-bins Total-counts Missing-counts Min-value Max-value
# Bin Coord Count Count/Total
```

In the first line, ID is replaced with the fix-ID. The second line describes the six values that are printed at the first of each section of output. The third describes the 4 values printed for each bin in the histogram.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix produces a global vector and global array which can be accessed by various output commands. The values can only be accessed on timesteps that are multiples of *Nfreq* since that is when a histogram is generated. The global vector has 4 values:

- 1 = total counts in the histogram
- 2 = values that were not histogrammed (see *beyond* keyword)
- 3 = min value of all input values, including ones not histogrammed
- 4 = max value of all input values, including ones not histogrammed

The global array has # of rows = Nbins and # of columns = 3. The first column has the bin coordinate, the 2nd column has the count of values in that histogram bin, and the 3rd column has the bin count divided by the total count (not including missing counts), so that the values in the 3rd column sum to 1.0.

The vector and array values calculated by this fix are all treated as "intensive". If this is not the case, e.g. due to histogramming per-atom input values, then you will need to account for that when interpreting the values produced by this fix.

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

compute, fix ave/atom, fix ave/spatial, fix ave/time, variable, fix ave/correlate,

Default: none

The option defaults are mode = scalar, ave = one, start = 0, no file output, beyond = ignore, and title 1,2,3 = strings as described above.

fix ave/spatial command

Syntax:

```
fix ID group-ID ave/spatial Nevery Nrepeat Nfreq dim origin delta ... value1 value2 ... keyword args
```

- ID, group-ID are documented in fix command
- ave/spatial = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of times to use input values for calculating averages
- Nfreq = calculate averages every this many timesteps
- dim, origin, delta can be repeated 1, 2, or 3 times for 1d, 2d, or 3d bins

```
dim = x or y or z
origin = lower or center or upper or coordinate value (distance units)
delta = thickness of spatial bins in dim (distance units)
```

- one or more input values can be listed
- value = vx, vy, vz, fx, fy, fz, density/mass, density/number, c_ID, c_ID[I], f_ID, f_ID[I], v_name

```
vx,vy,vz,fx,fy,fz = atom attribute (velocity, force component)
density/number, density/mass = number or mass density
c_ID = per-atom vector calculated by a compute with ID
c_ID[I] = Ith column of per-atom array calculated by a compute with ID
f_ID = per-atom vector calculated by a fix with ID
f_ID[I] = Ith column of per-atom array calculated by a fix with ID
v_name = per-atom vector calculated by an atom-style variable with name
```

- zero or more keyword/arg pairs may be appended
- keyword = *region* or *bound* or *discard* or *norm* or *ave* or *units* or *file* or *overwrite* or *title1* or *title2* or *title3*

```
region arg = region-ID
  bound args = x/y/z lo hi
    x/y/z = x or y or z to bound bins in this dimension
    lo = lower or coordinate value (distance units)
    hi = upper or coordinate value (distance units)
  discard arg = mixed or no or yes
    mixed = discard atoms outside bins only if bin bounds are explicitly set
    no = always keep out-of-bounds atoms
    yes = always discard out-of-bounds atoms
  norm arg = all or sample
    region-ID = ID of region atoms must be in to contribute to spatial averaging
  ave args = one or running or window M
    one = output new average value every Nfreq steps
    running = output cumulative average of all previous Nfreq steps
    window M = output average of M most recent Nfreq steps
  units arg = box or lattice or reduced
  file arg = filename
    filename = file to write results to
  overwrite arg = none = overwrite output file with only latest output
  title1 arg = string
    string = text to print as 1st line of output file
  title2 arg = string
    string = text to print as 2nd line of output file
  title3 arg = string
    string = text to print as 3rd line of output file
```

Examples:

```
fix 1 all ave/spatial 10000 1 10000 z lower 0.02 c_myCentro units reduced &
                      title1 "My output values"
fix 1 flow ave/spatial 100 10 1000 y 0.0 1.0 vx vz norm sample file vel.profile
fix 1 flow ave/spatial 100 5 1000 z lower 1.0 y 0.0 2.5 density/mass ave running
fix 1 flow ave/spatial 100 5 1000 z lower 1.0 y 0.0 2.5 density/mass bound y 5.0 20.0 discard yes av
```

NOTE:

The fix ave/spatial command has been replaced by the more flexible fix ave/chunk and compute chunk/atom commands. The fix ave/spatial command will be removed from LAMMPS sometime in the summer of 2015.

Any fix ave/spatial command can be replaced by the two new commands. You simply need to split the fix ave/spatial arguments across the two new commands. For example, this command:

```
fix 1 flow ave/spatial 100 10 1000 y 0.0 1.0 vx vz norm sample file vel.profile
```

could be replaced by:

```
compute cc1 flow chunk/atom bin/1d y 0.0 1.0
fix 1 flow ave/chunk 100 10 1000 cc1 vx vz norm sample file vel.profile
```

Description:

Use one or more per-atom vectors as inputs every few timesteps, bin their values spatially into 1d, 2d, or 3d bins based on current atom coordinates, and average the bin values over longer timescales. The resulting bin averages can be used by other output commands such as thermo_style custom, and can also be written to a file.

The group specified with the command means only atoms within the group contribute to bin averages. If the *region* keyword is used, the atom must be in both the specified group and the specified geometric region in order to contribute to bin averages.

Each listed value can be an atom attribute (position, velocity, force component), a mass or number density, or the result of a compute or fix or the evaluation of an atom-style variable. In the latter cases, the compute, fix, or variable must produce a per-atom quantity, not a global quantity. If you wish to time-average global quantities from a compute, fix, or variable, then see the fix ave/time command.

Computes that produce per-atom quantities are those which have the word *atom* in their style name. See the doc pages for individual fixes to determine which ones produce per-atom quantities. Variables of style *atom* are the only ones that can be used with this fix since all other styles of variable produce global quantities.

The per-atom values of each input vector are binned and averaged independently of the per-atom values in other input vectors.

The size and dimensionality of the bins (1d = layers or slabs, 2d = pencils, 3d = boxes) are determined by the *dim*, *origin*, and *delta* settings and how many times they are specified (1, 2, or 3). See details below.

NOTE: This fix works by creating an array of size Nbins by Nvalues on each processor. Nbins is the total number of bins; Nvalues is the number of input values specified. Each processor loops over its atoms, tallying its values to the appropriate bin. Then the entire array is summed across all processors. This means that using a large number of bins (easy to do for 2d or 3d bins) will incur an overhead in memory and computational cost (summing across processors), so be careful to use reasonable numbers of bins.

The *Nevery*, *Nrepeat*, and *Nfreq* arguments specify on what timesteps the input values will be used to bin them and contribute to the average. The final averaged quantities are generated on timesteps that are a multiples of *Nfreq*. The average is over *Nrepeat* quantities, computed in the preceding portion of the simulation every *Nevery* timesteps. *Nfreq* must be a multiple of *Nevery* and *Nevery* must be non-zero even if *Nrepeat* is 1. Also, the timesteps contributing to the average value cannot overlap, i.e. Nrepeat*Nevery can not exceed Nfreq.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then values on timesteps 90,92,94,96,98,100 will be used to compute the final average on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc. If Nrepeat=1 and Nfreq = 100, then no time averaging is done; values are simply generated on timesteps 100,200,etc.

Each per-atom property is also averaged over atoms in each bin. The way the averaging is one across the *Nrepeat* timesteps to produce output on the *Nfreq* timesteps, and across multiple *Nfreq* outputs, is determined by the *norm* and *av* keyword settings, as discussed below.

Bins can be 1d layers or slabs, 2d pencils, or 3d boxes. This depends on how many times (1, 2, or 3) the *dim*, *origin*, and *delta* settings are specified in the fix ave/spatial command. For 2d or 3d bins, there is no restriction on specifying dim = x before dim = y, or dim = y before dim = z. Bins in a particular *dim* have a bin size in that dimension given by *delta*. Every Nfreq steps, when averaging is being performed and the per-atom property is calculated for the first time, the number of bins and the bin sizes and boundaries are computed. Thus if the simulation box changes size during a simulation, the number of bins and their boundaries may also change. In each dimension, bins are defined relative to a specified *origin*, which may be the lower/upper edge of the simulation box in that dimension, or its center point, or a specified coordinate value. Starting at the origin, sufficient bins are created in both directions to completely span the bin extent in that dimension. By default the bin extent is the entire simulation box.

The *bound* keyword can be used one or more times to limit the extent of bin coverage in specified dimensions, i.e. to only bin a portion of the box. If the *lo* setting is *lower* or the *hi* setting is *upper*, the bin extent in that direction extends to the box boundary. If a numeric value is used for *lo* and/or *hi*, then the bin extent in the *lo* or *hi* direction extends only to that value, which is assumed to be inside (or at least near) the simulation box boundaries, though LAMMPS does not check for this.

On each sampling timestep, each atom is mapped to the bin it currently belongs to, based on its current position. Note that the group-ID and region keyword can exclude specific atoms from this operation, as discussed above. Note that between reneighboring timesteps, atoms can move outside the current simulation box. If the box is periodic (in that dimension) the atom is remapping into the periodic box for purposes of binning. If the box in not periodic, the atom may have moved outside the bounds of any bin.

The *discard* keyword determines what is done with any atom which is outside the bounds of any bin. If *discard* is set to *yes*, the atom will be ignored and not contribute to any bin averages. If *discard* is set to *no*, the atom will be counted as if it were in the first or last bin in that dimension. If (discard is set to *mixed*, which is the default, it will only be counted in the first or last bin if bins extend to the box boundary in that dimension. This is the case if the *bound* keyword settings are *lower* and *upper*, which is the default. If the *bound* keyword settings are numeric values, then the atom will be ignored if it is outside the bounds of any bin. Note that in this case, it is possible that the first or last bin extends beyond the numeric *bounds* settings, depending on the specified *origin*. If this is the case, the atom is only ignored if it is outside the first or last bin, not if it is simply outside the numeric *bounds* setting.

For orthogonal simulation boxes, the bins are also layers, pencils, or boxes aligned with the xyz coordinate axes. For triclinic (non-orthogonal) simulation boxes, the bins are so that they are parallel to the tilted faces of the simulation box. See this section of the manual for a discussion of the geometry of triclinic boxes in LAMMPS. As described there, a tilted simulation box has edge vectors a,b,c. In that nomenclature, bins in the x dimension have

faces with normals in the "b" cross "c" direction. Bins in y have faces normal to the "a" cross "c" direction. And bins in z have faces normal to the "a" cross "b" direction. Note that in order to define the size and position of these bins in an unambiguous fashion, the *units* option must be set to *reduced* when using a triclinic simulation box, as noted below.

The atom attribute values (vx,vy,vz,fx,fy,fz) are self-explanatory. Note that other atom attributes (including atom postitions x,y,z) can be used as inputs to this fix by using the compute property/atom command and then specifying an input value from that compute.

The *density/number* value means the number density is computed in each bin, i.e. a weighting of 1 for each atom. The *density/mass* value means the mass density is computed in each bind, i.e. each atom is weighted by its mass. The resulting density is normalized by the volume of the bin so that units of number/volume or density are output. See the units command doc page for the definition of density for each choice of units, e.g. gram/cm^3.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If no bracketed integer is appended, the per-atom vector calculated by the compute is used. If a bracketed integer is appended, the Ith column of the per-atom array calculated by the compute is used. Users can also write code for their own compute styles and add them to LAMMPS.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If no bracketed integer is appended, the per-atom vector calculated by the fix is used. If a bracketed integer is appended, the Ith column of the per-atom array calculated by the fix is used. Note that some fixes only produce their values on certain timesteps, which must be compatible with *Nevery*, else an error results. Users can also write code for their own fix styles and add them to LAMMPS.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. Variables of style *atom* can reference thermodynamic keywords and various per-atom attributes, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of generating per-atom quantities to spatially average.

Additional optional keywords also affect the operation of this fix. The *region*, *bound*, and *discard* keywords were discussed above.

The *norm* keyword affects how averaging is done for the output produced every *Nfreq* timesteps. For an *all* setting, a bin quantity is summed over all atoms in all *Nrepeat* samples, as is the count of atoms in the bin. The printed value for the bin is Total-quantity / Total-count. In other words it is an average over the entire *Nfreq* timescale.

For a *sample* setting, the bin quantity is summed over atoms for only a single sample, as is the count, and a "average sample value" is computed, i.e. Sample-quantity / Sample-count. The printed value for the bin is the average of the *Nrepeat* "average sample values", In other words it is an average of an average.

The *ave* keyword determines how the bin values produced every *Nfreq* steps are averaged with bin values produced on previous steps that were multiples of *Nfreq*, before they are accessed by another output command or written to a file.

If the *ave* setting is *one*, then the bin values produced on timesteps that are multiples of *Nfreq* are independent of each other; they are output as-is without further averaging.

If the *ave* setting is *running*, then the bin values produced on timesteps that are multiples of *Nfreq* are summed and averaged in a cumulative sense before being output. Each output bin value is thus the average of the bin value produced on that timestep with all preceding values for the same bin. This running average begins when the fix is

defined; it can only be restarted by deleting the fix via the unfix command, or re-defining the fix by re-specifying it.

If the *ave* setting is *window*, then the bin values produced on timesteps that are multiples of *Nfreq* are summed and averaged within a moving "window" of time, so that the last M values for the same bin are used to produce the output. E.g. if M = 3 and Nfreq = 1000, then the output on step 10000 will be the average of the individual bin values on steps 8000,9000,10000. Outputs on early steps will average over less than M values if they are not available.

The *units* keyword determines the meaning of the distance units used for the bin size *delta* and for *origin* and *bounds* values if they are coordinate value. For orthogonal simulation boxes, any of the 3 options may be used. For non-orthogonal (triclinic) simulation boxes, only the *reduced* option may be used.

A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacing. A *reduced* value means normalized unitless values between 0 and 1, which represent the lower and upper faces of the simulation box respectively. Thus an *origin* value of 0.5 means the center of the box in any dimension. A *delta* value of 0.1 means 10 bins span the box in that dimension.

Consider a non-orthogonal box, with bins that are 1d layers or slabs in the x dimension. No matter how the box is tilted, an *origin* of 0.0 means start layers at the lower "b" cross "c" plane of the simulation box and an *origin* of 1.0 means to start layers at the upper "b" cross "c" face of the box. A *delta* value of 0.1 means there will be 10 layers from 0.0 to 1.0, regardless of the current size or shape of the simulation box.

The *file* keyword allows a filename to be specified. Every *Nfreq* timesteps, a section of bin info will be written to a text file in the following format. A line with the timestep and number of bin is written. Then one line per bin is written, containing the bin ID (1-N), the coordinate of the center of the bin, the number of atoms in the bin, and one or more calculated values. The number of values in each line corresponds to the number of values specified in the fix ave/spatial command. The number of atoms and the value(s) are average quantities. If the value of the *units* keyword is *box* or *lattice*, the "coord" is printed in box units. If the value of the *units* keyword is *reduced*, the "coord" is printed in reduced units (0-1).

The *overwrite* keyword will continuously overwrite the output file with the latest output, so that it only contains one timestep worth of output. This option can only be used with the *ave running* setting.

The *title1* and *title2* and *title3* keywords allow specification of the strings that will be printed as the first 3 lines of the output file, assuming the *file* keyword was used. LAMMPS uses default values for each of these, so they do not need to be specified.

By default, these header lines are as follows:

```
# Spatial-averaged data for fix ID and group name
# Timestep Number-of-bins
# Bin Coord1 Coord2 Coord3 Count value1 value2 ...
```

In the first line, ID and name are replaced with the fix-ID and group name. The second line describes the two values that are printed at the first of each section of output. In the third line the values are replaced with the appropriate fields from the fix ave/spatial command. The Coord2 and Coord3 entries in the third line only appear for 2d and 3d bins respectively. For 1d bins, the word Coord1 is replaced by just Coord.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global array of values which can be accessed by various output commands. The values can only be accessed on timesteps that are multiples of *Nfreq* since that is when averaging is performed. The global array has # of rows = Nbins and # of columns = Ndim+1+Nvalues, where Ndim = 1,2,3 for 1d,2d,3d bins. The first 1 or 2 or 3 columns have the bin coordinates (center of the bin) in the appropriate dimensions, the next column has the count of atoms in that bin, and the remaining columns are the Nvalue quantities. When the array is accessed with an I that exceeds the current number of bins, than a 0.0 is returned by the fix instead of an error, since the number of bins can vary as a simulation runs, depending on the simulation box size. 2d or 3d bins are ordered so that the last dimension(s) vary fastest. The array values calculated by this fix are "intensive", since they are already normalized by the count of atoms in each bin.

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

When the *ave* keyword is set to *running* or *window* then the number of bins must remain the same during the simulation, so that the appropriate averaging can be done. This will be the case if the simulation box size doesn't change or if the *units* keyword is set to *reduced*.

Related commands:

compute, fix ave/atom, fix ave/histo, fix ave/time, variable, fix ave/correlate, fix ave/spatial/sphere

Default:

The option defaults are bound = lower and upper in all dimensions, discard = mixed, norm = all, ave = one, units = lattice, no file output, and title 1,2,3 = strings as described above.

fix ave/spatial/sphere command

Syntax:

```
fix ID group-ID ave/spatial/sphere Nevery Nrepeat Nfreq origin_x origin_y origin_z r_min r_max nbins
```

- ID, group-ID are documented in fix command
- ave/spatial = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of times to use input values for calculating averages
- Nfreq = calculate averages every this many timesteps
- origin_x, origin_y, origin_z = center of the sphere. can be the result of variables or computes (see below)
- r_min = radial distance at which binning begins
- r_max = radial distance at which binning ends
- nbins = number of spherical shells to create between r_min and r_max
- one or more input values can be listed
- value = vx, vy, vz, fx, fy, fz, density/mass, density/number, c_ID, c_ID[I], f_ID, f_ID[I], v_name

```
vx,vy,vz,fx,fy,fz = atom attribute (velocity, force component)
density/number, density/mass = number or mass density
c_ID = per-atom vector calculated by a compute with ID
c_ID[I] = Ith column of per-atom array calculated by a compute with ID
f_ID = per-atom vector calculated by a fix with ID
f_ID[I] = Ith column of per-atom array calculated by a fix with ID
v_name = per-atom vector calculated by an atom-style variable with name
```

- zero or more keyword/arg pairs may be appended
- keyword = *region* or *norm* or *units* or *ave* or *file* or *overwrite* or *title1* or *title2* or *title3*

```
region arg = region-ID
    region-ID = ID of region atoms must be in to contribute to spatial averaging
  norm arg = all or sample
  units arg = box or lattice or reduced
  ave args = one or running or window M
    one = output new average value every Nfreq steps
    running = output cumulative average of all previous Nfreq steps
    window M = output average of M most recent Nfreq steps
  file arg = filename
    filename = file to write results to
  overwrite arg = none = overwrite output file with only latest output
  title1 arg = string
    string = text to print as 1st line of output file
  title2 arg = string
    string = text to print as 2nd line of output file
  title3 arg = string
    string = text to print as 3rd line of output file
```

Examples:

```
fix 1 all ave/spatial/sphere 10000 1 10000 0.5 0.5 0.5 0.1 0.5 5 density/number vx vy vz units reduc
fix 1 flow ave/spatial/sphere 100 10 1000 20.0 20.0 20.0 0.0 20.0 20 vx vz norm sample file vel.prof
```

Description:

Use one or more per-atom vectors as inputs every few timesteps, bin their values spatially into spherical shells based on current atom coordinates, and average the bin values over longer timescales. The resulting bin averages

can be used by other output commands such as thermo_style custom, and can also be written to a file.

The group specified with the command means only atoms within the group contribute to bin averages. If the *region* keyword is used, the atom must be in both the group and the specified geometric region in order to contribute to bin averages.

Each listed value can be an atom attribute (position, velocity, force component), a mass or number density, or the result of a compute or fix or the evaluation of an atom-style variable. In the latter cases, the compute, fix, or variable must produce a per-atom quantity, not a global quantity. If you wish to time-average global quantities from a compute, fix, or variable, then see the fix ave/time command.

Computes that produce per-atom quantities are those which have the word *atom* in their style name. See the doc pages for individual fixes to determine which ones produce per-atom quantities. Variables of style *atom* are the only ones that can be used with this fix since all other styles of variable produce global quantities.

The per-atom values of each input vector are binned and averaged independently of the per-atom values in other input vectors.

Nbins specifies the number of spherical shells which will be created between r_min and r_max centered at (origin_x, origin_y, origin_z).

NOTE: This fix works by creating an array of size Nbins by Nvalues on each processor. Nbins is the total number of bins; Nvalues is the number of input values specified. Each processor loops over its atoms, tallying its values to the appropriate bin. Then the entire array is summed across all processors. This means that using a large number of bins will incur an overhead in memory and computational cost (summing across processors), so be careful to use reasonable numbers of bins.

The *Nevery*, *Nrepeat*, and *Nfreq* arguments specify on what timesteps the input values will be used to bin them and contribute to the average. The final averaged quantities are generated on timesteps that are a multiples of *Nfreq*. The average is over *Nrepeat* quantities, computed in the preceding portion of the simulation every *Nevery* timesteps. *Nfreq* must be a multiple of *Nevery* and *Nevery* must be non-zero even if *Nrepeat* is 1. Also, the timesteps contributing to the average value cannot overlap, i.e. Nrepeat*Nevery can not exceed Nfreq.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then values on timesteps 90,92,94,96,98,100 will be used to compute the final average on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc. If Nrepeat=1 and Nfreq = 100, then no time averaging is done; values are simply generated on timesteps 100,200,etc.

The *origin_x*, *origin_y*, and *origin_z* parameters may be specified by either a compute or a variable. This allows, for example, the center of the spherical bins to be attached to the center of mass of a group of atoms. If a variable origin is used and periodic boundary conditions are in effect, then the origin will be wrapped across periodic boundaries whenever it changes so that it is always inside the simulation box.

The atom attribute values (vx,vy,vz,fx,fy,fz) are self-explanatory. Note that other atom attributes (including atom postitions x,y,z) can be used as inputs to this fix by using the compute property/atom command and then specifying an input value from that compute.

The *density/number* value means the number density is computed in each bin, i.e. a weighting of 1 for each atom. The *density/mass* value means the mass density is computed in each bin, i.e. each atom is weighted by its mass. The resulting density is normalized by the volume of the bin so that units of number/volume or density are output. See the units command doc page for the definition of density for each choice of units, e.g. gram/cm^3. The bin volume will always be calculated in box units, independent of the use of the *units* keyword in this command.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If no bracketed integer is appended, the per-atom vector calculated by the compute is used. If a bracketed integer is appended, the Ith column of the per-atom array calculated by the compute is used. Users can also write code for their own compute styles and add them to LAMMPS.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If no bracketed integer is appended, the per-atom vector calculated by the fix is used. If a bracketed integer is appended, the Ith column of the per-atom array calculated by the fix is used. Note that some fixes only produce their values on certain timesteps, which must be compatible with *Nevery*, else an error results. Users can also write code for their own fix styles and add them to LAMMPS.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. Variables of style *atom* can reference thermodynamic keywords and various per-atom attributes, or invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of generating per-atom quantities to spatially average.

Additional optional keywords also affect the operation of this fix. The *region* keyword was discussed above.

The *norm* keyword affects how averaging is done for the output produced every *Nfreq* timesteps. For an *all* setting, a bin quantity is summed over all atoms in all *Nrepeat* samples, as is the count of atoms in the bin. The printed value for the bin is Total-quantity / Total-count. In other words it is an average over the entire *Nfreq* timescale.

For a *sample* setting, the bin quantity is summed over atoms for only a single sample, as is the count, and a "average sample value" is computed, i.e. Sample-quantity / Sample-count. The printed value for the bin is the average of the *Nrepeat* "average sample values", In other words it is an average of an average.

The *ave* keyword determines how the bin values produced every *Nfreq* steps are averaged with bin values produced on previous steps that were multiples of *Nfreq*, before they are accessed by another output command or written to a file.

If the *ave* setting is *one*, then the bin values produced on timesteps that are multiples of *Nfreq* are independent of each other; they are output as-is without further averaging.

If the *ave* setting is *running*, then the bin values produced on timesteps that are multiples of *Nfreq* are summed and averaged in a cumulative sense before being output. Each output bin value is thus the average of the bin value produced on that timestep with all preceding values for the same bin. This running average begins when the fix is defined; it can only be restarted by deleting the fix via the unfix command, or re-defining the fix by re-specifying it.

If the *ave* setting is *window*, then the bin values produced on timesteps that are multiples of *Nfreq* are summed and averaged within a moving "window" of time, so that the last M values for the same bin are used to produce the output. E.g. if M = 3 and Nfreq = 1000, then the output on step 10000 will be the average of the individual bin values on steps 8000,9000,10000. Outputs on early steps will average over less than M values if they are not available.

The *units* keyword determines the meaning of the distance units used for the sphere origin and the two radial lengths. For orthogonal simulation boxes, any of the 3 options may be used. For non-orthogonal (triclinic) simulation boxes, only the *reduced* option may be used.

A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The lattice command must have been

previously used to define the lattice spacing.

NOTE: The *lattice* style may only be used if the lattice spacing is the same in each direction.

A *reduced* value means normalized unitless values between 0 and 1, which represent the lower and upper faces of the simulation box respectively. Thus an *origin* value of 0.5 means the center of the box in any dimension.

The *file* keyword allows a filename to be specified. Every *Nfreq* timesteps, a section of bin info will be written to a text file in the following format. A line with the timestep and number of bin is written. Then one line per bin is written, containing the bin ID (1-N), the coordinate of the center of the bin, the number of atoms in the bin, and one or more calculated values. The number of values in each line corresponds to the number of values specified in the fix ave/spatial command. The number of atoms and the value(s) are average quantities. If the value of the *units* keyword is *box* or *lattice*, the "coord" is printed in box units. If the value of the *units* keyword is *reduced*, the "coord" is printed in reduced units (0-1).

The *overwrite* keyword will continuously overwrite the output file with the latest output, so that it only contains one timestep worth of output. This option can only be used with the *ave running* setting.

The *title1* and *title2* and *title3* keywords allow specification of the strings that will be printed as the first 3 lines of the output file, assuming the *file* keyword was used. LAMMPS uses default values for each of these, so they do not need to be specified.

By default, these header lines are as follows:

```
# Spatial-averaged data for fix ID and group name
# Timestep Number-of-bins
# Bin r Count value1 value2 ...
```

In the first line, ID and name are replaced with the fix-ID and group name. The second line describes the two values that are printed at the first of each section of output. In the third line the values are replaced with the appropriate fields from the fix ave/spatial command. The Coord2 and Coord3 entries in the third line only appear for 2d and 3d bins respectively. For 1d bins, the word Coord1 is replaced by just Coord.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global array of values which can be accessed by various output commands. The values can only be accessed on timesteps that are multiples of *Nfreq* since that is when averaging is performed. The global array has # of rows = Nbins and # of columns = 2+Nvalues. The first column contains the radius at the center of the shell. For units *reduced*, this is in reduced units, while for units *box* and *lattice* this is in box units. The next column has the count of atoms in that bin, and the remaining columns are the Nvalue quantities. When the array is accessed with an I that exceeds the current number of bins, than a 0.0 is returned by the fix instead of an error. The array values calculated by this fix are "intensive", since they are already normalized by the count of atoms in each bin.

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

When the *ave* keyword is set to *running* or *window* then the number of bins must remain the same during the simulation, so that the appropriate averaging can be done. This will be the case if the simulation box size doesn't change or if the *units* keyword is set to *reduced*.

This style is part of the USER-MISC package. It is only enabled if LAMMPS is build with that package. See the Making of LAMMPS section for more info.

Related commands:

compute, fix ave/atom, fix ave/histo, fix ave/time, variable, fix ave/correlate, fix ave/spatial,

Default:

The option defaults are norm = all, ave = one, units = lattice, no file output, and title 1,2,3 = strings as described above.

fix ave/time command

Syntax:

```
fix ID group-ID ave/time Nevery Nrepeat Nfreq value1 value2 ... keyword args ...
```

- ID, group-ID are documented in fix command
- ave/time = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of times to use input values for calculating averages
- Nfreq = calculate averages every this many timesteps
- one or more input values can be listed
- value = c_ID, c_ID[N], f_ID, f_ID[N], v_name

```
c_ID = global scalar, vector, or array calculated by a compute with ID
c_ID[I] = Ith component of global vector or Ith column of global array calculated by a compu
f_ID = global scalar, vector, or array calculated by a fix with ID
f_ID[I] = Ith component of global vector or Ith column of global array calculated by a fix v
v_name = global value calculated by an equal-style variable with name
```

- zero or more keyword/arg pairs may be appended
- keyword = *mode* or *file* or *ave* or *start* or *off* or *overwrite* or *title1* or *title2* or *title3*

```
mode arg = scalar or vector
    scalar = all input values are global scalars
    vector = all input values are global vectors or global arrays
  ave args = one or running or window M
    one = output a new average value every Nfreq steps
    running = output cummulative average of all previous Nfreq steps
    window M = output average of M most recent Nfreq steps
  start args = Nstart
    Nstart = start averaging on this timestep
  off arg = M = do not average this value
    M = value # from 1 to Nvalues
  file arg = filename
    filename = name of file to output time averages to
  overwrite arg = none = overwrite output file with only latest output
  format arg = string
    string = C-style format string
  title1 arg = string
    string = text to print as 1st line of output file
  title2 arg = string
    string = text to print as 2nd line of output file
  title3 arg = string
    string = text to print as 3rd line of output file, only for vector mode
```

Examples:

```
fix 1 all ave/time 100 5 1000 c_myTemp c_thermo_temp file temp.profile
fix 1 all ave/time 100 5 1000 c_thermo_press[2] ave window 20 &
                              title1 "My output values"
fix 1 all ave/time 1 100 1000 f_indent f_indent[1] file temp.indent off 1
```

Description:

Use one or more global values as inputs every few timesteps, and average them over longer timescales. The resulting averages can be used by other output commands such as thermo_style custom, and can also be written to

a file. Note that if no time averaging is done, this command can be used as a convenient way to simply output one or more global values to a file.

The group specified with this command is ignored. However, note that specified values may represent calculations performed by computes and fixes which store their own "group" definitions.

Each listed value can be the result of a compute or fix or the evaluation of an equal-style variable. In each case, the compute, fix, or variable must produce a global quantity, not a per-atom or local quantity. If you wish to spatial- or time-average or histogram per-atom quantities from a compute, fix, or variable, then see the fix ave/spatial, fix ave/atom, or fix ave/histo commands. If you wish to sum a per-atom quantity into a single global quantity, see the compute reduce command.

Computes that produce global quantities are those which do not have the word *atom* in their style name. Only a few fixes produce global quantities. See the doc pages for individual fixes for info on which ones produce such values. Variables of style *equal* are the only ones that can be used with this fix. Variables of style *atom* cannot be used, since they produce per-atom values.

The input values must either be all scalars or all vectors (or arrays), depending on the setting of the *mode* keyword. In both cases, the averaging is performed independently on each input value. I.e. each input scalar is averaged independently and each element of each input vector (or array) is averaged independently.

If *mode* = vector, then the input values may either be vectors or arrays and all must be the same "length", which is the length of the vector or number of rows in the array. If a global array is listed, then it is the same as if the individual columns of the array had been listed one by one. E.g. these 2 fix ave/time commands are equivalent, since the compute rdf command creates, in this case, a global array with 3 columns, each of length 50:

```
compute myRDF all rdf 50 1 2
fix 1 all ave/time 100 1 100 c_myRDF file tmp1.rdf mode vector
fix 2 all ave/time 100 1 100 c_myRDF[1] c_myRDF[2] c_myRDF[3] file tmp2.rdf mode vector
```

The *Nevery*, *Nrepeat*, and *Nfreq* arguments specify on what timesteps the input values will be used in order to contribute to the average. The final averaged quantities are generated on timesteps that are a mlutiple of *Nfreq*. The average is over *Nrepeat* quantities, computed in the preceding portion of the simulation every *Nevery* timesteps. *Nfreq* must be a multiple of *Nevery* and *Nevery* must be non-zero even if *Nrepeat* is 1. Also, the timesteps contributing to the average value cannot overlap, i.e. Nrepeat*Nevery can not exceed Nfreq.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then values on timesteps 90,92,94,96,98,100 will be used to compute the final average on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc. If Nrepeat=1 and Nfreq = 100, then no time averaging is done; values are simply generated on timesteps 100,200,etc.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If *mode* = scalar, then if no bracketed term is appended, the global scalar calculated by the compute is used. If a bracketed term is appended, the Ith element of the global vector calculated by the compute is used. If *mode* = vector, then if no bracketed term is appended, the global vector calculated by the compute is used. Or if the compute calculates an array, all of the columns of the global array are used as if they had been specified as individual vectors (see description above). If a bracketed term is appended, the Ith column of the global array calculated by the compute is used.

Note that there is a compute reduce command which can sum per-atom quantities into a global scalar or vector which can thus be accessed by fix ave/time. Or it can be a compute defined not in your input script, but by thermodynamic output or other fixes such as fix nvt or fix temp/rescale. See the doc pages for these commands which give the IDs of these computes. Users can also write code for their own compute styles and add them to

LAMMPS.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If *mode* = scalar, then if no bracketed term is appended, the global scalar calculated by the fix is used. If a bracketed term is appended, the Ith element of the global vector calculated by the fix is used. If *mode* = vector, then if no bracketed term is appended, the global vector calculated by the fix is used. Or if the fix calculates an array, all of the columns of the global array are used as if they had been specified as individual vectors (see description above). If a bracketed term is appended, the Ith column of the global array calculated by the fix is used.

Note that some fixes only produce their values on certain timesteps, which must be compatible with *Nevery*, else an error will result. Users can also write code for their own fix styles and add them to LAMMPS.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. Variables can only be used as input for *mode* = scalar. Only equal-style variables can be referenced. See the variable command for details. Note that variables of style *equal* define a formula which can reference individual atom properties or thermodynamic keywords, or they can invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of specifying quantities to time average.

Additional optional keywords also affect the operation of this fix.

If the *mode* keyword is set to *scalar*, then all input values must be global scalars, or elements of global vectors. If the *mode* keyword is set to *vector*, then all input values must be global vectors, or columns of global arrays. They can also be global arrays, which are converted into a series of global vectors (one per column), as explained above.

The *ave* keyword determines how the values produced every *Nfreq* steps are averaged with values produced on previous steps that were multiples of *Nfreq*, before they are accessed by another output command or written to a file.

If the *ave* setting is *one*, then the values produced on timesteps that are multiples of *Nfreq* are independent of each other; they are output as-is without further averaging.

If the *ave* setting is *running*, then the values produced on timesteps that are multiples of *Nfreq* are summed and averaged in a cummulative sense before being output. Each output value is thus the average of the value produced on that timestep with all preceding values. This running average begins when the fix is defined; it can only be restarted by deleting the fix via the unfix command, or by re-defining the fix by re-specifying it.

If the *ave* setting is *window*, then the values produced on timesteps that are multiples of *Nfreq* are summed and averaged within a moving "window" of time, so that the last M values are used to produce the output. E.g. if M = 3 and Nfreq = 1000, then the output on step 10000 will be the average of the individual values on steps 8000,9000,10000. Outputs on early steps will average over less than M values if they are not available.

The *start* keyword specifies what timestep averaging will begin on. The default is step 0. Often input values can be 0.0 at time 0, so setting *start* to a larger value can avoid including a 0.0 in a running or windowed average.

The *off* keyword can be used to flag any of the input values. If a value is flagged, it will not be time averaged. Instead the most recent input value will always be stored and output. This is useful if one of more of the inputs produced by a compute or fix or variable are effectively constant or are simply current values. E.g. they are being written to a file with other time-averaged values for purposes of creating well-formatted output.

The *file* keyword allows a filename to be specified. Every *Nfreq* steps, one quantity or vector of quantities is written to the file for each input value specified in the fix ave/time command. For *mode* = scalar, this means a

single line is written each time output is performed. Thus the file ends up to be a series of lines, i.e. one column of numbers for each input value. For *mode* = vector, an array of numbers is written each time output is performed. The number of rows is the length of the input vectors, and the number of columns is the number of values. Thus the file ends up to be a series of these array sections.

The *overwrite* keyword will continuously overwrite the output file with the latest output, so that it only contains one timestep worth of output. This option can only be used with the *ave running* setting.

The *format* keyword sets the numeric format of each value when it is printed to a file via the *file* keyword. Note that all values are floating point quantities. The default format is %g. You can specify a higher precision if desired, e.g. %20.16g.

The *title1* and *title2* and *title3* keywords allow specification of the strings that will be printed as the first 2 or 3 lines of the output file, assuming the *file* keyword was used. LAMMPS uses default values for each of these, so they do not need to be specified.

By default, these header lines are as follows for *mode* = scalar:

```
# Time-averaged data for fix ID
# TimeStep value1 value2 ...
```

In the first line, ID is replaced with the fix-ID. In the second line the values are replaced with the appropriate fields from the fix ave/time command. There is no third line in the header of the file, so the *title3* setting is ignored when *mode* = scalar.

By default, these header lines are as follows for *mode* = vector:

```
# Time-averaged data for fix ID
# TimeStep Number-of-rows
# Row value1 value2 ...
```

In the first line, ID is replaced with the fix-ID. The second line describes the two values that are printed at the first of each section of output. In the third line the values are replaced with the appropriate fields from the fix ave/time command.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix produces a global scalar or global vector or global array which can be accessed by various output commands. The values can only be accessed on timesteps that are multiples of *Nfreq* since that is when averaging is performed.

A scalar is produced if only a single input value is averaged and *mode* = scalar. A vector is produced if multiple input values are averaged for *mode* = scalar, or a single input value for *mode* = vector. In the first case, the length of the vector is the number of inputs. In the second case, the length of the vector is the same as the length of the input vector. An array is produced if multiple input values are averaged and *mode* = vector. The global array has # of rows = length of the input vectors and # of columns = number of inputs.

If the fix prouduces a scalar or vector, then the scalar and each element of the vector can be either "intensive" or "extensive", depending on whether the values contributing to the scalar or vector element are "intensive" or "extensive". If the fix produces an array, then all elements in the array must be the same, either "intensive" or

"extensive". If a compute or fix provides the value being time averaged, then the compute or fix determines whether the value is intensive or extensive; see the doc page for that compute or fix for further info. Values produced by a variable are treated as intensive.

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

compute, fix ave/atom, fix ave/spatial, fix ave/histo, variable, fix ave/correlate,

Default:

The option defaults are mode = scalar, ave = one, start = 0, no file output, format = %g, title 1,2,3 = strings as described above, and no off settings for any input values.

fix aveforce command

fix aveforce/cuda command

Syntax:

```
fix ID group-ID aveforce fx fy fz keyword value ...
```

- ID, group-ID are documented in fix command
- aveforce = style name of this fix command
- fx,fy,fz = force component values (force units)

```
  any of fx,fy,fz can be a variable (see below)
```

- zero or more keyword/value pairs may be appended to args
- keyword = *region*

```
region value = region-ID
    region-ID = ID of region atoms must be in to have added force
```

Examples:

```
fix pressdown topwall aveforce 0.0 -1.0 0.0
fix 2 bottomwall aveforce NULL -1.0 0.0 region top
fix 2 bottomwall aveforce NULL -1.0 v_oscillate region top
```

Description:

Apply an additional external force to a group of atoms in such a way that every atom experiences the same force. This is useful for pushing on wall or boundary atoms so that the structure of the wall does not change over time.

The existing force is averaged for the group of atoms, component by component. The actual force on each atom is then set to the average value plus the component specified in this command. This means each atom in the group receives the same force.

Any of the fx,fy,fz values can be specified as NULL which means the force in that dimension is not changed. Note that this is not the same as specifying a 0.0 value, since that sets all forces to the same average value without adding in any additional force.

Any of the 3 quantities defining the force components can be specified as an equal-style variable, namely *fx*, *fy*, *fz*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the average force.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent average force.

If the *region* keyword is used, the atom must also be in the specified geometric region in order to have force added to it.

Styles with a *cuda* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual.

The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global 3-vector of forces, which can be accessed by various output commands. This is the total force on the group of atoms before the forces on individual atoms are changed by the fix. The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command. You should not specify force components with a variable that has time-dependence for use with a minimizer, since the minimizer increments the timestep as the iteration count during the minimization.

Restrictions: none

Related commands:

fix setforce, fix addforce

Default: none

fix balance command

Syntax:

```
fix ID group-ID balance Nfreq thresh style args keyword value ...
```

- ID, group-ID are documented in fix command
- balance = style name of this fix command
- Nfreq = perform dynamic load balancing every this many steps
- thresh = imbalance threshhold that must be exceeded to perform a re-balance
- style = *shift* or *rcb*

```
  shift args = dimstr Niter stopthresh
    dimstr = sequence of letters containing "x" or "y" or "z", each not more than once
    Niter = # of times to iterate within each dimension of dimstr sequence
    stopthresh = stop balancing when this imbalance threshhold is reached
  rcb args = none
```

- zero or more keyword/value pairs may be appended
- keyword = *out*

```
out value = filename
    filename = write each processor's sub-domain to a file, at each re-balancing
```

Examples:

```
fix 2 all balance 1000 1.05 shift x 10 1.05
fix 2 all balance 100 0.9 shift xy 20 1.1 out tmp.balance
fix 2 all balance 1000 1.1 rcb
```

Description:

This command adjusts the size and shape of processor sub-domains within the simulation box, to attempt to balance the number of particles and thus the computational cost (load) evenly across processors. The load balancing is "dynamic" in the sense that rebalancing is performed periodically during the simulation. To perform "static" balancing, before or between runs, see the balance command.

Load-balancing is typically only useful if the particles in the simulation box have a spatially-varying density distribution. E.g. a model of a vapor/liquid interface, or a solid with an irregular-shaped geometry containing void regions. In this case, the LAMMPS default of dividing the simulation box volume into a regular-spaced grid of 3d bricks, with one equal-volume sub-domain per processor, may assign very different numbers of particles per processor. This can lead to poor performance when the simulation is run in parallel.

Note that the processors command allows some control over how the box volume is split across processors. Specifically, for a Px by Py by Pz grid of processors, it allows choice of Px, Py, and Pz, subject to the constraint that Px * Py * Pz = P, the total number of processors. This is sufficient to achieve good load-balance for some problems on some processor counts. However, all the processor sub-domains will still have the same shape and same volume.

On a particular timestep, a load-balancing operation is only performed if the current "imbalance factor" in particles owned by each processor exceeds the specified *thresh* parameter. The imbalance factor is defined as the maximum number of particles owned by any processor, divided by the average number of particles per processor. Thus an imbalance factor of 1.0 is perfect balance.

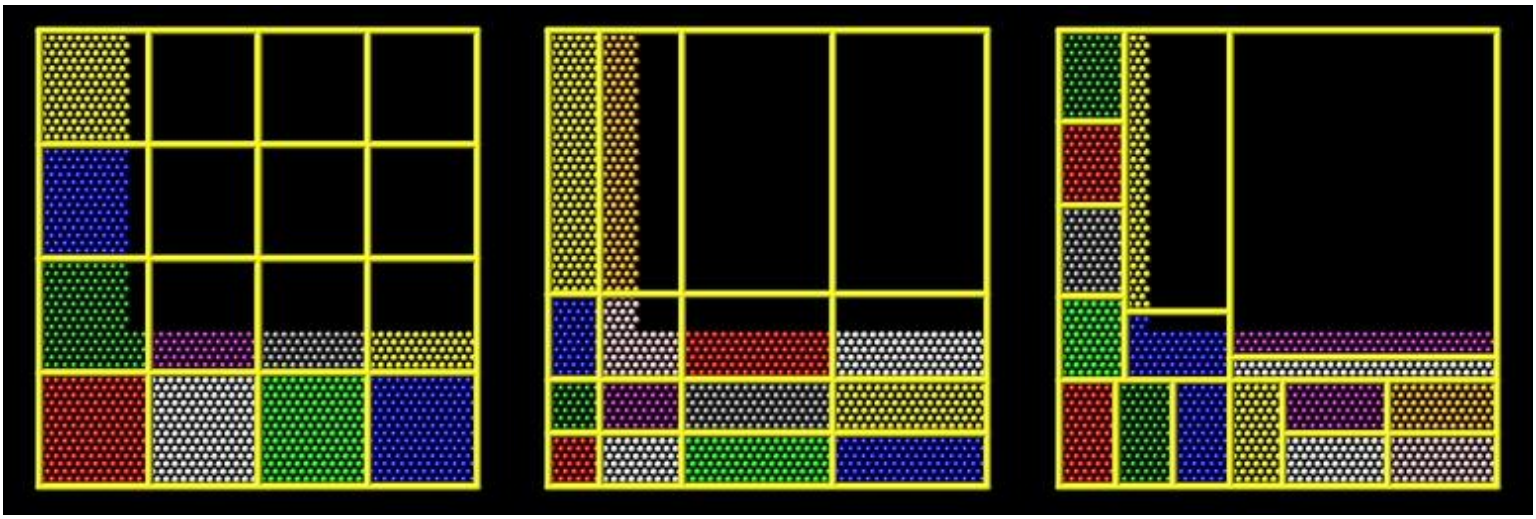
As an example, for 10000 particles running on 10 processors, if the most heavily loaded processor has 1200 particles, then the factor is 1.2, meaning there is a 20% imbalance. Note that re-balances can be forced even if the current balance is perfect (1.0) be specifying a *thresh* < 1.0.

NOTE: This command attempts to minimize the imbalance factor, as defined above. But depending on the method a perfect balance (1.0) may not be achieved. For example, "grid" methods (defined below) that create a logical 3d grid cannot achieve perfect balance for many irregular distributions of particles. Likewise, if a portion of the system is a perfect lattice, e.g. the initial system is generated by the create_atoms command, then "grid" methods may be unable to achieve exact balance. This is because entire lattice planes will be owned or not owned by a single processor.

NOTE: The imbalance factor is also an estimate of the maximum speed-up you can hope to achieve by running a perfectly balanced simulation versus an imbalanced one. In the example above, the 10000 particle simulation could run up to 20% faster if it were perfectly balanced, versus when imbalanced. However, computational cost is not strictly proportional to particle count, and changing the relative size and shape of processor sub-domains may lead to additional computational and communication overheads, e.g. in the PPPM solver used via the kspace_style command. Thus you should benchmark the run times of a simulation before and after balancing.

The method used to perform a load balance is specified by one of the listed styles, which are described in detail below. There are 2 kinds of styles.

The *shift* style is a "grid" method which produces a logical 3d grid of processors. It operates by changing the cutting planes (or lines) between processors in 3d (or 2d), to adjust the volume (area in 2d) assigned to each processor, as in the following 2d diagram where processor sub-domains are shown and atoms are colored by the processor that owns them. The leftmost diagram is the default partitioning of the simulation box across processors (one sub-box for each of 16 processors); the middle diagram is after a "grid" method has been applied.



The *rcb* style is a "tiling" method which does not produce a logical 3d grid of processors. Rather it tiles the simulation domain with rectangular sub-boxes of varying size and shape in an irregular fashion so as to have equal numbers of particles in each sub-box, as in the rightmost diagram above.

The "grid" methods can be used with either of the comm_style command options, *brick* or *tiled*. The "tiling" methods can only be used with comm_style tiled.

When a "grid" method is specified, the current domain partitioning can be either a logical 3d grid or a tiled partitioning. In the former case, the current logical 3d grid is used as a starting point and changes are made to improve the imbalance factor. In the latter case, the tiled partitioning is discarded and a logical 3d grid is created

with uniform spacing in all dimensions. This is the starting point for the balancing operation.

When a "tiling" method is specified, the current domain partitioning ("grid" or "tiled") is ignored, and a new partitioning is computed from scratch.

The *group-ID* is currently ignored. In the future it may be used to determine what particles are considered for balancing. Normally it would only makes sense to use the *all* group. But in some cases it may be useful to balance on a subset of the particles, e.g. when modeling large nanoparticles in a background of small solvent particles.

The *Nfreq* setting determines how often a rebalance is performed. If *Nfreq* > 0, then rebalancing will occur every *Nfreq* steps. Each time a rebalance occurs, a reneighboring is triggered, so *Nfreq* should not be too small. If *Nfreq* = 0, then rebalancing will be done every time reneighboring normally occurs, as determined by the the neighbor and neigh_modify command settings.

On rebalance steps, rebalancing will only be attempted if the current imbalance factor, as defined above, exceeds the *thresh* setting.

The *shift* style invokes a "grid" method for balancing, as described above. It changes the positions of cutting planes between processors in an iterative fashion, seeking to reduce the imbalance factor.

The *dimstr* argument is a string of characters, each of which must be an "x" or "y" or "z". Eacn character can appear zero or one time, since there is no advantage to balancing on a dimension more than once. You should normally only list dimensions where you expect there to be a density variation in the particles.

Balancing proceeds by adjusting the cutting planes in each of the dimensions listed in *dimstr*, one dimension at a time. For a single dimension, the balancing operation (described below) is iterated on up to *Niter* times. After each dimension finishes, the imbalance factor is re-computed, and the balancing operation halts if the *stopthresh* criterion is met.

A rebalance operation in a single dimension is performed using a density-dependent recursive multisectioning algorithm, where the position of each cutting plane (line in 2d) in the dimension is adjusted independently. This is similar to a recursive bisectioning for a single value, except that the bounds used for each bisectioning take advantage of information from neighboring cuts if possible, as well as counts of particles at the bounds on either side of each cuts, which themselves were cuts in previous iterations. The latter is used to infer a density of pariticles near each of the current cuts. At each iteration, the count of particles on either side of each plane is tallied. If the counts do not match the target value for the plane, the position of the cut is adjusted based on the local density. The low and high bounds are adjusted on each iteration, using new count information, so that they become closer together over time. Thus as the recursion progresses, the count of particles on either side of the plane gets closer to the target value.

The density-dependent part of this algorithm is often an advantage when you rebalance a system that is already nearly balanced. It typically converges more quickly than the geometric bisectioning algorithm used by the balance command. However, if can be a disadvantage if you attempt to rebalance a system that is far from balanced, and converge more slowly. In this case you probably want to use the balance command before starting a run, so that you begin the run with a balanced system.

Once the rebalancing is complete and final processor sub-domains assigned, particles migrate to their new owning processor as part of the normal reneighboring procedure.

NOTE: At each rebalance operation, the bisectioning for each cutting plane (line in 2d) typcially starts with low and high bounds separated by the extent of a processor's sub-domain in one dimension. The size of this bracketing region shrinks based on the local density, as described above, which should typically be 1/2 or more every

iteration. Thus if *Niter* is specified as 10, the cutting plane will typically be positioned to better than 1 part in 1000 accuracy (relative to the perfect target position). For *Niter* = 20, it will be accurate to better than 1 part in a million. Thus there is no need to set *Niter* to a large value. This is especially true if you are rebalancing often enough that each time you expect only an incremental adjustement in the cutting planes is necessary. LAMMPS will check if the threshold accuracy is reached (in a dimension) is less iterations than *Niter* and exit early.

The *rcb* style invokes a "tiled" method for balancing, as described above. It performs a recursive coordinate bisectioning (RCB) of the simulation domain. The basic idea is as follows.

The simulation domain is cut into 2 boxes by an axis-aligned cut in the longest dimension, leaving one new box on either side of the cut. All the processors are also partitioned into 2 groups, half assigned to the box on the lower side of the cut, and half to the box on the upper side. (If the processor count is odd, one side gets an extra processor.) The cut is positioned so that the number of atoms in the lower box is exactly the number that the processors assigned to that box should own for load balance to be perfect. This also makes load balance for the upper box perfect. The positioning is done iteratively, by a bisectioning method. Note that counting atoms on either side of the cut requires communication between all processors at each iteration.

That is the procedure for the first cut. Subsequent cuts are made recursively, in exactly the same manner. The subset of processors assigned to each box make a new cut in the longest dimension of that box, splitting the box, the subset of processsors, and the atoms in the box in two. The recursion continues until every processor is assigned a sub-box of the entire simulation domain, and owns the atoms in that sub-box.

The *out* keyword writes a text file to the specified *filename* with the results of each rebalancing operation. The file contains the bounds of the sub-domain for each processor after the balancing operation completes. The format of the file is compatible with the Pizza.py *mdump* tool which has support for manipulating and visualizing mesh files. An example is shown here for a balancing by 4 processors for a 2d problem:

```
ITEM: TIMESTEP
0
ITEM: NUMBER OF NODES
16
ITEM: BOX BOUNDS
0 10
0 10
0 10
ITEM: NODES
1 1 0 0 0
2 1 5 0 0
3 1 5 5 0
4 1 0 5 0
5 1 5 0 0
6 1 10 0 0
7 1 10 5 0
8 1 5 5 0
9 1 0 5 0
10 1 5 5 0
11 1 5 10 0
12 1 10 5 0
13 1 5 5 0
14 1 10 5 0
15 1 10 10 0
16 1 5 10 0
ITEM: TIMESTEP
0
ITEM: NUMBER OF SQUARES
4
ITEM: SQUARES
1 1 1 2 3 4
```

```
2 1 5 6 7 8
3 1 9 10 11 12
4 1 13 14 15 16
```

The coordinates of all the vertices are listed in the NODES section, 5 per processor. Note that the 4 sub-domains share vertices, so there will be duplicate nodes in the list.

The "SQUARES" section lists the node IDs of the 4 vertices in a rectangle for each processor (1 to 4).

For a 3d problem, the syntax is similar with 8 vertices listed for each processor, instead of 4, and "SQUARES" replaced by "CUBES".

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global scalar which is the imbalance factor after the most recent rebalance and a global vector of length 3 with additional information about the most recent rebalancing. The 3 values in the vector are as follows:

- 1 = max # of particles per processor
- 2 = total # iterations performed in last rebalance
- 3 = imbalance factor right before the last rebalance was performed

As explained above, the imbalance factor is the ratio of the maximum number of particles on any processor to the average number of particles per processor.

These quantities can be accessed by various output commands. The scalar and vector values calculated by this fix are "intensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

For 2d simulations, a "z" cannot appear in *dimstr* for the *shift* style.

Related commands:

processors, balance

Default: none

fix bond/break command

Syntax:

```
fix ID group-ID bond/break Nevery bondtype Rmax keyword values ...
```

- ID, group-ID are documented in fix command
- bond/break = style name of this fix command
- Nevery = attempt bond breaking every this many steps
- bondtype = type of bonds to break
- Rmax = bond longer than Rmax can break (distance units)
- zero or more keyword/value pairs may be appended to args
- keyword = *prob*

```
  prob values = fraction seed
      fraction = break a bond with this probability if otherwise eligible
      seed = random number seed (positive integer)
```

Examples:

```
fix 5 all bond/break 10 2 1.2
fix 5 polymer bond/break 1 1 2.0 prob 0.5 49829
```

Description:

Break bonds between pairs of atoms as a simulation runs according to specified criteria. This can be used to model the dissolution of a polymer network due to stretching of the simulation box or other deformations. In this context, a bond means an interaction between a pair of atoms computed by the bond_style command. Once the bond is broken it will be permanently deleted, as will all angle, dihedral, and improper interactions that bond is part of.

This is different than a pairwise bond-order potential such as Tersoff or AIREBO which infers bonds and many-body interactions based on the current geometry of a small cluster of atoms and effectively creates and destroys bonds and higher-order many-body interactions from timestep to timestep as atoms move.

A check for possible bond breakage is performed every *Nevery* timesteps. If two bonded atoms I,J are further than a distance *Rmax* of each other, if the bond is of type *bondtype*, and if both I and J are in the specified fix group, then I,J is labeled as a "possible" bond to break.

If several bonds involving an atom are stretched, it may have multiple possible bonds to break. Every atom checks its list of possible bonds to break and labels the longest such bond as its "sole" bond to break. After this is done, if atom I is bonded to atom J in its sole bond, and atom J is bonded to atom I in its sole bond, then the I,J bond is "eligible" to be broken.

Note that these rules mean an atom will only be part of at most one broken bond on a given timestep. It also means that if atom I chooses atom J as its sole partner, but atom J chooses atom K is its sole partner (due to Rjk > Rij), then this means atom I will not be part of a broken bond on this timestep, even if it has other possible bond partners.

The *prob* keyword can effect whether an eligible bond is actually broken. The *fraction* setting must be a value between 0.0 and 1.0. A uniform random number between 0.0 and 1.0 is generated and the eligible bond is only

broken if the random number < fraction.

When a bond is broken, data structures within LAMMPS that store bond topology are updated to reflect the breakage. Likewise, if the bond is part of a 3-body (angle) or 4-body (dihedral, improper) interaction, that interaction is removed as well. These changes typically affect pairwise interactions between atoms that used to be part of bonds, angles, etc.

NOTE: One data structure that is not updated when a bond breaks are the molecule IDs stored by each atom. Even though one molecule becomes two moleclues due to the broken bond, all atoms in both new moleclues retain their original molecule IDs.

Computationally, each timestep this fix operates, it loops over all the bonds in the system and computes distances between pairs of bonded atoms. It also communicates between neighboring processors to coordinate which bonds are broken. Moreover, if any bonds are broken, neighbor lists must be immediately updated on the same timestep. This is to insure that any pairwise interactions that should be turned "on" due to a bond breaking, because they are no longer excluded by the presence of the bond and the settings of the special_bonds command, will be immediately recognized. All of these operations increase the cost of a timestep. Thus you should be cautious about invoking this fix too frequently.

You can dump out snapshots of the current bond topology via the dump local command.

NOTE: Breaking a bond typically alters the energy of a system. You should be careful not to choose bond breaking criteria that induce a dramatic change in energy. For example, if you define a very stiff harmonic bond and break it when 2 atoms are separated by a distance far from the equilibribum bond length, then the 2 atoms will be dramatically released when the bond is broken. More generally, you may need to thermostat your system to compensate for energy changes resulting from broken bonds (and angles, dihedrals, impropers).

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes two statistics which it stores in a global vector of length 2, which can be accessed by various output commands. The vector values calculated by this fix are "intensive".

These are the 2 quantities:

- (1) # of bonds broken on the most recent breakage timestep
- (2) cummulative # of bonds broken

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the MC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix bond/create, fix bond/swap, dump local, special_bonds

Default:

The option defaults are prob = 1.0.

fix bond/create command

Syntax:

```
fix ID group-ID bond/create Nevery itype jtype Rmin bondtype keyword values ...
```

- ID, group-ID are documented in fix command
- bond/create = style name of this fix command
- Nevery = attempt bond creation every this many steps
- itype,jtype = atoms of itype can bond to atoms of jtype
- Rmin = 2 atoms separated by less than Rmin can bond (distance units)
- bondtype = type of created bonds
- zero or more keyword/value pairs may be appended to args
- keyword = *iparam* or *jparam* or *prob* or *atype* or *dtype* or *itype*

```
  iparam values = maxbond, newtype
      maxbond = max # of bonds of bondtype the itype atom can have
      newtype = change the itype atom to this type when maxbonds exist
    jparam values = maxbond, newtype
      maxbond = max # of bonds of bondtype the jtype atom can have
      newtype = change the jtype atom to this type when maxbonds exist
    prob values = fraction seed
      fraction = create a bond with this probability if otherwise eligible
      seed = random number seed (positive integer)
    atype value = angletype
      angletype = type of created angles
    dtype value = dihedraltype
      dihedraltype = type of created dihedrals
    itype value = impropertype
      impropertype = type of created impropers
```

Examples:

```
fix 5 all bond/create 10 1 2 0.8 1
fix 5 all bond/create 1 3 3 0.8 1 prob 0.5 85784 iparam 2 3
fix 5 all bond/create 1 3 3 0.8 1 prob 0.5 85784 iparam 2 3 atype 1 dtype 2
```

Description:

Create bonds between pairs of atoms as a simulation runs according to specified criteria. This can be used to model cross-linking of polymers, the formation of a percolation network, etc. In this context, a bond means an interaction between a pair of atoms computed by the bond_style command. Once the bond is created it will be permanently in place. Optionally, the creation of a bond can also create angle, dihedral, and improper interactions that bond is part of. See the discussion of the *atype*, *dtype*, and *itype* keywords below.

This is different than a pairwise bond-order potential such as Tersoff or AIREBO which infers bonds and many-body interactions based on the current geometry of a small cluster of atoms and effectively creates and destroys bonds and higher-order many-body interactions from timestep to timestep as atoms move.

A check for possible new bonds is performed every *Nevery* timesteps. If two atoms I,J are within a distance *Rmin* of each other, if I is of atom type *itype*, if J is of atom type *jtype*, if both I and J are in the specified fix group, if a bond does not already exist between I and J, and if both I and J meet their respective *maxbond* requirement (explained below), then I,J is labeled as a "possible" bond pair.

If several atoms are close to an atom, it may have multiple possible bond partners. Every atom checks its list of possible bond partners and labels the closest such partner as its "sole" bond partner. After this is done, if atom I has atom J as its sole partner, and atom J has atom I as its sole partner, then the I,J bond is "eligible" to be formed.

Note that these rules mean an atom will only be part of at most one created bond on a given timestep. It also means that if atom I chooses atom J as its sole partner, but atom J chooses atom K is its sole partner (due to Rjk < Rij), then this means atom I will not form a bond on this timestep, even if it has other possible bond partners.

It is permissible to have *itype* = *jtype*. *Rmin* must be <= the pairwise cutoff distance between *itype* and *jtype* atoms, as defined by the pair_style command.

The *iparam* and *jparam* keywords can be used to limit the bonding functionality of the participating atoms. Each atom keeps track of how many bonds of *bondtype* it already has. If atom I of itype already has *maxbond* bonds (as set by the *iparam* keyword), then it will not form any more. Likewise for atom J. If *maxbond* is set to 0, then there is no limit on the number of bonds that can be formed with that atom.

The *newtype* value for *iparam* and *jparam* can be used to change the atom type of atom I or J when it reaches *maxbond* number of bonds of type *bondtype*. This means it can now interact in a pairwise fashion with other atoms in a different way by specifying different pair_coeff coefficients. If you do not wish the atom type to change, simply specify *newtype* as *itype* or *jtype*.

The *prob* keyword can also effect whether an eligible bond is actually created. The *fraction* setting must be a value between 0.0 and 1.0. A uniform random number between 0.0 and 1.0 is generated and the eligible bond is only created if the random number < fraction.

Any bond that is created is assigned a bond type of *bondtype*

When a bond is created, data structures within LAMMPS that store bond topology are updated to reflect the creation. If the bond is part of new 3-body (angle) or 4-body (dihedral, improper) interactions, you can choose to create new angles, dihedrals, impropers as well, using the *atype*, *dtype*, and *itype* keywords. All of these changes typically affect pairwise interactions between atoms that are now part of new bonds, angles, etc.

NOTE: One data structure that is not updated when a bond breaks are the molecule IDs stored by each atom. Even though two molecules become one moleclue due to the created bond, all atoms in the new moleclue retain their original molecule IDs.

If the *atype* keyword is used and if an angle potential is defined via the angle_style command, then any new 3-body interactions inferred by the creation of a bond will create new angles of type *angletype*, with parameters assigned by the corresponding angle_coeff command. Likewise, the *dtype* and *itype* keywords will create new dihedrals and impropers of type *dihedraltype* and *impropertype*.

NOTE: To create a new bond, the internal LAMMPS data structures that store this information must have space for it. When LAMMPS is initialized from a data file, the list of bonds is scanned and the maximum number of bonds per atom is tallied. If some atom will acquire more bonds than this limit as this fix operates, then the "extra bond per atom" parameter must be set to allow for it. Ditto for "extra angle per atom", "extra dihedral per atom", and "extra improper per atom" if angles, dihedrals, or impropers are being added when bonds are created. See the read_data or create_box command for more details. Note that a data file with no atoms can be used if you wish to add unbonded atoms via the create atoms command, e.g. for a percolation simulation.

NOTE: LAMMPS stores and maintains a data structure with a list of the 1st, 2nd, and 3rd neighbors of each atom (within the bond topology of the system) for use in weighting pairwise interactions for bonded atoms. Note that adding a single bond always adds a new 1st neighbor but may also induce *many* new 2nd and 3rd neighbors,

depending on the molecular topology of your system. The "extra special per atom" parameter must typically be set to allow for the new maximum total size (1st + 2nd + 3rd neighbors) of this per-atom list. There are 3 ways to do this. See the read_data or create_box or "special_bonds extra" commands for details.

NOTE: Even if you do not use the *atype*, *dtype*, or *itype* keywords, the list of topological neighbors is updated for atoms affected by the new bond. This in turn affects which neighbors are considered for pairwise interactions, using the weighting rules set by the special_bonds command. Consider a new bond created between atoms I,J. If J has a bonded neighbor K, then K becomes a 2nd neighbor of I. Even if the *atype* keyword is not used to create angle I-J-K, the pairwise interaction between I and K will be potentially turned off or weighted by the 1-3 weighting specified by the special_bonds command. This is the case even if the "angle yes" option was used with that command. The same is true for 3rd neighbors (1-4 interactions), the *dtype* keyword, and the "dihedral yes" option used with the special_bonds command.

Note that even if your simulation starts with no bonds, you must define a bond_style and use the bond_coeff command to specify coefficients for the *bondtype*. Similarly, if new atom types are specified by the *iparam* or *jparam* keywords, they must be within the range of atom types allowed by the simulation and pairwise coefficients must be specified for the new types.

Computationally, each timestep this fix operates, it loops over neighbor lists and computes distances between pairs of atoms in the list. It also communicates between neighboring processors to coordinate which bonds are created. Moreover, if any bonds are created, neighbor lists must be immediately updated on the same timestep. This is to insure that any pairwise interactions that should be turned "off" due to a bond creation, because they are now excluded by the presence of the bond and the settings of the special_bonds command, will be immediately recognized. All of these operations increase the cost of a timestep. Thus you should be cautious about invoking this fix too frequently.

You can dump out snapshots of the current bond topology via the dump local command.

NOTE: Creating a bond typically alters the energy of a system. You should be careful not to choose bond creation criteria that induce a dramatic change in energy. For example, if you define a very stiff harmonic bond and create it when 2 atoms are separated by a distance far from the equilibribum bond length, then the 2 atoms will oscillate dramatically when the bond is formed. More generally, you may need to thermostat your system to compensate for energy changes resulting from created bonds (and angles, dihedrals, impropers).

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes two statistics which it stores in a global vector of length 2, which can be accessed by various output commands. The vector values calculated by this fix are "intensive".

These are the 2 quantities:

- (1) # of bonds created on the most recent creation timestep
- (2) cummulative # of bonds created

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the MC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix bond/break, fix bond/swap, dump local, special_bonds

Default:

The option defaults are iparam = (0,itype), jparam = (0,jtype), and prob = 1.0.

fix bond/swap command

Syntax:

```
fix ID group-ID bond/swap Nevery fraction cutoff seed
```

- ID, group-ID are documented in fix command
- bond/swap = style name of this fix command
- Nevery = attempt bond swapping every this many steps
- fraction = fraction of group atoms to consider for swapping
- cutoff = distance at which swapping will be considered (distance units)
- seed = random # seed (positive integer)

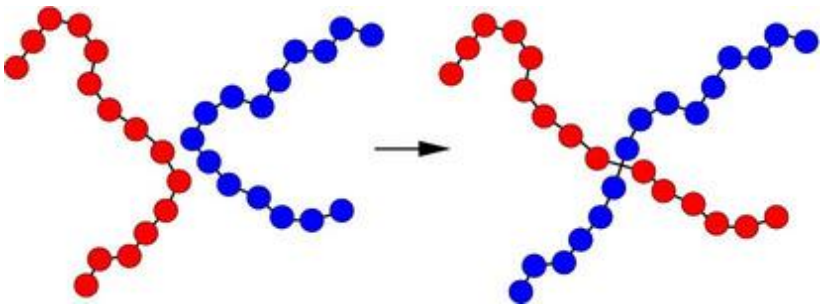
Examples:

```
fix 1 all bond/swap 50 0.5 1.3 598934
```

Description:

In a simulation of polymer chains, this command attempts to swap bonds between two different chains, effectively grafting the end of one chain onto another chain and vice versa. This is done via Monte Carlo rules using the Boltzmann acceptance criterion. The purpose is to equilibrate the polymer chain conformations more rapidly than dynamics alone would do it, by enabling instantaneous large conformational changes in a dense polymer melt. The polymer chains should thus more rapidly converge to the proper end-to-end distances and radii of gyration. It is designed for use with systems of FENE or harmonic bead-spring polymer chains where each polymer is a linear chain of monomers, but LAMMPS does not enforce this requirement, i.e. any bond_style can be used.

A schematic of the kinds of bond swaps that can occur is shown here:



On the left, the red and blue chains have two monomers A1 and B1 close to each other, which are currently bonded to monomers A2 and B2 respectively within their own chains. The bond swap operation will attempt to delete the A1-A2 and B1-B2 bonds and replace them with A1-B2 and B1-A2 bonds. If the swap is energetically favorable, the two chains on the right are the result and each polymer chain has undergone a dramatic conformational change. This reference, (Sides) provides more details on how the algorithm works and its application:

The bond swapping operation is invoked every *Nevery* timesteps. If any bond is swapped, a re-build of the neighbor lists is triggered, since a swap alters the list of which neighbors are considered for pairwise interaction. At each invocation, each processor considers a random specified *fraction* of its atoms as potential swapping monomers for this timestep. Choosing a small *fraction* value can reduce the likelihood of a reverse swap

occurring soon after an initial swap.

For each monomer A1, its neighbors are examined to find a possible B1 monomer. Both A1 and B1 must be in the fix group, their separation must be less than the specified *cutoff*, and the molecule IDs of A1 and B1 must be the same (see below). If a suitable partner is found, the energy change due to swapping the 2 bonds is computed. This includes changes in pairwise, bond, and angle energies due to the altered connectivity of the 2 chains. Dihedral and improper interactions are not allowed to be defined when this fix is used.

If the energy decreases due to the swap operation, the bond swap is accepted. If the energy increases it is accepted with probability exp(-delta/kT) where delta is the increase in energy, k is the Boltzmann constant, and T is the current temperature of the system. Whether the swap is accepted or rejected, no other swaps are attempted by this processor on this timestep.

The criterion for matching molecule IDs is how bond swaps performed by this fix conserve chain length. To use this features you must setup the molecule IDs for your polymer chains in a certain way, typically in the data file, read by the read_data comand. Consider a system of 6-mer chains. You have 2 choices. If the molecule IDs for monomers on each chain are set to 1,2,3,4,5,6 then swaps will conserve chain length. For a particular momoner there will be only one other monomer on another chain which is a potential swap partner. If the molecule IDs for monomers on each chain are set to 1,2,3,3,2,1 then swaps will conserve chain length but swaps will be able to occur at either end of a chain. Thus for a particular monomer there will be 2 possible swap partners on another chain. In this scenario, swaps can also occur within a single chain, i.e. the two ends of a chain swap with each other.

NOTE: If your simulation uses molecule IDs in the usual way, where all monomers on a single chain are assigned the same ID (different for each chain), then swaps will only occur within the same chain. If you assign the same molecule ID to all monomers in all chains then inter-chain swaps will occur, but they will not conserve chain length. Neither of these scenarios is probably what you want for this fix.

NOTE: When a bond swap occurs the image flags of monomers in the new polymer chains can become inconsistent. See the dump command for a discussion of image flags. This is not an issue for running dynamics, but can affect calculation of some diagnostic quantities or the printing of unwrapped coordinates to a dump file.

This fix computes a temperature each time it is invoked for use by the Boltzmann criterion. To do this, the fix creates its own compute of style *temp*, as if this command had been issued:

```
compute fix-ID_temp all temp
```

See the compute temp command for details. Note that the ID of the new compute is the fix-ID with underscore + "temp" appended and the group for the new compute is "all", so that the temperature of the entire system is used.

Note that this is NOT the compute used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp*. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the compute_modify command or print this temperature during thermodyanmic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* will have no effect on this fix.

Restart, fix_modify, thermo output, run start/stop, minimize info:

No information about this fix is written to binary restart files. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior. Also note that each processor generates possible swaps independently of other processors.

Thus if you repeat the same simulation on a different number of processors, the specific swaps performed will be different.

The fix_modify *temp* option is supported by this fix. You can use it to assign a compute you have defined to this fix which will be used to compute the temperature for the Boltzmann criterion.

This fix computes two statistical quantities as a global 2-vector of output, which can be accessed by various output commands. The first component of the vector is the cummulative number of swaps performed by all processors. The second component of the vector is the cummulative number of swaps attempted (whether accepted or rejected). Note that a swap "attempt" only occurs when swap partners meeting the criteria described above are found on a particular timestep. The vector values calculated by this fix are "intensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the MC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The setings of the "special_bond" command must be 0,1,1 in order to use this fix, which is typical of bead-spring chains with FENE or harmonic bonds. This means that pairwise interactions between bonded atoms are turned off, but are turned on between atoms two or three hops away along the chain backbone.

Currently, energy changes in dihedral and improper interactions due to a bond swap are not considered. Thus a simulation that uses this fix cannot use a dihedral or improper potential.

Related commands:

fix atom/swap

Default: none

(Sides) Sides, Grest, Stevens, Plimpton, J Polymer Science B, 42, 199-208 (2004).

fix box/relax command

Syntax:

```
fix ID group-ID box/relax keyword value ...
```

- ID, group-ID are documented in fix command
- box/relax = style name of this fix command

```
one or more keyword value pairs may be appended
keyword = iso or aniso or tri or x or y or z or xy or yz or xz or couple or nreset or vmax or
  iso or aniso or tri value = Ptarget = desired pressure (pressure units)
  x or y or z or xy or yz or xz value = Ptarget = desired pressure (pressure units)
  couple = none or xyz or xy or yz or xz
  nreset value = reset reference cell every this many minimizer iterations
  vmax value = fraction = max allowed volume change in one iteration
  dilate value = all or partial
  scaleyz value = yes or no = scale yz with lz
  scalexz value = yes or no = scale xz with lz
  scalexy value = yes or no = scale xy with ly
  fixedpoint values = x y z
    x,y,z = perform relaxation dilation/contraction around this point (distance units)
```

Examples:

```
fix 1 all box/relax iso 0.0 vmax 0.001
fix 2 water box/relax aniso 0.0 dilate partial
fix 2 ice box/relax tri 0.0 couple xy nreset 100
```

Description:

Apply an external pressure or stress tensor to the simulation box during an energy minimization. This allows the box size and shape to vary during the iterations of the minimizer so that the final configuration will be both an energy minimum for the potential energy of the atoms, and the system pressure tensor will be close to the specified external tensor. Conceptually, specifying a positive pressure is like squeezing on the simulation box; a negative pressure typically allows the box to expand.

The external pressure tensor is specified using one or more of the *iso*, *aniso*, *tri*, *x*, *y*, *z*, *xy*, *xz*, *yz*, and *couple* keywords. These keywords give you the ability to specify all 6 components of an external stress tensor, and to couple various of these components together so that the dimensions they represent are varied together during the mimimization.

Orthogonal simulation boxes have 3 adjustable dimensions (x,y,z). Triclinic (non-orthogonal) simulation boxes have 6 adjustable dimensions (x,y,z,xy,xz,yz). The create_box, read data, and read_restart commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the xy,xz,yz tilt factors.

The target pressures *Ptarget* for each of the 6 components of the stress tensor can be specified independently via the *x*, *y*, *z*, *xy*, *xz*, *yz* keywords, which correspond to the 6 simulation box dimensions. For example, if the *y* keyword is used, the y-box length will change during the minimization. If the *xy* keyword is used, the xy tilt factor will change. A box dimension will not change if that component is not specified.

Note that in order to use the *xy*, *xz*, or *yz* keywords, the simulation box must be triclinic, even if its initial tilt factors are 0.0.

When the size of the simulation box changes, all atoms are re-scaled to new positions, unless the keyword *dilate* is specified with a value of *partial*, in which case only the atoms in the fix group are re-scaled. This can be useful for leaving the coordinates of atoms in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

The *scaleyz*, *scalexz*, and *scalexy* keywords control whether or not the corresponding tilt factors are scaled with the associated box dimensions when relaxing triclinic periodic cells. The default values *yes* will turn on scaling, which corresponds to adjusting the linear dimensions of the cell while preserving its shape. Choosing *no* ensures that the tilt factors are not scaled with the box dimensions. See below for restrictions and default values in different situations. In older versions of LAMMPS, scaling of tilt factors was not performed. The old behavior can be recovered by setting all three scale keywords to *no*.

The *fixedpoint* keyword specifies the fixed point for cell relaxation. By default, it is the center of the box. Whatever point is chosen will not move during the simulation. For example, if the lower periodic boundaries pass through (0,0,0), and this point is provided to *fixedpoint*, then the lower periodic boundaries will remain at (0,0,0), while the upper periodic boundaries will move twice as far. In all cases, the particle positions at each iteration are unaffected by the chosen value, except that all particles are displaced by the same amount, different on each iteration.

NOTE: Appling an external pressure to tilt dimensions *xy*, *xz*, *yz* can sometimes result in arbitrarily large values of the tilt factors, i.e. a dramatically deformed simulation box. This typically indicates that there is something badly wrong with how the simulation was constructed. The two most common sources of this error are applying a shear stress to a liquid system or specifying an external shear stress tensor that exceeds the yield stress of the solid. In either case the minimization may converge to a bogus conformation or not converge at all. Also note that if the box shape tilts to an extreme shape, LAMMPS will run less efficiently, due to the large volume of communication needed to acquire ghost atoms around a processor's irregular-shaped sub-domain. For extreme values of tilt, LAMMPS may also lose atoms and generate an error.

NOTE: Performing a minimization with this fix is not a mathematically well-defined minimization problem. This is because the objective function being minimized changes if the box size/shape changes. In practice this means the minimizer can get "stuck" before you have reached the desired tolerance. The solution to this is to restart the minmizer from the new adjusted box size/shape, since that creates a new objective function valid for the new box size/shape. Repeat as necessary until the box size/shape has reached its new equilibrium.

The *couple* keyword allows two or three of the diagonal components of the pressure tensor to be "coupled" together. The value specified with the keyword determines which are coupled. For example, *xz* means the *Pxx* and *Pzz* components of the stress tensor are coupled. *Xyz* means all 3 diagonal components are coupled. Coupling means two things: the instantaneous stress will be computed as an average of the corresponding diagonal components, and the coupled box dimensions will be changed together in lockstep, meaning coupled dimensions will be dilated or contracted by the same percentage every timestep. The *Ptarget* values for any coupled dimensions must be identical. *Couple xyz* can be used for a 2d simulation; the *z* dimension is simply ignored.

The *iso*, *aniso*, and *tri* keywords are simply shortcuts that are equivalent to specifying several other keywords together.

The keyword *iso* means couple all 3 diagonal components together when pressure is computed (hydrostatic pressure), and dilate/contract the dimensions together. Using "iso Ptarget" is the same as specifying these 4

keywords:

```
x Ptarget
y Ptarget
z Ptarget
couple xyz
```

The keyword *aniso* means *x*, *y*, and *z* dimensions are controlled independently using the *Pxx*, *Pyy*, and *Pzz* components of the stress tensor as the driving forces, and the specified scalar external pressure. Using "aniso Ptarget" is the same as specifying these 4 keywords:

```
x Ptarget
y Ptarget
z Ptarget
couple none
```

The keyword *tri* means *x*, *y*, *z*, *xy*, *xz*, and *yz* dimensions are controlled independently using their individual stress components as the driving forces, and the specified scalar pressure as the external normal stress. Using "tri Ptarget" is the same as specifying these 7 keywords:

```
x Ptarget
y Ptarget
z Ptarget
xy 0.0
yz 0.0
xz 0.0
couple none
```

The *vmax* keyword can be used to limit the fractional change in the volume of the simulation box that can occur in one iteration of the minimizer. If the pressure is not settling down during the minimization this can be because the volume is fluctuating too much. The specified fraction must be greater than 0.0 and should be << 1.0. A value of 0.001 means the volume cannot change by more than 1/10 of a percent in one iteration when *couple xyz* has been specified. For any other case it means no linear dimension of the simulation box can change by more than 1/10 of a percent.

With this fix, the potential energy used by the minimizer is augmented by an additional energy provided by the fix. The overall objective function then is:

$$E = U + P_t \left(V - V_0 \right) + E_{strain}$$

where *U* is the system potential energy, *P*_t is the desired hydrostatic pressure, *V* and *V*_0 are the system and reference volumes, respectively. *E_strain* is the strain energy expression proposed by Parrinello and Rahman (Parrinello1981). Taking derivatives of *E* w.r.t. the box dimensions, and setting these to zero, we find that at the minimum of the objective function, the global system stress tensor **P** will satisfy the relation:

$$\mathbf{P} = P_t \mathbf{I} + \mathbf{S}_t \left(\mathbf{h}_0^{-1} \right)^t \mathbf{h}_{0d}$$

where **I** is the identity matrix, **h**_0 is the box dimension tensor of the reference cell, and **h**_0*d* is the diagonal part of **h**_0. **S**_*t* is a symmetric stress tensor that is chosen by LAMMPS so that the upper-triangular components of **P** equal the stress tensor specified by the user.

This equation only applies when the box dimensions are equal to those of the reference dimensions. If this is not the case, then the converged stress tensor will not equal that specified by the user. We can resolve this problem by periodically resetting the reference dimensions. The keyword *nreset_ref* controls how often this is done. If this keyword is not used, or is given a value of zero, then the reference dimensions are set to those of the initial simulation domain and are never changed. A value of *nstep* means that every *nstep* minimization steps, the reference dimensions are set to those of the current simulation domain. Note that resetting the reference dimensions changes the objective function and gradients, which sometimes causes the minimization to fail. This can be resolved by changing the value of *nreset*, or simply continuing the minimization from a restart file.

NOTE: As normally computed, pressure includes a kinetic- energy or temperature-dependent component; see the compute pressure command. However, atom velocities are ignored during a minimization, and the applied pressure(s) specified with this command are assumed to only be the virial component of the pressure (the non-kinetic portion). Thus if atoms have a non-zero temperature and you print the usual thermodynamic pressure, it may not appear the system is converging to your specified pressure. The solution for this is to either (a) zero the velocities of all atoms before performing the minimization, or (b) make sure you are monitoring the pressure without its kinetic component. The latter can be done by outputting the pressure from the fix this command creates (see below) or a pressure fix you define yourself.

NOTE: Because pressure is often a very sensitive function of volume, it can be difficult for the minimizer to equilibrate the system the desired pressure with high precision, particularly for solids. Some techniques that seem to help are (a) use the "min_modify line quadratic" option when minimizing with box relaxations, (b) minimize several times in succession if need be, to drive the pressure closer to the target pressure, (c) relax the atom positions before relaxing the box, and (d) relax the box to the target hydrostatic pressure before relaxing to a target shear stress state. Also note that some systems (e.g. liquids) will not sustain a non-hydrostatic applied pressure, which means the minimizer will not converge.

This fix computes a temperature and pressure each timestep. The temperature is used to compute the kinetic contribution to the pressure, even though this is subsequently ignored by default. To do this, the fix creates its own computes of style "temp" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp group-ID temp
compute fix-ID_press group-ID pressure fix-ID_temp virial
```

See the compute temp and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is the same as the fix group. Also note that the pressure compute does not include a kinetic component.

Note that these are NOT the computes used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the compute_modify command or print this temperature or pressure during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *temp* and *press* options are supported by this fix. You can use them to assign a compute you have

defined to this fix which will be used in its temperature and pressure calculation, as described above. Note that as described above, if you assign a pressure compute to this fix that includes a kinetic energy component it will affect the minimization, most likely in an undesirable way.

NOTE: If both the *temp* and *press* keywords are used in a single thermo_modify command (or in two separate commands), then the order in which the keywords are specified is important. Note that a pressure compute defines its own temperature compute as an argument when it is specified. The *temp* keyword will override this (for the pressure compute being used by fix npt), but only if the *temp* keyword comes after the *press* keyword. If the *temp* keyword comes before the *press* keyword, then the new pressure compute specified by the *press* keyword will be unaffected by the *temp* setting.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the pressure-volume energy, plus the strain energy, if it exists.

No parameter of this fix can be used with the *start/stop* keywords of the run command.

This fix is invoked during energy minimization, but not for the purpose of adding a contribution to the energy or forces being minimized. Instead it alters the simulation box geometry as described above.

Restrictions:

Only dimensions that are available can be adjusted by this fix. Non-periodic dimensions are not available. *z*, *xz*, and *yz*, are not available for 2D simulations. *xy*, *xz*, and *yz* are only available if the simulation domain is non-orthogonal. The create_box, read data, and read_restart commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the xy,xz,yz tilt factors.

The *scaleyz yes* and *scalexz yes* keyword/value pairs can not be used for 2D simulations. *scaleyz yes*, *scalexz yes*, and *scalexy yes* options can only be used if the 2nd dimension in the keyword is periodic, and if the tilt factor is not coupled to the barostat via keywords *tri*, *yz*, *xz*, and *xy*.

Related commands:

fix npt, minimize

Default:

The keyword defaults are dilate = all, vmax = 0.0001, nreset = 0.

(Parrinello1981) Parrinello and Rahman, J Appl Phys, 52, 7182 (1981).

fix colvars command

Syntax:

```
fix ID group-ID colvars configfile keyword values ...
```

- ID, group-ID are documented in fix command
- colvars = style name of this fix command
- configfile = the configuration file for the colvars module
- keyword = *input* or *output* or *seed* or *tstat*

```
  input arg = colvars.state file name or prefix or NULL (default: NULL)
    output arg = output filename prefix (default: out)
    seed arg = seed for random number generator (default: 1966)
    unwrap arg = yes or no
      use unwrapped coordinates in collective variables (default: yes)
    tstat arg = fix id of a thermostat or NULL (default: NULL)
```

Examples:

```
fix mtd all colvars peptide.colvars.inp seed 2122 input peptide.colvars.state output peptide
fix abf all colvars colvars.inp tstat 1
```

Description:

This fix interfaces LAMMPS to a "collective variables" or "colvars" module library which allows to calculate potentials of mean force (PMFs) for any set of colvars, using different sampling methods: currently implemented are the Adaptive Biasing Force (ABF) method, metadynamics, Steered Molecular Dynamics (SMD) and Umbrella Sampling (US) via a flexible harmonic restraint bias. The colvars library is hosted at http://colvars.github.io/

This documentation describes only the fix colvars command itself and LAMMPS specific parts of the code. The full documentation of the colvars library is available as this supplementary PDF document

A detailed discussion of the implementation of the portable collective variable library is in (Fiorin). Additional information can be found in (Henin).

There are some example scripts for using this package with LAMMPS in the examples/USER/colvars directory.

The only mandatory argument to the fix is the filename to the colvars input file that contains the input that is independent from the MD program in which the colvars library has been integrated.

The *group-ID* entry is ignored. The collective variable module will always apply to the entire system and there can only be one instance of the colvars fix at a time. The colvars fix will only communicate the minimum information necessary and the colvars library supports multiple, completely independent collective variables, so there is no restriction to functionaliry by limiting the number of colvars fixes.

The *input* keyword allows to specify a state file that would contain the restart information required in order to continue a calculation from a prerecorded state. Fix colvars records it state in binary restart files, so when using the read_restart command, this is usually not needed.

The *output* keyword allows to specify the output prefix. All output files generated will use this prefix followed by

the ".colvars." and a word like "state" or "traj".

The *seed* keyword contains the seed for the random number generator that will be used in the colvars module.

The *unwrap* keyword controls whether wrapped or unwrapped coordinates are passed to the colvars library for calculation of the collective variables and the resulting forces. The default is *yes*, i.e. to use the image flags to reconstruct the absolute atom positions. Setting this to *no* will use the current local coordinates that are wrapped back into the simulation cell at each re-neighboring instead.

The *tstat* keyword can be either NULL or the label of a thermostating fix that thermostats all atoms in the fix colvars group. This will be used to provide the colvars module with the current thermostat target temperature.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the current status of the colvars module into binary restart files. This is in addition to the text mode status file that is written by the colvars module itself and the kind of information in both files is identical.

The fix_modify *energy* option is supported by this fix to add the energy change from the biasing force added by the fix to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the cummulative energy change due to this fix. The scalar value calculated by this fix is "extensive".

Restrictions:

This fix is part of the USER-COLVARS package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

There can only be one colvars fix active at a time. Since the interface communicates only the minimum amount of information and colvars module itself can handle an arbitrary number of collective variables, this is not a limitation of functionality.

Related commands:

fix smd

Default:

The default options are input = NULL, output = out, seed = 1966, unwrap yes, and tstat = NULL.

(Fiorin) Fiorin , Klein, Henin, Mol. Phys., DOI:10.1080/00268976.2013.813594

(Henin) Henin, Fiorin, Chipot, Klein, J. Chem. Theory Comput., 6, 35-47 (2010)

fix deform command

fix deform/kk command

Syntax:

```
fix ID group-ID deform N parameter args ... keyword value ...
```

- ID, group-ID are documented in fix command
- deform = style name of this fix command
- N = perform box deformation every this many timesteps
- one or more parameter/arg pairs may be appended

```
parameter = x or y or z or xy or xz or yz
  x, y, z args = style value(s)
    style = final or delta or scale or vel or erate or trate or volume or wiggle or variable
      final values = lo hi
        lo hi = box boundaries at end of run (distance units)
      delta values = dlo dhi
        dlo dhi = change in box boundaries at end of run (distance units)
      scale values = factor
        factor = multiplicative factor for change in box length at end of run
      vel value = V
        V = change box length at this velocity (distance/time units),
            effectively an engineering strain rate
      erate value = R
        R = engineering strain rate (1/time units)
      trate value = R
        R = true strain rate (1/time units)
      volume value = none = adjust this dim to preserve volume of system
      wiggle values = A Tp
        A = amplitude of oscillation (distance units)
        Tp = period of oscillation (time units)
      variable values = v_name1 v_name2
        v_name1 = variable with name1 for box length change as function of time
        v_name2 = variable with name2 for change rate as function of time
  xy, xz, yz args = style value
    style = final or delta or vel or erate or trate or wiggle
      final value = tilt
        tilt = tilt factor at end of run (distance units)
      delta value = dtilt
        dtilt = change in tilt factor at end of run (distance units)
      vel value = V
        V = change tilt factor at this velocity (distance/time units),
            effectively an engineering shear strain rate
      erate value = R
        R = engineering shear strain rate (1/time units)
      trate value = R
        R = true shear strain rate (1/time units)
      wiggle values = A Tp
        A = amplitude of oscillation (distance units)
        Tp = period of oscillation (time units)
      variable values = v_name1 v_name2
        v_name1 = variable with name1 for tilt change as function of time
        v_name2 = variable with name2 for change rate as function of time
```

- zero or more keyword/value pairs may be appended
- keyword = *remap* or *flip* or *units*

```
      remap value = x or v or none
          x = remap coords of atoms in group into deforming box
          v = remap velocities of all atoms when they cross periodic boundaries
          none = no remapping of x or v
        flip value = yes or no
          allow or disallow box flips when it becomes highly skewed
        units value = lattice or box
          lattice = distances are defined in lattice units
          box = distances are defined in simulation box units
```

Examples:

```
fix 1 all deform 1 x final 0.0 9.0 z final 0.0 5.0 units box
fix 1 all deform 1 x trate 0.1 y volume z volume
fix 1 all deform 1 xy erate 0.001 remap v
fix 1 all deform 10 y delta -0.5 0.5 xz vel 1.0
```

Description:

Change the volume and/or shape of the simulation box during a dynamics run. Orthogonal simulation boxes have 3 adjustable parameters (x,y,z). Triclinic (non-orthogonal) simulation boxes have 6 adjustable parameters (x,y,z,xy,xz,yz). Any or all of them can be adjusted independently and simultaneously by this command. This fix can be used to perform non-equilibrium MD (NEMD) simulations of a continuously strained system. See the fix nvt/sllod and compute temp/deform commands for more details.

For the *x*, *y*, *z* parameters, the associated dimension cannot be shrink-wrapped. For the *xy*, *yz*, *xz* parameters, the associated 2nd dimension cannot be shrink-wrapped. Dimensions not varied by this command can be periodic or non-periodic. Dimensions corresponding to unspecified parameters can also be controlled by a fix npt or fix nph command.

The size and shape of the simulation box at the beginning of the simulation run were either specified by the create_box or read_data or read_restart command used to setup the simulation initially if it is the first run, or they are the values from the end of the previous run. The create_box, read data, and read_restart commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the xy,xz,yz tilt factors. If fix deform changes the xy,xz,yz tilt factors, then the simulation box must be triclinic, even if its initial tilt factors are 0.0.

As described below, the desired simulation box size and shape at the end of the run are determined by the parameters of the fix deform command. Every Nth timestep during the run, the simulation box is expanded, contracted, or tilted to ramped values between the initial and final values.

For the *x*, *y*, and *z* parameters, this is the meaning of their styles and values.

The *final*, *delta*, *scale*, *vel*, and *erate* styles all change the specified dimension of the box via "constant displacement" which is effectively a "constant engineering strain rate". This means the box dimension changes linearly with time from its initial to final value.

For style *final*, the final lo and hi box boundaries of a dimension are specified. The values can be in lattice or box distance units. See the discussion of the units keyword below.

For style *delta*, plus or minus changes in the lo/hi box boundaries of a dimension are specified. The values can be in lattice or box distance units. See the discussion of the units keyword below.

For style *scale*, a multiplicative factor to apply to the box length of a dimension is specified. For example, if the initial box length is 10, and the factor is 1.1, then the final box length will be 11. A factor less than 1.0 means

compression.

For style *vel*, a velocity at which the box length changes is specified in units of distance/time. This is effectively a "constant engineering strain rate", where rate = V/L0 and L0 is the initial box length. The distance can be in lattice or box distance units. See the discussion of the units keyword below. For example, if the initial box length is 100 Angstroms, and V is 10 Angstroms/psec, then after 10 psec, the box length will have doubled. After 20 psec, it will have tripled.

The *erate* style changes a dimension of the the box at a "constant engineering strain rate". The units of the specified strain rate are 1/time. See the units command for the time units associated with different choices of simulation units, e.g. picoseconds for "metal" units). Tensile strain is unitless and is defined as delta/L0, where L0 is the original box length and delta is the change relative to the original length. The box length L as a function of time will change as

```
L(t) = L0 (1 + erate*dt)
```

where dt is the elapsed time (in time units). Thus if *erate* R is specified as 0.1 and time units are picoseconds, this means the box length will increase by 10% of its original length every picosecond. I.e. strain after 1 psec = 0.1, strain after 2 psec = 0.2, etc. R = -0.01 means the box length will shrink by 1% of its original length every picosecond. Note that for an "engineering" rate the change is based on the original box length, so running with R = 1 for 10 picoseconds expands the box length by a factor of 11 (strain of 10), which is different that what the *trate* style would induce.

The *trate* style changes a dimension of the box at a "constant true strain rate". Note that this is not an "engineering strain rate", as the other styles are. Rather, for a "true" rate, the rate of change is constant, which means the box dimension changes non-linearly with time from its initial to final value. The units of the specified strain rate are 1/time. See the units command for the time units associated with different choices of simulation units, e.g. picoseconds for "metal" units). Tensile strain is unitless and is defined as delta/L0, where L0 is the original box length and delta is the change relative to the original length.

The box length L as a function of time will change as

```
L(t) = L0 exp(trate*dt)
```

where dt is the elapsed time (in time units). Thus if *trate* R is specified as ln(1.1) and time units are picoseconds, this means the box length will increase by 10% of its current (not original) length every picosecond. I.e. strain after 1 psec = 0.1, strain after 2 psec = 0.21, etc. R = ln(2) or ln(3) means the box length will double or triple every picosecond. R = ln(0.99) means the box length will shrink by 1% of its current length every picosecond. Note that for a "true" rate the change is continuous and based on the current length, so running with R = ln(2) for 10 picoseconds does not expand the box length by a factor of 11 as it would with *erate*, but by a factor of 1024 since the box length will double every picosecond.

Note that to change the volume (or cross-sectional area) of the simulation box at a constant rate, you can change multiple dimensions via *erate* or *trate*. E.g. to double the box volume in a picosecond picosecond, you could set "x erate M", "y erate M", "z erate M", with M = pow(2,1/3) - 1 = 0.26, since if each box dimension grows by 26%, the box volume doubles. Or you could set "x trate M", "y trate M", "z trate M", with M = ln(1.26) = 0.231, and the box volume would double every picosecond.

The *volume* style changes the specified dimension in such a way that the box volume remains constant while other box dimensions are changed explicitly via the styles discussed above. For example, "x scale 1.1 y scale 1.1 z volume" will shrink the z box length as the x,y box lengths increase, to keep the volume constant (product of x,y,z lengths). If "x scale 1.1 z volume" is specified and parameter *y* is unspecified, then the z box length will shrink as x increases to keep the product of x,z lengths constant. If "x scale 1.1 y volume z volume" is specified, then both

the y,z box lengths will shrink as x increases to keep the volume constant (product of x,y,z lengths). In this case, the y,z box lengths shrink so as to keep their relative aspect ratio constant.

For solids or liquids, note that when one dimension of the box is expanded via fix deform (i.e. tensile strain), it may be physically undesirable to hold the other 2 box lengths constant (unspecified by fix deform) since that implies a density change. Using the *volume* style for those 2 dimensions to keep the box volume constant may make more physical sense, but may also not be correct for materials and potentials whose Poisson ratio is not 0.5. An alternative is to use fix npt aniso with zero applied pressure on those 2 dimensions, so that they respond to the tensile strain dynamically.

The *wiggle* style oscillates the specified box length dimension sinusoidally with the specified amplitude and period. I.e. the box length L as a function of time is given by

```
L(t) = L0 + A sin(2*pi t/Tp)
```

where L0 is its initial length. If the amplitude A is a positive number the box initially expands, then contracts, etc. If A is negative then the box initially contracts, then expands, etc. The amplitude can be in lattice or box distance units. See the discussion of the units keyword below.

The *variable* style changes the specified box length dimension by evaluating a variable, which presumably is a function of time. The variable with *name1* must be an equal-style variable and should calculate a change in box length in units of distance. Note that this distance is in box units, not lattice units; see the discussion of the *units* keyword below. The formula associated with variable *name1* can reference the current timestep. Note that it should return the "change" in box length, not the absolute box length. This means it should evaluate to 0.0 when invoked on the initial timestep of the run following the definition of fix deform. It should evaluate to a value > 0.0 to dilate the box at future times, or a value < 0.0 to compress the box.

The variable *name2* must also be an equal-style variable and should calculate the rate of box length change, in units of distance/time, i.e. the time-derivative of the *name1* variable. This quantity is used internally by LAMMPS to reset atom velocities when they cross periodic boundaries. It is computed internally for the other styles, but you must provide it when using an arbitrary variable.

Here is an example of using the *variable* style to perform the same box deformation as the *wiggle* style formula listed above, where we assume that the current timestep = 0.

```
variable A equal 5.0
variable Tp equal 10.0
variable displace equal "v_A * sin(2*PI * step*dt/v_Tp)"
variable rate equal "2*PI*v_A/v_Tp * cos(2*PI * step*dt/v_Tp)"
fix 2 all deform 1 x variable v_displace v_rate remap v
```

For the *scale*, *vel*, *erate*, *trate*, *volume*, *wiggle*, and *variable* styles, the box length is expanded or compressed around its mid point.

For the *xy*, *xz*, and *yz* parameters, this is the meaning of their styles and values. Note that changing the tilt factors of a triclinic box does not change its volume.

The *final*, *delta*, *vel*, and *erate* styles all change the shear strain at a "constant engineering shear strain rate". This means the tilt factor changes linearly with time from its initial to final value.

For style *final*, the final tilt factor is specified. The value can be in lattice or box distance units. See the discussion of the units keyword below.

For style *delta*, a plus or minus change in the tilt factor is specified. The value can be in lattice or box distance units. See the discussion of the units keyword below.

For style *vel*, a velocity at which the tilt factor changes is specified in units of distance/time. This is effectively an "engineering shear strain rate", where rate = V/L0 and L0 is the initial box length perpendicular to the direction of shear. The distance can be in lattice or box distance units. See the discussion of the units keyword below. For example, if the initial tilt factor is 5 Angstroms, and the V is 10 Angstroms/psec, then after 1 psec, the tilt factor will be 15 Angstroms. After 2 psec, it will be 25 Angstroms.

The *erate* style changes a tilt factor at a "constant engineering shear strain rate". The units of the specified shear strain rate are 1/time. See the units command for the time units associated with different choices of simulation units, e.g. picoseconds for "metal" units). Shear strain is unitless and is defined as offset/length, where length is the box length perpendicular to the shear direction (e.g. y box length for xy deformation) and offset is the displacement distance in the shear direction (e.g. x direction for xy deformation) from the unstrained orientation.

The tilt factor T as a function of time will change as

```
T(t) = T0 + L0*erate*dt
```

where T0 is the initial tilt factor, L0 is the original length of the box perpendicular to the shear direction (e.g. y box length for xy deformation), and dt is the elapsed time (in time units). Thus if *erate* R is specified as 0.1 and time units are picoseconds, this means the shear strain will increase by 0.1 every picosecond. I.e. if the xy shear strain was initially 0.0, then strain after 1 psec = 0.1, strain after 2 psec = 0.2, etc. Thus the tilt factor would be 0.0 at time 0, 0.1*ybox at 1 psec, 0.2*ybox at 2 psec, etc, where ybox is the original y box length. R = 1 or 2 means the tilt factor will increase by 1 or 2 every picosecond. R = -0.01 means a decrease in shear strain by 0.01 every picosecond.

The *trate* style changes a tilt factor at a "constant true shear strain rate". Note that this is not an "engineering shear strain rate", as the other styles are. Rather, for a "true" rate, the rate of change is constant, which means the tilt factor changes non-linearly with time from its initial to final value. The units of the specified shear strain rate are 1/time. See the units command for the time units associated with different choices of simulation units, e.g. picoseconds for "metal" units). Shear strain is unitless and is defined as offset/length, where length is the box length perpendicular to the shear direction (e.g. y box length for xy deformation) and offset is the displacement distance in the shear direction (e.g. x direction for xy deformation) from the unstrained orientation.

The tilt factor T as a function of time will change as

```
T(t) = T0 exp(trate*dt)
```

where T0 is the initial tilt factor and dt is the elapsed time (in time units). Thus if *trate* R is specified as ln(1.1) and time units are picoseconds, this means the shear strain or tilt factor will increase by 10% every picosecond. I.e. if the xy shear strain was initially 0.1, then strain after 1 psec = 0.11, strain after 2 psec = 0.121, etc. R = ln(2) or ln(3) means the tilt factor will double or triple every picosecond. R = ln(0.99) means the tilt factor will shrink by 1% every picosecond. Note that the change is continuous, so running with R = ln(2) for 10 picoseconds does not change the tilt factor by a factor of 10, but by a factor of 1024 since it doubles every picosecond. Note that the initial tilt factor must be non-zero to use the *trate* option.

Note that shear strain is defined as the tilt factor divided by the perpendicular box length. The *erate* and *trate* styles control the tilt factor, but assume the perpendicular box length remains constant. If this is not the case (e.g. it changes due to another fix deform parameter), then this effect on the shear strain is ignored.

The *wiggle* style oscillates the specified tilt factor sinusoidally with the specified amplitude and period. I.e. the tilt factor T as a function of time is given by

```
T(t) = T0 + A sin(2*pi t/Tp)
```

where T0 is its initial value. If the amplitude A is a positive number the tilt factor initially becomes more positive, then more negative, etc. If A is negative then the tilt factor initially becomes more negative, then more positive, etc. The amplitude can be in lattice or box distance units. See the discussion of the units keyword below.

The *variable* style changes the specified tilt factor by evaluating a variable, which presumably is a function of time. The variable with *name1* must be an equal-style variable and should calculate a change in tilt in units of distance. Note that this distance is in box units, not lattice units; see the discussion of the *units* keyword below. The formula associated with variable *name1* can reference the current timestep. Note that it should return the "change" in tilt factor, not the absolute tilt factor. This means it should evaluate to 0.0 when invoked on the initial timestep of the run following the definition of fix deform.

The variable *name2* must also be an equal-style variable and should calculate the rate of tilt change, in units of distance/time, i.e. the time-derivative of the *name1* variable. This quantity is used internally by LAMMPS to reset atom velocities when they cross periodic boundaries. It is computed internally for the other styles, but you must provide it when using an arbitrary variable.

Here is an example of using the *variable* style to perform the same box deformation as the *wiggle* style formula listed above, where we assume that the current timestep = 0.

```
variable A equal 5.0
variable Tp equal 10.0
variable displace equal "v_A * sin(2*PI * step*dt/v_Tp)"
variable rate equal "2*PI*v_A/v_Tp * cos(2*PI * step*dt/v_Tp)"
fix 2 all deform 1 xy variable v_displace v_rate remap v
```

All of the tilt styles change the xy, xz, yz tilt factors during a simulation. In LAMMPS, tilt factors (xy,xz,yz) for triclinic boxes are normally bounded by half the distance of the parallel box length. See the discussion of the *flip* keyword below, to allow this bound to be exceeded, if desired.

For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = ..., -15, -5, 5, 15, 25, ... are all equivalent.

To obey this constraint and allow for large shear deformations to be applied via the *xy*, *xz*, or *yz* parameters, the following algorithm is used. If *prd* is the associated parallel box length (10 in the example above), then if the tilt factor exceeds the accepted range of -5 to 5 during the simulation, then the box is flipped to the other limit (an equivalent box) and the simulation continues. Thus for this example, if the initial xy tilt factor was 0.0 and "xy final 100.0" was specified, then during the simulation the xy tilt factor would increase from 0.0 to 5.0, the box would be flipped so that the tilt factor becomes -5.0, the tilt factor would increase from -5.0 to 5.0, the box would be flipped again, etc. The flip occurs 10 times and the final tilt factor at the end of the simulation would be 0.0. During each flip event, atoms are remapped into the new box in the appropriate manner.

The one exception to this rule is if the 1st dimension in the tilt factor (x for xy) is non-periodic. In that case, the limits on the tilt factor are not enforced, since flipping the box in that dimension does not change the atom positions due to non-periodicity. In this mode, if you tilt the system to extreme angles, the simulation will simply become inefficient due to the highly skewed simulation box.

Each time the box size or shape is changed, the *remap* keyword determines whether atom positions are remapped to the new box. If *remap* is set to *x* (the default), atoms in the fix group are remapped; otherwise they are not. Note that their velocities are not changed, just their positions are altered. If *remap* is set to *v*, then any atom in the

fix group that crosses a periodic boundary will have a delta added to its velocity equal to the difference in velocities between the lo and hi boundaries. Note that this velocity difference can include tilt components, e.g. a delta in the x velocity when an atom crosses the y periodic boundary. If *remap* is set to *none*, then neither of these remappings take place.

Conceptually, setting *remap* to *x* forces the atoms to deform via an affine transformation that exactly matches the box deformation. This setting is typically appropriate for solids. Note that though the atoms are effectively "moving" with the box over time, it is not due to their having a velocity that tracks the box change, but only due to the remapping. By contrast, setting *remap* to *v* is typically appropriate for fluids, where you want the atoms to respond to the change in box size/shape on their own and acquire a velocity that matches the box change, so that their motion will naturally track the box without explicit remapping of their coordinates.

NOTE: When non-equilibrium MD (NEMD) simulations are performed using this fix, the option "remap v" should normally be used. This is because fix nvt/sllod adjusts the atom positions and velocities to induce a velocity profile that matches the changing box size/shape. Thus atom coordinates should NOT be remapped by fix deform, but velocities SHOULD be when atoms cross periodic boundaries, since that is consistent with maintaining the velocity profile already created by fix nvt/sllod. LAMMPS will warn you if the *remap* setting is not consistent with fix nvt/sllod.

NOTE: For non-equilibrium MD (NEMD) simulations using "remap v" it is usually desirable that the fluid (or flowing material, e.g. granular particles) stream with a velocity profile consistent with the deforming box. As mentioned above, using a thermostat such as fix nvt/sllod or fix lavgevin (with a bias provided by compute temp/deform), will typically accomplish that. If you do not use a thermostat, then there is no driving force pushing the atoms to flow in a manner consistent with the deforming box. E.g. for a shearing system the box deformation velocity may vary from 0 at the bottom to 10 at the top of the box. But the stream velocity profile of the atoms may vary from -5 at the bottom to +5 at the top. You can monitor these effects using the fix ave/spatial, compute temp/deform, and compute temp/profile commands. One way to induce atoms to stream consistent with the box deformation is to give them an initial velocity profile, via the velocity ramp command, that matches the box deformation rate. This also typically helps the system come to equilibrium more quickly, even if a thermostat is used.

NOTE: If a fix rigid is defined for rigid bodies, and *remap* is set to *x*, then the center-of-mass coordinates of rigid bodies will be remapped to the changing simulation box. This will be done regardless of whether atoms in the rigid bodies are in the fix deform group or not. The velocity of the centers of mass are not remapped even if *remap* is set to *v*, since fix nvt/sllod does not currently do anything special for rigid particles. If you wish to perform a NEMD simulation of rigid particles, you can either thermostat them independently or include a background fluid and thermostat the fluid via fix nvt/sllod.

The *flip* keyword allows the tilt factors for a triclinic box to exceed half the distance of the parallel box length, as discussed above. If the *flip* value is set to *yes*, the bound is enforced by flipping the box when it is exceeded. If the *flip* value is set to *no*, the tilt will continue to change without flipping. Note that if you apply large deformations, this means the box shape can tilt dramatically LAMMPS will run less efficiently, due to the large volume of communication needed to acquire ghost atoms around a processor's irregular-shaped sub-domain. For extreme values of tilt, LAMMPS may also lose atoms and generate an error.

The *units* keyword determines the meaning of the distance units used to define various arguments. A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacing. Note that the units choice also affects the *vel* style parameters since it is defined in terms of distance/time. Also note that the units keyword does not affect the *variable* style. You should use the *xlat*, *ylat*, *zlat* keywords of the thermo_style command if you want to include lattice spacings in a variable formula.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands.

This fix can perform deformation over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

You cannot apply x, y, or z deformations to a dimension that is shrink-wrapped via the boundary comamnd.

You cannot apply xy, yz, or xz deformations to a 2nd dimension (y in xy) that is shrink-wrapped via the boundary comamnd.

Related commands:

change_box

Default:

The option defaults are remap = x, flip = yes, and units = lattice.

fix deposit command

Syntax:

```
fix ID group-ID deposit N type M seed keyword values ...
```

- ID, group-ID are documented in fix command
- deposit = style name of this fix command
- N = # of atoms or molecules to insert
- type = atom type to assign to inserted atoms (offset for moleclue insertion)
- M = insert a single atom or molecule every M steps
- seed = random # seed (positive integer)
- one or more keyword/value pairs may be appended to args
- keyword = *region* or *id* or *global* or *local* or *near* or *attempt* or *rate* or *vx* or *vy* or *vz* or *mol* or *rigid* or *shake* or *units*

```
region value = region-ID
    region-ID = ID of region to use as insertion volume
  id value = max or next
    max = atom ID for new atom(s) is max ID of all current atoms plus one
    next = atom ID for new atom(s) increments by one for every deposition
  global values = lo hi
    lo,hi = put new atom/molecule a distance lo-hi above all other atoms (distance units)
  local values = lo hi delta
    lo,hi = put new atom/molecule a distance lo-hi above any nearby atom beneath it (distance
    delta = lateral distance within which a neighbor is considered "nearby" (distance units)
  near value = R
    R = only insert atom/molecule if further than R from existing particles (distance units)
  attempt value = Q
    Q = attempt a single insertion up to Q times
  rate value = V
    V = z velocity (y in 2d) at which insertion volume moves (velocity units)
  vx values = vxlo vxhi
    vxlo,vxhi = range of x velocities for inserted atom/molecule (velocity units)
  vy values = vylo vyhi
    vylo,vyhi = range of y velocities for inserted atom/molecule (velocity units)
  vz values = vzlo vzhi
    vzlo,vzhi = range of z velocities for inserted atom/molecule (velocity units)
  target values = tx ty tz
    tx,ty,tz = location of target point (distance units)
  mol value = template-ID
    template-ID = ID of molecule template specified in a separate molecule command
  molfrac values = f1 f2 ... fN
    f1 to fN = relative probability of creating each of N molecules in template-ID
  rigid value = fix-ID
    fix-ID = ID of fix rigid/small command
  shake value = fix-ID
    fix-ID = ID of fix shake command
  units value = lattice or box
    lattice = the geometry is defined in lattice units
    box = the geometry is defined in simulation box units
```

Examples:

```
fix 3 all deposit 1000 2 100 29494 region myblock local 1.0 1.0 1.0 units box
fix 2 newatoms deposit 10000 1 500 12345 region disk near 2.0 vz -1.0 -0.8
fix 4 sputter deposit 1000 2 500 12235 region sphere vz -1.0 -1.0 target 5.0 5.0 0.0 units lattice
```

Description:

Insert a single atom or molecule into the simulation domain every M timesteps until N atoms or molecules have been inserted. This is useful for simulating deposition onto a surface. For the remainder of this doc page, a single inserted atom or molecule is referred to as a "particle".

If inserted particles are individual atoms, they are assigned the specified atom type. If they are molecules, the type of each atom in the inserted molecule is specified in the file read by the molecule command, and those values are added to the specified atom type. E.g. if the file specifies atom types 1,2,3, and those are the atom types you want for inserted molecules, then specify *type* = 0. If you specify *type* = 2, the in the inserted molecule will have atom types 3,4,5.

All atoms in the inserted particle are assigned to two groups: the default group "all" and the group specified in the fix deposit command (which can also be "all").

If you are computing temperature values which include inserted particles, you will want to use the compute_modify dynamic option, which insures the current number of atoms is used as a normalizing factor each time the temperature is computed.

Care must be taken that inserted particles are not too near existing atoms, using the options described below. When inserting particles above a surface in a non-periodic box (see the boundary command), the possibility of a particle escaping the surface and flying upward should be considered, since the particle may be lost or the box size may grow infinitely large. A fix wall/reflect command can be used to prevent this behavior. Note that if a shrink-wrap boundary is used, it is OK to insert the new particle outside the box, however the box will immediately be expanded to include the new particle. When simulating a sputtering experiment it is probably more realistic to ignore those atoms using the thermo_modify command with the *lost ignore* option and a fixed boundary.

The fix deposit command must use the *region* keyword to define an insertion volume. The specified region must have been previously defined with a region command. It must be defined with side = *in*.

NOTE: LAMMPS checks that the specified region is wholly inside the simulation box. It can do this correctly for orthonormal simulation boxes. However for triclinic boxes, it only tests against the larger orthonormal box that bounds the tilted simulation box. If the specified region includes volume outside the tilted box, then an insertion will likely fail, leading to a "lost atoms" error. Thus for triclinic boxes you should insure the specified region is wholly inside the simulation box.

Individual atoms are inserted, unless the *mol* keyword is used. It specifies a *template-ID* previously defined using the molecule command, which reads files that define one or more molecules. The coordinates, atom types, charges, etc, as well as any bond/angle/etc and special neighbor information for the molecule can be specified in the molecule file. See the molecule command for details. The only settings required to be in each file are the coordinates and types of atoms in the molecule.

If the molecule template contains more than one molecule, the relative probability of depositing each molecule can be specified by the *molfrac* keyword. N relative probablities, each from 0.0 to 1.0, are specified, where N is the number of molecules in the template. Each time a molecule is deposited, a random number is used to sample from the list of relative probabilities. The N values must sum to 1.0.

If you wish to insert molecules via the *mol* keyword, that will be treated as rigid bodies, use the *rigid* keyword, specifying as its value the ID of a separate fix rigid/small command which also appears in your input script.

If you wish to insert molecules via the *mol* keyword, that will have their bonds or angles constrained via SHAKE,

use the *shake* keyword, specifying as its value the ID of a separate fix shake command which also appears in your input script.

Each timestep a particle is inserted, the coordinates for its atoms are chosen as follows. For insertion of individual atoms, the "position" referred to in the following description is the coordinate of the atom. For insertion of molecule, the "position" is the geometric center of the molecule; see the molecule doc page for details. A random rotation of the molecule around its center point is performed, which determines the coordinates all the individual atoms.

A random position within the region insertion volume is generated. If neither the *global* or *local* keyword is used, the random position is the trial position. If the *global* keyword is used, the random x,y values are used, but the z position of the new particle is set above the highest current atom in the simulation by a distance randomly chosen between lo/hi. (For a 2d simulation, this is done for the y position.) If the *local* keyword is used, the z position is set a distance between lo/hi above the highest current atom in the simulation that is "nearby" the chosen x,y position. In this context, "nearby" means the lateral distance (in x,y) between the new and old particles is less than the *delta* setting.

Once a trial x,y,z position has been selected, the insertion is only performed if no current atom in the simulation is within a distance R of any atom in the new particle, including the effect of periodic boundary conditions if applicable. R is defined by the *near* keyword. Note that the default value for R is 0.0, which will allow atoms to strongly overlap if you are inserting where other atoms are present. This distance test is performed independently for each atom in an inserted molecule, based on the randomly rotated configuration of the molecule. If this test fails, a new random position within the insertion volume is chosen and another trial is made. Up to Q attempts are made. If the particle is not successfully inserted, LAMMPS prints a warning message.

NOTE: If you are inserting finite size particles or a molecule or rigid body consisting of finite-size particles, then you should typically set R larger than the distance at which any inserted particle may overlap with either a previouly inserted particle or an existing particle. LAMMPS will issue a warning if R is smaller than this value, based on the radii of existing and inserted particles.

The *rate* option moves the insertion volume in the z direction (3d) or y direction (2d). This enables particles to be inserted from a successively higher height over time. Note that this parameter is ignored if the *global* or *local* keywords are used, since those options choose a z-coordinate for insertion independently.

The vx, vy, and vz components of velocity for the inserted particle are set using the values specified for the *vx*, *vy*, and *vz* keywords. Note that normally, new particles should be a assigned a negative vertical velocity so that they move towards the surface. For molecules, the same velocity is given to every particle (no rotation or bond vibration).

If the *target* option is used, the velocity vector of the inserted particle is changed so that it points from the insertion position towards the specified target point. The magnitude of the velocity is unchanged. This can be useful, for example, for simulating a sputtering process. E.g. the target point can be far away, so that all incident particles strike the surface as if they are in an incident beam of particles at a prescribed angle.

The *id* keyword determines how atom IDs and molecule IDs are assigned to newly deposited particles. Molecule IDs are only assigned if molecules are being inserted. For the *max* setting, the atom and molecule IDs of all current atoms are checked. Atoms in the new particle are assigned IDs starting with the current maximum plus one. If a molecule is inserted it is assigned an ID = current maximum plus one. This means that if particles leave the system, the new IDs may replace the lost ones. For the *next* setting, the maximum ID of any atom and molecule is stored at the time the fix is defined. Each time a new particle is added, this value is incremented to assign IDs to the new atom(s) or molecule. Thus atom and molecule IDs for deposited particles will be consecutive even if particles leave the system over time.

The *units* keyword determines the meaning of the distance units used for the other deposition parameters. A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacing. Note that the units choice affects all the keyword values that have units of distance or velocity.

NOTE: If you are monitoring the temperature of a system where the atom count is changing due to adding particles, you typically should use the compute_modify dynamic yes command for the temperature compute you are using.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the deposition to binary restart files. This includes information about how many particles have been depositied, the random number generator seed, the next timestep for deposition, etc. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The specified insertion region cannot be a "dynamic" region, as defined by the region command.

Related commands:

fix_pour, region

Default:

Insertions are performed for individual atoms, i.e. no *mol* setting is defined. If the *mol* keyword is used, the default for *molfrac* is an equal probabilities for all molecules in the template. Additional option defaults are id = max, delta = 0.0, near = 0.0, attempt = 10, rate = 0.0, vx = 0.0 0.0, vy = 0.0 0.0, vz = 0.0 0.0, and units = lattice.

fix drag command

Syntax:

```
fix ID group-ID drag x y z fmag delta
```

- ID, group-ID are documented in fix command
- drag = style name of this fix command
- x,y,z = coord to drag atoms towards
- fmag = magnitude of force to apply to each atom (force units)
- delta = cutoff distance inside of which force is not applied (distance units)

Examples:

```
fix center small-molecule drag 0.0 10.0 0.0 5.0 2.0
```

Description:

Apply a force to each atom in a group to drag it towards the point (x,y,z). The magnitude of the force is specified by fmag. If an atom is closer than a distance delta to the point, then the force is not applied.

Any of the x,y,z values can be specified as NULL which means do not include that dimension in the distance calculation or force application.

This command can be used to steer one or more atoms to a new location in the simulation.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global 3-vector of forces, which can be accessed by various output commands. This is the total force on the group of atoms by the drag force. The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

fix spring, fix spring/self, fix spring/rg, fix smd

Default: none

fix drude command

Syntax:

```
fix ID group-ID drude flag1 flag2 ... flagN
```

- ID, group-ID are documented in fix command
- drude = style name of this fix command
- flag1 flag2 ... flagN = Drude flag for each atom type (1 to N) in the system

Examples:

```
fix 1 all drude 1 1 0 1 0 2 2 2
fix 1 all drude C C N C N D D D
```

Description:

Assign each atom type in the system to be one of 3 kinds of atoms within the Drude polarization model. This fix is designed to be used with the thermalized Drude oscillator model. Polarizable models in LAMMPS are described in this Section.

The three possible types can be designated with an integer (0,1,2) or capital letter (N,C,D):

- 0 or N = non-polarizable atom (not part of Drude model)
- 1 or C = Drude core
- 2 or D = Drude electron

Restrictions:

This fix should be invoked before any other commands that implement the Drude oscillator model, such as fix langevin/drude, fix drude/transform, compute temp/drude, pair_style thole.

Related commands:

fix langevin/drude, fix drude/transform, compute temp/drude, pair_style thole

Default: None

fix drude/transform/direct command

fix drude/transform/inverse command

Syntax:

```
fix ID group-ID style keyword value ...
```

- ID, group-ID are documented in fix command
- style = *drude/transform/direct* or *drude/transform/inverse*

Examples:

```
fix 3 all drude/transform/direct
fix 1 all drude/transform/inverse
```

Description:

Transform the coordinates of Drude oscillators from real to reduced and back for thermalizing the Drude oscillators as described in (Lamoureux) using a Nose-Hoover thermostat. This fix is designed to be used with the thermalized Drude oscillator model. Polarizable models in LAMMPS are described in this Section.

Drude oscillators are a pair of atoms representing a single polarizable atom. Ideally, the mass of Drude particles would vanish and their positions would be determined self-consistently by iterative minimization of the energy, the cores' positions being fixed. It is however more efficient and it yields comparable results, if the Drude oscillators (the motion of the Drude particle relative to the core) are thermalized at a low temperature. In that case, the Drude particles need a small mass.

The thermostats act on the reduced degrees of freedom, which are defined by the following equations. Note that in these equations upper case denotes atomic or center of mass values and lower case denotes Drude particle or dipole values. Primes denote the transformed (reduced) values, while bare letters denote the original values.

Masses: \begin{equation} M' = M + m \end{equation} \begin{equation} m' = \frac {M\, m } {M'} \end{equation} Positions: \begin{equation} X' = \frac {M\, X + m\, x} {M'} \end{equation} \begin{equation} x' = x - X \end{equation} Velocities: \begin{equation} V' = \frac {M\, V + m\, v} {M'} \end{equation} \begin{equation} v' = v - V \end{equation} Forces: \begin{equation} F' = F + f \end{equation} \begin{equation} f' = \frac { M\, f - m\, F} {M'} \end{equation}

This transform conserves the total kinetic energy \begin{equation} \frac 1 2 \, (M\, V^2\ + m\, v^2) = \frac 1 2 \, (M'\, V'^2\ + m'\, v'^2) \end{equation} and the virial defined with absolute positions \begin{equation} X\, F + x\, f = X'\, F' + x'\, f' \end{equation}

This fix requires each atom know whether it is a Drude particle or not. You must therefore use the fix drude command to specify the Drude status of each atom type.

NOTE: only the Drude core atoms need to be in the group specified for this fix. A Drude electron will be transformed together with its core even if it is not itself in the group. It is safe to include Drude electrons or non-polarizable atoms in the group. The non-polarizable atoms will simply not be transformed.

This fix does NOT perform time integration. It only transform masses, coordinates, velocities and forces. Thus you must use separate time integration fixes, like fix nve or fix npt to actually update the velocities and positions of atoms. In order to thermalize the reduced degrees of freedom at different temperatures, two Nose-Hoover thermostats must be defined, acting on two distinct groups.

NOTE: The *fix drude/transform/direct* command must appear before any Nose-Hoover thermostating fixes. The *fix drude/transform/inverse* command must appear after any Nose-Hoover thermostating fixes.

Example:

```
fix fDIRECT all drude/transform/direct
fix fNVT gCORES nvt temp 300.0 300.0 100
fix fNVT gDRUDES nvt temp 1.0 1.0 100
fix fINVERSE all drude/transform/inverse
compute TDRUDE all temp/drude
thermo_style custom step cpu etotal ke pe ebond ecoul elong press vol temp c_TDRUDE[1] c_TDRUDE[2]
```

In this example, *gCORES* is the group of the atom cores and *gDRUDES* is the group of the Drude particles (electrons). The centers of mass of the Drude oscillators will be thermostated at 300.0 and the internal degrees of freedom will be thermostated at 1.0. The temperatures of cores and Drude particles, in center-of-mass and relative coordinates, are calculated using compute temp/drude

In addition, if you want to use a barostat to simulate a system at constant pressure, only one of the Nose-Hoover fixes must be *npt*, the other one should be *nvt*. You must add a *compute temp/com* and a *fix_modify* command so that the temperature of the *npt* fix be just that of its group (the Drude cores) but the pressure be the overall pressure *thermo_press*.

Example:

```
compute cTEMP_CORE gCORES temp/com
fix fDIRECT all drude/transform/direct
fix fNPT gCORES npt temp 298.0 298.0 100 iso 1.0 1.0 500
fix_modify fNPT temp cTEMP_CORE press thermo_press
fix fNVT gDRUDES nvt temp 5.0 5.0 100
fix fINVERSE all drude/transform/inverse
```

In this example, *gCORES* is the group of the atom cores and *gDRUDES* is the group of the Drude particles. The centers of mass of the Drude oscillators will be thermostated at 298.0 and the internal degrees of freedom will be thermostated at 5.0. The whole system will be barostated at 1.0.

In order to avoid the flying ice cube problem (irreversible transfer of linear momentum to the center of mass of the system), you may need to add a *fix momentum* command:

```
fix fMOMENTUM all momentum 100 linear 1 1 1
```

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

Restrictions: none

Related commands:

fix drude, fix langevin/drude, compute temp/drude, pair_style thole

Default: none

(Lamoureux) Lamoureux and Roux, J Chem Phys, 119, 3025-3039 (2003).

fix dt/reset command

Syntax:

```
fix ID group-ID dt/reset N Tmin Tmax Xmax keyword values ...
```

- ID, group-ID are documented in fix command
- dt/reset = style name of this fix command
- N = recompute dt every N timesteps
- Tmin = minimum dt allowed which can be NULL (time units)
- Tmax = maximum dt allowed which can be NULL (time units)
- Xmax = maximum distance for an atom to move in one timestep (distance units)
- zero or more keyword/value pairs may be appended
- keyword = *units*

```
units value = lattice or box
    lattice = Xmax is defined in lattice units
    box = Xmax is defined in simulation box units
```

Examples:

```
fix 5 all dt/reset 10 1.0e-5 0.01 0.1
fix 5 all dt/reset 10 0.01 2.0 0.2 units box
```

Description:

Reset the timestep size every N steps during a run, so that no atom moves further than Xmax, based on current atom velocities and forces. This can be useful when starting from a configuration with overlapping atoms, where forces will be large. Or it can be useful when running an impact simulation where one or more high-energy atoms collide with a solid, causing a damage cascade.

This fix overrides the timestep size setting made by the timestep command. The new timestep size *dt* is computed in the following manner.

For each atom, the timestep is computed that would cause it to displace *Xmax* on the next integration step, as a function of its current velocity and force. Since performing this calculation exactly would require the solution to a quartic equation, a cheaper estimate is generated. The estimate is conservative in that the atom's displacement is guaranteed not to exceed *Xmax*, though it may be smaller.

Given this putative timestep for each atom, the minimum timestep value across all atoms is computed. Then the *Tmin* and *Tmax* bounds are applied, if specified. If one (or both) is specified as NULL, it is not applied.

When the run style is *respa*, this fix resets the outer loop (largest) timestep, which is the same timestep that the timestep command sets.

Note that the cumulative simulation time (in time units), which accounts for changes in the timestep size as a simulation proceeds, can be accessed by the thermo_style time keyword.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global scalar which can be accessed by various output commands. The scalar stores the last timestep on which the timestep was reset to a new value.

The scalar value calculated by this fix is "intensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

timestep

Default:

The option defaults is units = lattice.

fix efield command

Syntax:

```
fix ID group-ID efield ex ey ez keyword value ...
```

- ID, group-ID are documented in fix command
- efield = style name of this fix command
- ex,ey,ez = E-field component values (electric field units)
- any of ex,ey,ez can be a variable (see below)
- zero or more keyword/value pairs may be appended to args
- keyword = *region* or *energy*

```
  region value = region-ID
      region-ID = ID of region atoms must be in to have added force
    energy value = v_name
      v_name = variable with name that calculates the potential energy of each atom in the added
```

Examples:

```
fix kick external-field efield 1.0 0.0 0.0
fix kick external-field efield 0.0 0.0 v_oscillate
```

Description:

Add a force F = qE to each charged atom in the group due to an external electric field being applied to the system. If the system contains point-dipoles, also add a torque on the dipoles due to the external electric field.

For charges, any of the 3 quantities defining the E-field components can be specified as an equal-style or atom-style variable, namely *ex*, *ey*, *ez*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the E-field component.

For point-dipoles, equal-style variables can be used, but atom-style variables are not currently supported, since they imply a spatial gradient in the electric field which means additional terms with gradients of the field are required for the force and torque on dipoles.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent E-field.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent E-field with optional time-dependence as well.

If the *region* keyword is used, the atom must also be in the specified geometric region in order to have force added to it.

Adding a force or torque to atoms implies a change in their potential energy as they move or rotate due to the applied E-field.

For dynamics via the "run" command, this energy can be optionally added to the system's potential energy for thermodynamic output (see below). For energy minimization via the "minimize" command, this energy must be added to the system's potential energy to formulate a self-consistent minimization problem (see below).

The *energy* keyword is not allowed if the added field is a constant vector (ex,ey,ez), with all components defined as numeric constants and not as variables. This is because LAMMPS can compute the energy for each charged particle directly as E = -x dot qE = -q (x*ex + y*ey + z*ez), so that -Grad(E) = F. Similarly for point-dipole particles the energy can be computed as E = -mu dot E = -(mux*ex + muy*ey + muz*ez).

The *energy* keyword is optional if the added force is defined with one or more variables, and if you are performing dynamics via the run command. If the keyword is not used, LAMMPS will set the energy to 0.0, which is typically fine for dynamics.

The *energy* keyword is required if the added force is defined with one or more variables, and you are performing energy minimization via the "minimize" command for charged particles. It is not required for point-dipoles, but a warning is issued since the minimizer in LAMMPS does not rotate dipoles, so you should not expect to be able to minimize the orientation of dipoles in an applied electric field.

The *energy* keyword specifies the name of an atom-style variable which is used to compute the energy of each atom as function of its position. Like variables used for *ex*, *ey*, *ez*, the energy variable is specified as v_name, where name is the variable name.

Note that when the *energy* keyword is used during an energy minimization, you must insure that the formula defined for the atom-style variable is consistent with the force variable formulas, i.e. that -Grad(E) = F. For example, if the force due to the electric field were a spring-like F = kx, then the energy formula should be E = -0.5kx^2. If you don't do this correctly, the minimization will not converge properly.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *energy* option is supported by this fix to add the potential "energy" inferred by the added force due to the electric field to the system's potential energy as part of thermodynamic output. This is a fictitious quantity but is needed so that the minimize command can include the forces added by this fix in a consistent manner. I.e. there is a decrease in potential energy when atoms move in the direction of the added force due to the electric field.

This fix computes a global scalar and a global 3-vector of forces, which can be accessed by various output commands. The scalar is the potential energy discussed above. The vector is the total force added to the group of atoms. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command. You should not specify force components with a variable that has time-dependence for use with a minimizer, since the minimizer increments the timestep as the iteration count during the minimization.

NOTE: If you want the fictitious potential energy associated with the added forces to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the fix_modify *energy* option for this fix.

Restrictions:

This fix is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix addforce

Default: none

fix enforce2d command

fix enforce2d/cuda command

Syntax:

```
fix ID group-ID enforce2d
```

- ID, group-ID are documented in fix command
- enforce2d = style name of this fix command

Examples:

```
fix 5 all enforce2d
```

Description:

Zero out the z-dimension velocity and force on each atom in the group. This is useful when running a 2d simulation to insure that atoms do not move from their initial z coordinate.

Styles with a *cuda* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command.

Restrictions: none

Related commands: none

Default: none

fix eos/cv command

Syntax:

```
fix ID group-ID eos/cv cv
```

- ID, group-ID are documented in fix command
- eos/cv = style name of this fix command
- cv = constant-volume heat capacity (energy/temperature units)

Examples:

```
fix 1 all eos/cv 0.01
```

Description:

Fix *eos/cv* applies a mesoparticle equation of state to relate the particle internal energy (u_i) to the particle internal temperature (dpdTheta_i). The *eos/cv* mesoparticle equation of state requires the constant-volume heat capacity, and is defined as follows:

$$u_i = u_i^{mech} + u_i^{cond} = C_V \theta_i$$

where Cv is the constant-volume heat capacity, u_cond is the internal conductive energy, and u_mech is the internal mechanical energy. Note that alternative definitions of the mesoparticle equation of state are possible.

Restrictions:

The fix *eos/cv* is only available if LAMMPS is built with the USER-DPD package.

Related commands:

fix shardlow, pair dpd/fdt

Default: none

(Larentzos) J.P. Larentzos, J.K. Brennan, J.D. Moore, and W.D. Mattson, "LAMMPS Implementation of Constant Energy Dissipative Particle Dynamics (DPD-E)", ARL-TR-6863, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD (2014).

fix eos/table command

Syntax:

```
fix ID group-ID eos/table style file N keyword
```

- ID, group-ID are documented in fix command
- eos/table = style name of this fix command
- style = *linear* = method of interpolation
- file = filename containing the tabulated equation of state
- N = use N values in *linear* tables
- keyword = name of table keyword correponding to table file

Examples:

```
fix 1 all eos/table linear eos.table 100000 KEYWORD
```

Description:

Fix *eos/table* applies a tabulated mesoparticle equation of state to relate the particle internal energy (u_i) to the particle internal temperature (dpdTheta_i).

Fix *eos/table* creates interpolation tables of length *N* from internal energy values listed in a file as a function of internal temperature.

The interpolation tables are created by fitting cubic splines to the file values and interpolating energy values at each of *N* internal temperatures, and vice-versa. During a simulation, these tables are used to interpolate internal energy or temperature values as needed. The interpolation is done with the *linear* style.

For the *linear* style, the internal temperature is used to find 2 surrounding table values from which an internal energy is computed by linear interpolation, and vice-versa.

The filename specifies a file containing tabulated internal temperature and internal energy values. The keyword specifies a section of the file. The format of this file is described below.

The format of a tabulated file is as follows (without the parenthesized comments):

```
# EOS TABLE                (one or more comment or blank lines)

KEYWORD                    (keyword is first text on line)
N 500                      (N  parameter)
                           (blank)
1   1.00 0.000             (index, internal temperature, internal energy)
2   1.02 0.001
...
500 10.0 0.500
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the fix command.

The next line lists the number of table entries. The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the *N* specified in the fix eos/table command. Let Ntable = *N* in the fix command, and Nfile = "N" in the tabulated file. What LAMMPS does is a preliminary interpolation by creating splines using the Nfile tabulated values as nodal points. It uses these to interpolate as needed to generate energy and temperature values at Ntable different points. The resulting tables of length Ntable are then used as described above, when computing energy and temperature relationships. This means that if you want the interpolation tables of length Ntable to match exactly what is in the tabulated file (with effectively no preliminary interpolation), you should set Ntable = Nfile.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is the internal temperature (in temperature units), the 3rd value is the internal energy (in energy units).

Note that the internal temperature and internal energy values must increase from one line to the next.

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

Restrictions:

The fix *eos/table* is only available if LAMMPS is built with the USER-DPD package.

The equation of state must be a monotonically increasing function.

An exit error will occur if the internal temperature or internal energies are not within the table cutoffs.

Related commands:

fix shardlow, pair dpd/fdt

Default: none

fix evaporate command

Syntax:

```
fix ID group-ID evaporate N M region-ID seed
```

- ID, group-ID are documented in fix command
- evaporate = style name of this fix command
- N = delete atoms every this many timesteps
- M = number of atoms to delete each time
- region-ID = ID of region within which to perform deletions
- seed = random number seed to use for choosing atoms to delete
- zero or more keyword/value pairs may be appended

```
keyword = molecule
  molecule value = no or yes
```

Examples:

```
fix 1 solvent evaporate 1000 10 surface 49892
fix 1 solvent evaporate 1000 10 surface 38277 molecule yes
```

Description:

Remove M atoms from the simulation every N steps. This can be used, for example, to model evaporation of solvent particles or moleclues (i.e. drying) of a system. Every N steps, the number of atoms in the fix group and within the specifed region are counted. M of these are chosen at random and deleted. If there are less than M eligible particles, then all of them are deleted.

If the setting for the *molecule* keyword is *no*, then only single atoms are deleted. In this case, you should insure you do not delete only a portion of a molecule (only some of its atoms), or LAMMPS will soon generate an error when it tries to find those atoms. LAMMPS will warn you if any of the atoms eligible for deletion have a non-zero molecule ID, but does not check for this at the time of deletion.

If the setting for the *molecule* keyword is *yes*, then when an atom is chosen for deletion, the entire molecule it is part of is deleted. The count of deleted atoms is incremented by the number of atoms in the molecule, which may make it exceed *M*. If the molecule ID of the chosen atom is 0, then it is assumed to not be part of a molecule, and just the single atom is deleted.

As an example, if you wish to delete 10 water molecules every *N* steps, you should set *M* to 30. If only the water's oxygen atoms were in the fix group, then two hydrogen atoms would be deleted when an oxygen atom is selected for deletion, whether the hydrogens are inside the evaporation region or not.

Note that neighbor lists are re-built on timesteps that atoms are removed. Thus you should not remove atoms too frequently or you will incur overhead due to the cost of building neighbor lists.

NOTE: If you are monitoring the temperature of a system where the atom count is changing due to evaporation, you typically should use the compute_modify dynamic yes command for the temperature compute you are using.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global scalar, which can be accessed by various output commands. The scalar is the cummulative number of deleted atoms. The scalar value calculated by this fix is "intensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix deposit

Default:

The option defaults are molecule = no.

fix external command

Syntax:

```
fix ID group-ID external mode args
```

- ID, group-ID are documented in fix command
- external = style name of this fix command
- mode = *pf/callback* or *pf/array*

```
  pf/callback args = Ncall Napply
      Ncall = make callback every Ncall steps
      Napply = apply callback forces every Napply steps
    pf/array args = Napply
      Napply = apply array forces every Napply steps
```

Examples:

```
fix 1 all external pf/callback 1 1
fix 1 all external pf/callback 100 1
fix 1 all external pf/array 10
```

Description:

This fix allows external programs that are running LAMMPS through its library interface to modify certain LAMMPS properties on specific timesteps, similar to the way other fixes do. The external driver can be a C/C++ or Fortran program or a Python script.

If mode is *pf/callback* then the fix will make a callback every *Ncall* timesteps or minimization iterations to the external program. The external program computes forces on atoms by setting values in an array owned by the fix. The fix then adds these forces to each atom in the group, once every *Napply* steps, similar to the way the fix addforce command works. Note that if *Ncall* > *Napply*, the force values produced by one callback will persist, and be used multiple times to update atom forces.

The callback function "foo" is invoked by the fix as:

```
foo(void *ptr, bigint timestep, int nlocal, int *ids, double **x, double **fexternal);
```

The arguments are as follows:

- ptr = pointer provided by and simply passed back to external driver
- timestep = current LAMMPS timestep
- nlocal = # of atoms on this processor
- ids = list of atom IDs on this processor
- x = coordinates of atoms on this processor
- fexternal = forces to add to atoms on this processor

Note that timestep is a "bigint" which is defined in src/lmptype.h, typically as a 64-bit integer.

Fexternal are the forces returned by the driver program.

The fix has a set_callback() method which the external driver can call to pass a pointer to its foo() function. See the couple/lammps_quest/lmpqst.cpp file in the LAMMPS distribution for an example of how this is done. This sample application performs classical MD using quantum forces computed by a density functional code Quest.

If mode is *pf/array* then the fix simply stores force values in an array. The fix adds these forces to each atom in the group, once every *Napply* steps, similar to the way the fix addforce command works.

The name of the public force array provided by the FixExternal class is

```
double **fexternal;
```

It is allocated by the FixExternal class as an (N,3) array where N is the number of atoms owned by a processor. The 3 corresponds to the fx, fy, fz components of force.

It is up to the external program to set the values in this array to the desired quantities, as often as desired. For example, the driver program might perform an MD run in stages of 1000 timesteps each. In between calls to the LAMMPS run command, it could retrieve atom coordinates from LAMMPS, compute forces, set values in fexternal, etc.

To use this fix during energy minimization, the energy corresponding to the added forces must also be set so as to be consistent with the added forces. Otherwise the minimization will not converge correctly.

This can be done from the external driver by calling this public method of the FixExternal class:

```
void set_energy(double eng);
```

where eng is the potential energy. Eng is an extensive quantity, meaning it should be the sum over per-atom energies of all affected atoms. It should also be provided in energy units consistent with the simulation. See the details below for how to insure this energy setting is used appropriately in a minimization.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *energy* option is supported by this fix to add the potential "energy" set by the external driver to the system's potential energy as part of thermodynamic output. This is a fictitious quantity but is needed so that the minimize command can include the forces added by this fix in a consistent manner. I.e. there is a decrease in potential energy when atoms move in the direction of the added force.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the potential energy discussed above. The scalar stored by this fix is "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command.

NOTE: If you want the fictitious potential energy associated with the added forces to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the fix_modify *energy* option for this fix.

Restrictions: none

Related commands: none

Default: none

fix freeze command

fix freeze/cuda command

Syntax:

```
fix ID group-ID freeze
```

- ID, group-ID are documented in fix command
- freeze = style name of this fix command

Examples:

```
fix 2 bottom freeze
```

Description:

Zero out the force and torque on a granular particle. This is useful for preventing certain particles from moving in a simulation. The granular pair styles also detect if this fix has been defined and compute interactions between frozen and non-frozen particles appropriately, as if the frozen particle has infinite mass. A similar functionality for normal (point) particles can be obtained using fix setforce.

Styles with a *cuda* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global 3-vector of forces, which can be accessed by various output commands. This is the total force on the group of atoms before the forces on individual atoms are changed by the fix. The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the GRANULAR package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

There can only be a single freeze fix defined. This is because other the granular pair styles treat frozen particles differently and need to be able to reference a single group to which this fix is applied.

Related commands:

atom_style sphere, fix setforce

Default: none

fix gcmc command

Syntax:

```
fix ID group-ID gcmc N X M type seed T mu displace keyword values ...
```

- ID, group-ID are documented in fix command
- gcmc = style name of this fix command
- N = invoke this fix every N steps
- X = average number of GCMC exchanges to attempt every N steps
- M = average number of MC moves to attempt every N steps
- type = atom type for inserted atoms (must be 0 if mol keyword used)
- seed = random # seed (positive integer)
- T = temperature of the ideal gas reservoir (temperature units)
- mu = chemical potential of the ideal gas reservoir (energy units)
- translate = maximum Monte Carlo translation distance (length units)
- zero or more keyword/value pairs may be appended to args

```
keyword = mol, region, maxangle, pressure, fugacity_coeff, full_energy, charge, group, groupty
  mol value = template-ID
    template-ID = ID of molecule template specified in a separate molecule command
  shake value = fix-ID
    fix-ID = ID of fix shake command
  region value = region-ID
    region-ID = ID of region where MC moves are allowed
  maxangle value = maximum molecular rotation angle (degrees)
  pressure value = pressure of the gas reservoir (pressure units)
  fugacity_coeff value = fugacity coefficient of the gas reservoir (unitless)
  full_energy = compute the entire system energy when performing MC moves
  charge value = charge of inserted atoms (charge units)
  group value = group-ID
    group-ID = group-ID for inserted atoms (string)
  grouptype values = type group-ID
    type = atom type (int)
    group-ID = group-ID for inserted atoms (string)
  intra_energy value = intramolecular energy (energy units)
  tfac_insert value = scale up/down temperature of inserted atoms (unitless)
```

Examples:

```
fix 2 gas gcmc 10 1000 1000 2 29494 298.0 -0.5 0.01
fix 3 water gcmc 10 100 100 0 3456543 3.0 -2.5 0.1 mol my_one_water maxangle 180 full_energy
fix 4 my_gas gcmc 1 10 10 1 123456543 300.0 -12.5 1.0 region disk
```

Description:

This fix performs grand canonical Monte Carlo (GCMC) exchanges of atoms or molecules of the given type with an imaginary ideal gas reservoir at the specified T and chemical potential (mu) as discussed in (Frenkel). If used with the fix nvt command, simulations in the grand canonical ensemble (muVT, constant chemical potential, constant volume, and constant temperature) can be performed. Specific uses include computing isotherms in microporous materials, or computing vapor-liquid coexistence curves.

Every N timesteps the fix attempts a number of GCMC exchanges (insertions or deletions) of gas atoms or molecules of the given type between the simulation cell and the imaginary reservoir. It also attempts a number of

Monte Carlo moves (translations and molecule rotations) of gas of the given type within the simulation cell or region. The average number of attempted GCMC exchanges is X. The average number of attempted MC moves is M. M should typically be chosen to be approximately equal to the expected number of gas atoms or molecules of the given type within the simulation cell or region, which will result in roughly one MC translation per atom or molecule per MC cycle.

For MC moves of molecular gasses, rotations and translations are each attempted with 50% probability. For MC moves of atomic gasses, translations are attempted 100% of the time. For MC exchanges of either molecular or atomic gasses, deletions and insertions are each attempted with 50% probability.

All inserted particles are always assigned to two groups: the default group "all" and the group specified in the fix gcmc command (which can also be "all"). In addition, particles are also added to any groups specified by the *group* and *grouptype* keywords. If inserted particles are individual atoms, they are assigned the atom type given by the type argument. If they are molecules, the type argument has no effect and must be set to zero. Instead, the type of each atom in the inserted molecule is specified in the file read by the molecule command.

This fix cannot be used to perform MC insertions of gas atoms or molecules other than the exchanged type, but MC deletions, translations, and rotations can be performed on any atom/molecule in the fix group. All atoms in the simulation cell can be moved using regular time integration translations, e.g. via fix_nvt, resulting in a hybrid GCMC+MD simulation. A smaller-than-usual timestep size may be needed when running such a hybrid simulation, especially if the inserted molecules are not well equilibrated.

This command may optionally use the *region* keyword to define an exchange and move volume. The specified region must have been previously defined with a region command. It must be defined with side = *in*. Insertion attempts occur only within the specified region. For non-rectangular regions, random trial points are generated within the rectangular bounding box until a point is found that lies inside the region. If no valid point is generated after 1000 trials, no insertion is performed, but it is counted as an attempted insertion. Move and deletion attempt candidates are selected from gas atoms or molecules within the region. If there are no candidates, no move or deletion is performed, but it is counted as an attempt move or deletion. If an attempted move places the atom or molecule center-of-mass outside the specified region, a new attempted move is generated. This process is repeated until the atom or molecule center-of-mass is inside the specified region.

If used with fix_nvt, the temperature of the imaginary reservoir, T, should be set to be equivalent to the target temperature used in fix_nvt. Otherwise, the imaginary reservoir will not be in thermal equilibrium with the simulation cell. Also, it is important that the temperature used by fix nvt be dynamic, which can be achieved as follows:

```
compute mdtemp mdatoms temp
compute_modify mdtemp dynamic yes
fix mdnvt mdatoms nvt temp 300.0 300.0 10.0
fix_modify mdnvt temp mdtemp
```

Note that neighbor lists are re-built every timestep that this fix is invoked, so you should not set N to be too small. However, periodic rebuilds are necessary in order to avoid dangerous rebuilds and missed interactions. Specifically, avoid performing so many MC translations per timestep that atoms can move beyond the neighbor list skin distance. See the neighbor command for details.

When an atom or molecule is to be inserted, its coordinates are chosen at a random position within the current simulation cell or region, and new atom velocities are randomly chosen from the specified temperature distribution given by T. The effective temperature for new atom velocities can be increased or decreased using the optional keyword *tfac_insert* (see below). Relative coordinates for atoms in a molecule are taken from the template molecule provided by the user. The center of mass of the molecule is placed at the insertion point. The orientation of the molecule is chosen at random by rotating about this point.

Individual atoms are inserted, unless the *mol* keyword is used. It specifies a *template-ID* previously defined using the molecule command, which reads a file that defines the molecule. The coordinates, atom types, charges, etc, as well as any bond/angle/etc and special neighbor information for the molecule can be specified in the molecule file. See the molecule command for details. The only settings required to be in this file are the coordinates and types of atoms in the molecule.

When not using the *mol* keyword, you should ensure you do not delete atoms that are bonded to other atoms, or LAMMPS will soon generate an error when it tries to find bonded neighbors. LAMMPS will warn you if any of the atoms eligible for deletion have a non-zero molecule ID, but does not check for this at the time of deletion.

If you wish to insert molecules via the *mol* keyword, that will have their bonds or angles constrained via SHAKE, use the *shake* keyword, specifying as its value the ID of a separate fix shake command which also appears in your input script.

Optionally, users may specify the maximum rotation angle for molecular rotations using the *maxangle* keyword and specifying the angle in degrees. Rotations are performed by generating a random point on the unit sphere and a random rotation angle on the range [0,maxangle). The molecule is then rotated by that angle about an axis passing through the molecule center of mass. The axis is parallel to the unit vector defined by the point on the unit sphere. The same procedure is used for randomly rotating molecules when they are inserted, except that the maximum angle is 360 degrees.

Note that fix GCMC does not use configurational bias MC or any other kind of sampling of intramolecular degrees of freedom. Inserted molecules can have different orientations, but they will all have the same intramolecular configuration, which was specified in the molecule command input.

For atomic gasses, inserted atoms have the specified atom type, but deleted atoms are any atoms that have been inserted or that belong to the user-specified fix group. For molecular gasses, exchanged molecules use the same atom types as in the template molecule supplied by the user. In both cases, exchanged atoms/molecules are assigned to two groups: the default group "all" and the group specified in the fix gcmc command (which can also be "all").

The gas reservoir pressure can be specified using the *pressure* keyword, in which case the user-specified chemical potential is ignored. For non-ideal gas reservoirs, the user may also specify the fugacity coefficient using the *fugacity_coeff* keyword.

The *full_energy* option means that fix GCMC will compute the total potential energy of the entire simulated system. The total system energy before and after the proposed GCMC move is then used in the Metropolis criterion to determine whether or not to accept the proposed GCMC move. By default, this option is off, in which case only partial energies are computed to determine the difference in energy that would be caused by the proposed GCMC move.

The *full_energy* option is needed for systems with complicated potential energy calculations, including the following:

- long-range electrostatics (kspace)
- many-body pair styles
- hybrid pair styles
- eam pair styles
- triclinic systems
- need to include potential energy contributions from other fixes

In these cases, LAMMPS will automatically apply the *full_energy* keyword and issue a warning message.

When the *mol* keyword is used, the *full_energy* option also includes the intramolecular energy of inserted and deleted molecules. If this is not desired, the *intra_energy* keyword can be used to define an amount of energy that is subtracted from the final energy when a molecule is inserted, and added to the initial energy when a molecule is deleted. For molecules that have a non-zero intramolecular energy, this will ensure roughly the same behavior whether or not the *full_energy* option is used.

Inserted atoms and molecules are assigned random velocities based on the specified temperature T. Because the relative velocity of all atoms in the molecule is zero, this may result in inserted molecules that are systematically too cold. In addition, the intramolecular potential energy of the inserted molecule may cause the kinetic energy of the molecule to quickly increase or decrease after insertion. The *tfac_insert* keyword allows the user to counteract these effects by changing the temperature used to assign velocities to inserted atoms and molecules by a constant factor. For a particular application, some experimentation may be required to find a value of *tfac_insert* that results in inserted molecules that equilibrate quickly to the correct temperature.

Some fixes have an associated potential energy. Examples of such fixes include: efield, gravity, addforce, langevin, restrain, temp/berendsen, temp/rescale, and wall fixes. For that energy to be included in the total potential energy of the system (the quantity used when performing GCMC moves), you MUST enable the fix_modify *energy* option for that fix. The doc pages for individual fix commands specify if this should be done.

Use the *charge* option to insert atoms with a user-specified point charge. Note that doing so will cause the system to become non-neutral. LAMMPS issues a warning when using long-range electrostatics (kspace) with non-neutral systems. See the compute_group_group documentation for more details about simulating non-neutral systems with kspace on.

Use of this fix typically will cause the number of atoms to fluctuate, therefore, you will want to use the compute_modify command to insure that the current number of atoms is used as a normalizing factor each time temperature is computed. Here is the necessary command:

```
compute_modify thermo_temp dynamic yes
```

If LJ units are used, note that a value of 0.18292026 is used by this fix as the reduced value for Planck's constant. This value was derived from LJ parameters for argon, where h* = h/sqrt(sigma^2 * epsilon * mass), sigma = 3.429 angstroms, epsilon/k = 121.85 K, and mass = 39.948 amu.

The *group* keyword assigns all inserted atoms to the group of the group-ID value. The *grouptype* keyword assigns all inserted atoms of the specified type to the group of the group-ID value.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the fix to binary restart files. This includes information about the random number generator seed, the next timestep for MC exchanges, etc. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

None of the fix_modify options are relevant to this fix.

This fix computes a global vector of length 8, which can be accessed by various output commands. The vector values are the following global cumulative quantities:

- 1 = translation attempts
- 2 = translation successes
- 3 = insertion attempts
- 4 = insertion successes

- 5 = deletion attempts
- 6 = deletion successes
- 7 = rotation attempts
- 8 = rotation successes

The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the MC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Do not set "neigh_modify once yes" or else this fix will never be called. Reneighboring is required.

Can be run in parallel, but aspects of the GCMC part will not scale well in parallel. Only usable for 3D simulations.

Note that very lengthy simulations involving insertions/deletions of billions of gas molecules may run out of atom or molecule IDs and trigger an error, so it is better to run multiple shorter-duration simulations. Likewise, very large molecules have not been tested and may turn out to be problematic.

Use of multiple fix gcmc commands in the same input script can be problematic if using a template molecule. The issue is that the user-referenced template molecule in the second fix gcmc command may no longer exist since it might have been deleted by the first fix gcmc command. An existing template molecule will need to be referenced by the user for each subsequent fix gcmc command.

Related commands:

fix atom/swap, fix nvt, neighbor, fix deposit, fix evaporate, delete_atoms

Default:

The option defaults are mol = no, maxangle = 10, full_energy = no, except for the situations where full_energy is required, as listed above.

(Frenkel) Frenkel and Smit, Understanding Molecular Simulation, Academic Press, London, 2002.

fix gld command

Syntax:

```
fix ID group-ID gld Tstart Tstop N_k seed series c_1 tau_1 ... c_N_k tau_N_k keyword values ...
```

- ID, group-ID are documented in fix command
- gld = style name of this fix command
- Tstart,Tstop = desired temperature at start/end of run (temperature units)
- N_k = number of terms in the Prony series representation of the memory kernel
- seed = random number seed to use for white noise (positive integer)
- series = *pprony* is presently the only available option
- c_k = the weight of the kth term in the Prony series (mass per time units)
- tau_k = the time constant of the kth term in the Prony series (time units)
- zero or more keyword/value pairs may be appended

```
keyword = frozen or zero
  frozen value = no or yes
    no = initialize extended variables using values drawn from equilibrium distribution at Tst
    yes = initialize extended variables to zero (i.e., from equilibrium distribution at zero t
  zero value = no or yes
    no = do not set total random force to zero
    yes = set total random force to zero
```

Examples:

```
fix 1 all gld 1.0 1.0 2 82885 pprony 0.5 1.0 1.0 2.0 frozen yes zero yes
fix 3 rouse gld 7.355 7.355 4 48823 pprony 107.1 0.02415 186.0 0.04294 428.6 0.09661 1714 0.38643
```

Description:

Applies Generalized Langevin Dynamics to a group of atoms, as described in (Baczewski). This is intended to model the effect of an implicit solvent with a temporally non-local dissipative force and a colored Gaussian random force, consistent with the Fluctuation-Dissipation Theorem. The functional form of the memory kernel associated with the temporally non-local force is constrained to be a Prony series.

NOTE: While this fix bears many similarities to fix langevin, it has one significant difference. Namely, fix gld performs time integration, whereas fix langevin does NOT. To this end, the specification of another fix to perform time integration, such as fix nve, is NOT necessary.

With this fix active, the force on the *j*th atom is given as

$$\mathbf{F}_j(t) = \mathbf{F}_j^C(t) - \int_0^t \Gamma_j(t-s)\mathbf{v}_j(s)\ \mathrm{d}s + \mathbf{F}_j^R(t)$$

$$\Gamma_j(t-s) = \sum_{k=1}^{N_k} \frac{c_k}{\tau_k} e^{-(t-s)/\tau_k}$$

$$\langle \mathbf{F}_j^R(t), \mathbf{F}_j^R(s) \rangle = \mathrm{k_B T}\ \Gamma_j(t-s)$$

Here, the first term is representative of all conservative (pairwise, bonded, etc) forces external to this fix, the second is the temporally non-local dissipative force given as a Prony series, and the third is the colored Gaussian random force.

The Prony series form of the memory kernel is chosen to enable an extended variable formalism, with a number of exemplary mathematical features discussed in (Baczewski). In particular, 3N_k extended variables are added to each atom, which effect the action of the memory kernel without having to explicitly evaluate the integral over time in the second term of the force. This also has the benefit of requiring the generation of uncorrelated random forces, rather than correlated random forces as specified in the third term of the force.

Presently, the Prony series coefficients are limited to being greater than or equal to zero, and the time constants are limited to being greater than zero. To this end, the value of series MUST be set to *pprony*, for now. Future updates will allow for negative coefficients and other representations of the memory kernel. It is with these updates in mind that the series option was included.

The units of the Prony series coefficients are chosen to be mass per time to ensure that the numerical integration scheme stably approaches the Newtonian and Langevin limits. Details of these limits, and the associated numerical concerns are discussed in (Baczewski).

The desired temperature at each timestep is ramped from *Tstart* to *Tstop* over the course of the next run.

The random # *seed* must be a positive integer. A Marsaglia random number generator is used. Each processor uses the input seed to generate its own unique seed and its own stream of random numbers. Thus the dynamics of the system will not be identical on two runs on different numbers of processors.

The keyword/value option pairs are used in the following ways.

The keyword *frozen* can be used to specify how the extended variables associated with the GLD memory kernel are initialized. Specifying no (the default), the initial values are drawn at random from an equilibrium distribution at *Tstart*, consistent with the Fluctuation-Dissipation Theorem. Specifying yes, initializes the extended variables to zero.

The keyword *zero* can be used to eliminate drift due to the thermostat. Because the random forces on different atoms are independent, they do not sum exactly to zero. As a result, this fix applies a small random force to the entire system, and the center-of-mass of the system undergoes a slow random walk. If the keyword *zero* is set to *yes*, the total random force is set exactly to zero by subtracting off an equal part of it from each atom in the group. As a result, the center-of-mass of a system with zero initial momentum will not drift over time.

Restart, run start/stop, minimize info:

The instantaneous values of the extended variables are written to binary restart files. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior.

None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix langevin, fix viscous, pair_style dpd/tstat

Default:

The option defaults are frozen = no, zero = no.

(Baczewski) A.D. Baczewski and S.D. Bond, J. Chem. Phys. 139, 044107 (2013).

fix gle command

Syntax:

```
fix ID id-group gle Ns Tstart Tstop seed Amatrix [noneq Cmatrix] [every stride]
```

- ID, group-ID are documented in fix command
- gle = style name of this fix command
- Ns = number of additional fictitious momenta
- Tstart, Tstop = temperature ramp during the run
- Amatrix = file to read the drift matrix A from
- seed = random number seed to use for generating noise (positive integer)
- zero or more keyword/value pairs may be appended keyword = *noneq* and/or *every noneq* Cmatrix = file to read the non-equilibrium covariance matrix from *every* stride = apply the GLE once every time steps. Reduces the accuracy of the integration of the GLE, but has *no effect* on the accuracy of equilibrium sampling. It might change sampling properties when used together with *noneq*.

Examples:

fix 3 boundary gle 6 300 300 31415 smart.A fix 1 all gle 6 300 300 31415 qt-300k.A noneq qt-300k.C

Description:

Apply a Generalized Langevin Equation (GLE) thermostat as described in (Ceriotti). The formalism allows one to obtain a number of different effects ranging from efficient sampling of all vibrational modes in the system to inexpensive (approximate) modelling of nuclear quantum effects. Contrary to fix langevin, this fix performs both thermostatting and evolution of the Hamiltonian equations of motion, so it should not be used together with fix nve -- at least not on the same atom groups.

Each degree of freedom in the thermostatted group is supplemented with Ns additional degrees of freedom s, and the equations of motion become

dq/dt=p/m d(p,s)/dt=(F,0) - A(p,s) + B dW/dt

where F is the physical force, A is the drift matrix (that generalizes the friction in Langevin dynamics), B is the diffusion term and dW/dt un-correlated Gaussian random forces. The A matrix couples the physical (q,p) dynamics with that of the additional degrees of freedom, and makes it possible to obtain effectively a history-dependent noise and friction kernel.

The drift matrix should be given as an external file *Afile*, as a (Ns+1 x Ns+1) matrix in inverse time units. Matrices that are optimal for a given application and the system of choice can be obtained from (GLE4MD).

Equilibrium sampling a temperature T is obtained by specifiying the target value as the *Tstart* and *Tstop* arguments, so that the diffusion matrix that gives canonical sampling for a given A is computed automatically. However, the GLE framework also allow for non-equilibrium sampling, that can be used for instance to model inexpensively zero-point energy effects (Ceriotti2). This is achieved specifying the *noneq* keyword followed by the name of the file that contains the static covariance matrix for the non-equilibrium dynamics.

Since integrating GLE dynamics can be costly when used together with simple potentials, one can use the *every* optional keyword to apply the Langevin terms only once every several MD steps, in a multiple time-step fashion.

This should be used with care when doing non-equilibrium sampling, but should have no effect on equilibrium averages when using canonical sampling.

The random number *seed* must be a positive integer. A Marsaglia random number generator is used. Each processor uses the input seed to generate its own unique seed and its own stream of random numbers. Thus the dynamics of the system will not be identical on two runs on different numbers of processors.

Note also that the Generalized Langevin Dynamics scheme that is implemented by the fix gld scheme is closely related to the present one. In fact, it should be always possible to cast the Prony series form of the memory kernel used by GLD into an appropriate input matrix for fix_gle. While the GLE scheme is more general, the form used by fix gld can be more directly related to the representation of an implicit solvent environment.

Restart, fix_modify, output, run start/stop, minimize info:

The instantaneous values of the extended variables are written to binary restart files. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior. Note however that you should use a different seed each time you restart, otherwise the same sequence of random numbers will be used each time, which might lead to stochastic synchronization and subtle artefacts in the sampling.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

The fix_modify *energy* option is supported by this fix to add the energy change induced by Langevin thermostatting to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the cummulative energy change due to this fix. The scalar value calculated by this fix is "extensive".

Restrictions:

The GLE thermostat in its current implementation should not be used with rigid bodies, SHAKE or RATTLE. It is expected that all the thermostatted degrees of freedom are fully flexible, and the sampled ensemble will not be correct otherwise.

In order to perform constant-pressure simulations please use fix press/berendsen, rather than fix_npt, to avoid duplicate integration of the equations of motion.

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix nvt, fix temp/rescale, fix viscous, fix nvt, pair_style dpd/tstat, fix_gld

---

(Ceriotti) Ceriotti, Bussi and Parrinello, J Chem Theory Comput 6, 1170-80 (2010)

(GLE4MD) http://epfl-cosmo.github.io/gle4md/

(Ceriotti2) Ceriotti, Bussi and Parrinello, Phys Rev Lett 103, 030603 (2009)

fix gravity command

fix gravity/cuda command

fix gravity/omp command

Syntax:

```
fix ID group gravity magnitude style args
```

- ID, group are documented in fix command
- gravity = style name of this fix command
- magnitude = size of acceleration (force/mass units)
- magnitude can be a variable (see below)
- style = *chute* or *spherical* or *gradient* or *vector*

```
  chute args = angle
      angle = angle in +x away from -z or -y axis in 3d/2d (in degrees)
      angle can be a variable (see below)
    spherical args = phi theta
      phi = azimuthal angle from +x axis (in degrees)
      theta = angle from +z or +y axis in 3d/2d (in degrees)
      phi or theta can be a variable (see below)
    vector args = x y z
      x y z = vector direction to apply the acceleration
      x or y or z can be a variable (see below)
```

Examples:

```
fix 1 all gravity 1.0 chute 24.0
fix 1 all gravity v_increase chute 24.0
fix 1 all gravity 1.0 spherical 0.0 -180.0
fix 1 all gravity 10.0 spherical v_phi v_theta
fix 1 all gravity 100.0 vector 1 1 0
```

Description:

Impose an additional acceleration on each particle in the group. This fix is typically used with granular systems to include a "gravity" term acting on the macroscopic particles. More generally, it can represent any kind of driving field, e.g. a pressure gradient inducing a Poiseuille flow in a fluid. Note that this fix operates differently than the fix addforce command. The addforce fix adds the same force to each atom, independent of its mass. This command imparts the same acceleration to each atom (force/mass).

The *magnitude* of the acceleration is specified in force/mass units. For granular systems (LJ units) this is typically 1.0. See the units command for details.

Style *chute* is typically used for simulations of chute flow where the specified *angle* is the chute angle, with flow occurring in the +x direction. For 3d systems, the tilt is away from the z axis; for 2d systems, the tilt is away from the y axis.

Style *spherical* allows an arbitrary 3d direction to be specified for the acceleration vector. *Phi* and *theta* are defined in the usual spherical coordinates. Thus for acceleration acting in the -z direction, *theta* would be 180.0

(or -180.0). *Theta* = 90.0 and *phi* = -90.0 would mean acceleration acts in the -y direction. For 2d systems, *phi* is ignored and *theta* is an angle in the xy plane where *theta* = 0.0 is the y-axis.

Style *vector* imposes an acceleration in the vector direction given by (x,y,z). Only the direction of the vector is important; it's length is ignored. For 2d systems, the *z* component is ignored.

Any of the quantities *magnitude*, *angle*, *phi*, *theta*, *x*, *y*, *z* which define the gravitational magnitude and direction, can be specified as an equal-style variable. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the quantity. You should insure that the variable calculates a result in the approriate units, e.g. force/mass or degrees.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent gravitational field.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *energy* option is supported by this fix to add the gravitational potential energy of the system to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar which can be accessed by various output commands. This scalar is the gravitational potential energy of the particles in the defined field, namely mass * (g dot x) for each particles, where x and mass are the particles position and mass, and g is the gravitational field. The scalar value calculated by this fix is "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

atom_style sphere, fix addforce

Default: none

fix heat command

Syntax:

```
fix ID group-ID heat N eflux
```

- ID, group-ID are documented in fix command
- heat = style name of this fix command
- N = add/subtract heat every this many timesteps
- eflux = rate of heat addition or subtraction (energy/time units)
- eflux can be a variable (see below)
- zero or more keyword/value pairs may be appended to args
- keyword = *region*

```
region value = region-ID
    region-ID = ID of region atoms must be in to have added force
```

Examples:

```
fix 3 qin heat 1 1.0
fix 3 qin heat 10 v_flux
fix 4 qout heat 1 -1.0 region top
```

Description:

Add non-translational kinetic energy (heat) to a group of atoms in a manner that conserves their aggregate momentum. Two of these fixes can be used to establish a temperature gradient across a simulation domain by adding heat (energy) to one group of atoms (hot reservoir) and subtracting heat from another (cold reservoir). E.g. a simulation sampling from the McDLT ensemble.

If the *region* keyword is used, the atom must be in both the group and the specified geometric region in order to have energy added or subtracted to it. If not specified, then the atoms in the group are affected wherever they may move to.

Heat addition/subtraction is performed every N timesteps. The *eflux* parameter can be specified as a numeric constant or as a variable (see below). If it is a numeric constant or equal-style variable which evaluates to a scalar value, then the *eflux* determines the change in aggregate energy of the entire group of atoms per unit time, e.g. in eV/psec for metal units. In this case it is an "extensive" quantity, meaning its magnitude should be scaled with the number of atoms in the group. Note that since *eflux* has per-time units (i.e. it is a flux), this means that a larger value of N will add/subtract a larger amount of energy each time the fix is invoked.

If *eflux* is specified as an atom-style variable (see below), then the variable computes one value per atom. In this case, each value is the energy flux for a single atom, again in units of energy per unit time. In this case, each value is an "intensive" quantity, which need not be scaled with the number of atoms in the group.

As mentioned above, the *eflux* parameter can be specified as an equal-style or atom_style variable. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value(s) used to determine the flux.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a

time-dependent flux.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent flux with optional time-dependence as well.

NOTE: If heat is subtracted from the system too aggressively so that the group's kinetic energy would go to zero, or any individual atom's kinetic energy would go to zero for the case where *eflux* is an atom-style variable, then LAMMPS will halt with an error message.

Fix heat is different from a thermostat such as fix nvt or fix temp/rescale in that energy is added/subtracted continually. Thus if there isn't another mechanism in place to counterbalance this effect, the entire system will heat or cool continuously. You can use multiple heat fixes so that the net energy change is 0.0 or use fix viscous to drain energy from the system.

This fix does not change the coordinates of its atoms; it only scales their velocities. Thus you must still use an integration fix (e.g. fix nve) on the affected atoms. This fix should not normally be used on atoms that have their temperature controlled by another fix - e.g. fix nvt or fix langevin fix.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global scalar which can be accessed by various output commands. This scalar is the most recent value by which velocites were scaled. The scalar value calculated by this fix is "intensive". If *eflux* is specified as an atom-style variable, this fix computes the average value by which the velocities were scaled for all of the atoms that had their velocities scaled.

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

compute temp, compute temp/region

Default: none

fix imd command

Syntax:

```
fix ID group-ID imd trate port keyword values ...
```

- ID, group-ID are documented in fix command
- imd = style name of this fix command
- port = port number on which the fix listens for an IMD client
- keyword = *unwrap* or *fscale* or *trate*

```
  unwrap arg = on or off
      off = coordinates are wrapped back into the principal unit cell (default)
      on = "unwrapped" coordinates using the image flags used
    fscale arg = factor
      factor = floating point number to scale IMD forces (default: 1.0)
    trate arg = transmission rate of coordinate data sets (default: 1)
    nowait arg = on or off
      off = LAMMPS waits to be connected to an IMD client before continuing (default)
      on = LAMMPS listens for an IMD client, but continues with the run
```

Examples:

```
fix vmd all imd 5678
fix comm all imd 8888 trate 5 unwrap on fscale 10.0
```

Description:

This fix implements the "Interactive MD" (IMD) protocol which allows realtime visualization and manipulation of MD simulations through the IMD protocol, as initially implemented in VMD and NAMD. Specifically it allows LAMMPS to connect an IMD client, for example the VMD visualization program, so that it can monitor the progress of the simulation and interactively apply forces to selected atoms.

If LAMMPS is compiled with the preprocessor flag -DLAMMPS_ASYNC_IMD then fix imd will use POSIX threads to spawn a IMD communication thread on MPI rank 0 in order to offload data reading and writing from the main execution thread and potentially lower the inferred latencies for slow communication links. This feature has only been tested under linux.

There are example scripts for using this package with LAMMPS in examples/USER/imd. Additional examples and a driver for use with the Novint Falcon game controller as haptic device can be found at: http://sites.google.com/site/akohlmey/software/vrpn-icms.

The source code for this fix includes code developed by the Theoretical and Computational Biophysics Group in the Beckman Institute for Advanced Science and Technology at the University of Illinois at Urbana-Champaign. We thank them for providing a software interface that allows codes like LAMMPS to hook to VMD.

Upon initialization of the fix, it will open a communication port on the node with MPI task 0 and wait for an incoming connection. As soon as an IMD client is connected, the simulation will continue and the fix will send the current coordinates of the fix's group to the IMD client at every trate MD step. When using r-RESPA, trate applies to the steps of the outmost RESPA level. During a run with an active IMD connection also the IMD client can request to apply forces to selected atoms of the fix group.

The port number selected must be an available network port number. On many machines, port numbers < 1024 are reserved for accounts with system manager privilege and specific applications. If multiple imd fixes would be active at the same time, each needs to use a different port number.

The *nowait* keyword controls the behavior of the fix when no IMD client is connected. With the default setting of *off*, LAMMPS will wait until a connection is made before continuing with the execution. Setting *nowait* to *on* will have the LAMMPS code be ready to connect to a client, but continue with the simulation. This can for example be used to monitor the progress of an ongoing calculation without the need to be permanently connected or having to download a trajectory file.

The *trate* keyword allows to select how often the coordinate data is sent to the IMD client. It can also be changed on request of the IMD client through an IMD protocol message. The *unwrap* keyword allows to send "unwrapped" coordinates to the IMD client that undo the wrapping back of coordinates into the principle unit cell, as done by default in LAMMPS. The *fscale* keyword allows to apply a scaling factor to forces transmitted by the IMD client. The IMD protocols stipulates that forces are transferred in kcal/mol/angstrom under the assumption that coordinates are given in angstrom. For LAMMPS runs with different units or as a measure to tweak the forces generated by the manipulation of the IMD client, this option allows to make adjustments.

To connect VMD to a listening LAMMPS simulation on the same machine with fix imd enabled, one needs to start VMD and load a coordinate or topology file that matches the fix group. When the VMD command prompts appears, one types the command line:

```
imd connect localhost 5678
```

This assumes that *fix imd* was started with 5678 as a port number for the IMD protocol.

The steps to do interactive manipulation of a running simulation in VMD are the following:

In the Mouse menu of the VMD Main window, select "Mouse -> Force -> Atom". You may alternately select "Residue", or "Fragment" to apply forces to whole residues or fragments. Your mouse can now be used to apply forces to your simulation. Click on an atom, residue, or fragment and drag to apply a force. Click quickly without moving the mouse to turn the force off. You can also use a variety of 3D position trackers to apply forces to your simulation. Game controllers or haptic devices with force-feedback such as the Novint Falcon or Sensable PHANTOM allow you to feel the resistance due to inertia or interactions with neighbors that the atoms experience you are trying to move, as if they were real objects. See the VMD IMD Homepage and the VRPN-ICMS Homepage for more details.

If IMD control messages are received, a line of text describing the message and its effect will be printed to the LAMMPS output screen, if screen output is active.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global scalar or vector or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

When used in combination with VMD, a topology or coordinate file has to be loaded, which matches (in number and ordering of atoms) the group the fix is applied to. The fix internally sorts atom IDs by ascending integer value; in VMD (and thus the IMD protocol) those will be assigned 0-based consecutive index numbers.

When using multiple active IMD connections at the same time, each needs to use a different port number.

Related commands: none

Default: none

fix indent command

Syntax:

```
fix ID group-ID indent K keyword values ...
```

- ID, group-ID are documented in fix command
- indent = style name of this fix command
- K = force constant for indenter surface (force/distance^2 units)
- one or more keyword/value pairs may be appended
- keyword = *sphere* or *cylinder* or *plane* or *side* or *units*

```
  sphere args = x y z R
      x,y,z = initial position of center of indenter (distance units)
      R = sphere radius of indenter (distance units)
      any of x,y,z,R can be a variable (see below)
    cylinder args = dim c1 c2 R
      dim = x or y or z = axis of cylinder
      c1,c2 = coords of cylinder axis in other 2 dimensions (distance units)
      R = cylinder radius of indenter (distance units)
      any of c1,c2,R can be a variable (see below)
    plane args = dim pos side
      dim = x or y or z = plane perpendicular to this dimension
      pos = position of plane in dimension x, y, or z (distance units)
      pos can be a variable (see below)
      side = lo or hi
    side value = in or out
      in = the indenter acts on particles inside the sphere or cylinder
      out = the indenter acts on particles outside the sphere or cylinder
    units value = lattice or box
      lattice = the geometry is defined in lattice units
      box = the geometry is defined in simulation box units
```

Examples:

```
fix 1 all indent 10.0 sphere 0.0 0.0 15.0 3.0
fix 1 all indent 10.0 sphere v_x v_y 0.0 v_radius side in
fix 2 flow indent 10.0 cylinder z 0.0 0.0 10.0 units box
```

Description:

Insert an indenter within a simulation box. The indenter repels all atoms in the group that touch it, so it can be used to push into a material or as an obstacle in a flow. Or it can be used as a constraining wall around a simulation; see the discussion of the *side* keyword below.

The indenter can either be spherical or cylindrical or planar. You must set one of those 3 keywords.

A spherical indenter exerts a force of magnitude

```
F(r) = - K (r - R)^2
```

on each atom where K is the specified force constant, r is the distance from the atom to the center of the indenter, and R is the radius of the indenter. The force is repulsive and F(r) = 0 for $r > R$.

A cylindrical indenter exerts the same force, except that *r* is the distance from the atom to the center axis of the cylinder. The cylinder extends infinitely along its axis.

Spherical and cylindrical indenters account for periodic boundaries in two ways. First, the center point of a spherical indenter (x,y,z) or axis of a cylindrical indenter (c1,c2) is remapped back into the simulation box, if the box is periodic in a particular dimension. This occurs every timestep if the indenter geometry is specified with a variable (see below), e.g. it is moving over time. Second, the calculation of distance to the indenter center or axis accounts for periodic boundaries. Both of these mean that an indenter can effectively move through and straddle one or more periodic boundaries.

A planar indenter is really an axis-aligned infinite-extent wall exerting the same force on atoms in the system, where *R* is the position of the plane and *r-R* is the distance from the plane. If the *side* parameter of the plane is specified as *lo* then it will indent from the lo end of the simulation box, meaning that atoms with a coordinate less than the plane's current position will be pushed towards the hi end of the box and atoms with a coordinate higher than the plane's current position will feel no force. Vice versa if *side* is specified as *hi*.

Any of the 4 quantities defining a spherical indenter's geometry can be specified as an equal-style variable, namely *x*, *y*, *z*, or *R*. Similarly, for a cylindrical indenter, any of *c1*, *c2*, or *R*, can be a variable. For a planar indenter, *pos* can be a variable. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to define the indenter geometry.

Note that equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify indenter properties that change as a function of time or span consecutive runs in a continuous fashion. For the latter, see the *start* and *stop* keywords of the run command and the *elaplong* keyword of thermo_style custom for details.

For example, if a spherical indenter's x-position is specfied as v_x, then this variable definition will keep it's center at a relative position in the simulation box, 1/4 of the way from the left edge to the right edge, even if the box size changes:

```
variable x equal "xlo + 0.25*lx"
```

Similarly, either of these variable definitions will move the indenter from an initial position at 2.5 at a constant velocity of 5:

```
variable x equal "2.5 + 5*elaplong*dt"
variable x equal vdisplace(2.5,5)
```

If a spherical indenter's radius is specified as v_r, then these variable definitions will grow the size of the indenter at a specfied rate.

```
variable r0 equal 0.0
variable rate equal 1.0
variable r equal "v_r0 + step*dt*v_rate"
```

If the *side* keyword is specified as *out*, which is the default, then particles outside the indenter are pushded away from its outer surface, as described above. This only applies to spherical or cylindrical indenters. If the *side* keyword is specified as *in*, the action of the indenter is reversed. Particles inside the indenter are pushed away from its inner surface. In other words, the indenter is now a containing wall that traps the particles inside it. If the radius shrinks over time, it will squeeze the particles.

The *units* keyword determines the meaning of the distance units used to define the indenter geometry. A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacing. The (x,y,z) coords of the indenter position are scaled by the x,y,z lattice spacings respectively. The radius of a spherical or cylindrical indenter is scaled by the x lattice spacing.

Note that the units keyword only affects indenter geometry parameters specified directly with numbers, not those specified as variables. In the latter case, you should use the *xlat*, *ylat*, *zlat* keywords of the thermo_style command if you want to include lattice spacings in a variable formula.

The force constant *K* is not affected by the *units* keyword. It is always in force/distance^2 units where force and distance are defined by the units command. If you wish K to be scaled by the lattice spacing, you can define K with a variable whose formula contains *xlat*, *ylat*, *zlat* keywords of the thermo_style command, e.g.

```
variable k equal 100.0/xlat/xlat
fix 1 all indent $k sphere ...
```

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *energy* option is supported by this fix to add the energy of interaction between atoms and the indenter to the system's potential energy as part of thermodynamic output. The energy of each particle interacting with the indenter is K/3 (r - R)^3.

This fix computes a global scalar energy and a global 3-vector of forces (on the indenter), which can be accessed by various output commands. The scalar and vector values calculated by this fix are "extensive".

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command. Note that if you define the indenter geometry with a variable using a time-dependent formula, LAMMPS uses the iteration count in the minimizer as the timestep. But it is almost certainly a bad idea to have the indenter change its position or size during a minimization. LAMMPS does not check if you have done this.

NOTE: If you want the atom/indenter interaction energy to be included in the total potential energy of the system (the quantity being minimized), you must enable the fix_modify *energy* option for this fix.

Restrictions: none

Related commands: none

Default:

The option defaults are side = out and units = lattice.

fix ipi command

Syntax:

```
fix ID group-ID ipi address port [unix]
```

- ID, group-ID are documented in fix command
- ipi = style name of this fix command
- address = internet address (FQDN or IP), or UNIX socket name
- port = port number (ignored for UNIX sockets)
- optional keyword = *unix*, if present uses a unix socket

Examples:

fix 1 all ipi my.server.com 12345 fix 1 all ipi mysocket 666 unix

Description:

This fix enables LAMMPS to be run as a client for the i-PI Python wrapper (IPI) for performing a path integral molecular dynamics (PIMD) simulation. The philosophy behind i-PI is described in the following publication (IPI-CPC).

A version of the i-PI package, containing only files needed for use with LAMMPS, is provided in the tools/i-pi directory. See the tools/i-pi/manual.pdf for an introduction to i-PI. The examples/USER/i-pi directory contains example scripts for using i-PI with LAMMPS.

In brief, the path integral molecular dynamics is performed by the Python wrapper, while the client (LAMMPS in this case) simply computes forces and energy for each configuration. The communication between the two components takes place using sockets, and is reduced to the bare minimum. All the parameters of the dynamics are specified in the input of i-PI, and all the parameters of the force field must be specified as LAMMPS inputs, preceding the *fix ipi* command.

The server address must be specified by the *address* argument, and can be either the IP address, the fully-qualified name of the server, or the name of a UNIX socket for local, faster communication. In the case of internet sockets, the *port* argument specifies the port number on which i-PI is listening, while the *unix* optional switch specifies that the socket is a UNIX socket.

Note that there is no check of data integrity, or that the atomic configurations make sense. It is assumed that the species in the i-PI input are listed in the same order as in the data file of LAMMPS. The initial configuration is ignored, as it will be substituted with the coordinates received from i-PI before forces are ever evaluated.

Restart, fix_modify, output, run start/stop, minimize info:

There is no restart information associated with this fix, since all the dynamical parameters are dealt with by i-PI.

Restrictions:

Using this fix on anything other than all atoms requires particular care, since i-PI will know nothing on atoms that are not those whose coordinates are transferred. However, one could use this strategy to define an external potential acting on the atoms that are moved by i-PI.

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info. Because of the use of UNIX domain sockets, this fix will only work in a UNIX environment.

Related commands:

fix nve

(IPI-CPC) Ceriotti, More and Manolopoulos, Comp Phys Comm, 185, 1019-1026 (2014).

(IPI) http://epfl-cosmo.github.io/gle4md/index.html?page=ipi

fix langevin command

fix langevin/kk command

Syntax:

```
fix ID group-ID langevin Tstart Tstop damp seed keyword values ...
```

- ID, group-ID are documented in fix command
- langevin = style name of this fix command
- Tstart,Tstop = desired temperature at start/end of run (temperature units)
- Tstart can be a variable (see below)
- damp = damping parameter (time units)
- seed = random number seed to use for white noise (positive integer)
- zero or more keyword/value pairs may be appended
- keyword = *angmom* or *omega* or *scale* or *tally* or *zero*

```
  angmom value = no or scale
      no = do not thermostat rotational degrees of freedom via the angular momentum
      factor = do thermostat rotational degrees of freedom via the angular momentum and apply nu
    gjf value = no or yes
      no = use standard formulation
      yes = use Gronbech-Jensen/Farago formulation
    omega value = no or yes
      no = do not thermostat rotational degrees of freedom via the angular velocity
      yes = do thermostat rotational degrees of freedom via the angular velocity
    scale values = type ratio
      type = atom type (1-N)
      ratio = factor by which to scale the damping coefficient
    tally value = no or yes
      no = do not tally the energy added/subtracted to atoms
      yes = do tally the energy added/subtracted to atoms
    zero value = no or yes
      no = do not set total random force to zero
      yes = set total random force to zero
```

Examples:

```
fix 3 boundary langevin 1.0 1.0 1000.0 699483
fix 1 all langevin 1.0 1.1 100.0 48279 scale 3 1.5
fix 1 all langevin 1.0 1.1 100.0 48279 angmom 3.333
```

Description:

Apply a Langevin thermostat as described in (Schneider) to a group of atoms which models an interaction with a background implicit solvent. Used with fix nve, this command performs Brownian dynamics (BD), since the total force on each atom will have the form:

```
F = Fc + Ff + Fr
Ff = - (m / damp) v
Fr is proportional to sqrt(Kb T m / (dt damp))
```

Fc is the conservative force computed via the usual inter-particle interactions (pair_style, bond_style, etc).

The Ff and Fr terms are added by this fix on a per-particle basis. See the pair_style dpd/tstat command for a thermostatting option that adds similar terms on a pairwise basis to pairs of interacting particles.

Ff is a frictional drag or viscous damping term proportional to the particle's velocity. The proportionality constant for each atom is computed as m/damp, where m is the mass of the particle and damp is the damping factor specified by the user.

Fr is a force due to solvent atoms at a temperature T randomly bumping into the particle. As derived from the fluctuation/dissipation theorem, its magnitude as shown above is proportional to sqrt(Kb T m / dt damp), where Kb is the Boltzmann constant, T is the desired temperature, m is the mass of the particle, dt is the timestep size, and damp is the damping factor. Random numbers are used to randomize the direction and magnitude of this force as described in (Dunweg), where a uniform random number is used (instead of a Gaussian random number) for speed.

Note that unless you use the *omega* or *angmom* keywords, the thermostat effect of this fix is applied to only the translational degrees of freedom for the particles, which is an important consideration for finite-size particles, which have rotational degrees of freedom, are being thermostatted. The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

NOTE: Unlike the fix nvt command which performs Nose/Hoover thermostatting AND time integration, this fix does NOT perform time integration. It only modifies forces to effect thermostatting. Thus you must use a separate time integration fix, like fix nve to actually update the velocities and positions of atoms using the modified forces. Likewise, this fix should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by fix nvt or fix temp/rescale commands.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

The desired temperature at each timestep is a ramped value during the run from *Tstart* to *Tstop*.

Tstart can be specified as an equal-style or atom-style variable. In this case, the *Tstop* setting is ignored. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the target temperature.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent temperature.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent temperature with optional time-dependence as well.

Like other fixes that perform thermostatting, this fix can be used with compute commands that remove a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or removing the x-component of velocity from the calculation. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute commands to determine which ones include a bias. In this case, the thermostat works in the following manner: bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

The *damp* parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 100.0 means to relax the temperature in a timespan of (roughly) 100 time units (tau or fmsec

or psec - see the units command). The damp factor can be thought of as inversely related to the viscosity of the solvent. I.e. a small relaxation time implies a hi-viscosity solvent and vice versa. See the discussion about gamma and viscosity in the documentation for the fix viscous command for more details.

The random # *seed* must be a positive integer. A Marsaglia random number generator is used. Each processor uses the input seed to generate its own unique seed and its own stream of random numbers. Thus the dynamics of the system will not be identical on two runs on different numbers of processors.

The keyword/value option pairs are used in the following ways.

The keyword *angmom* and *omega* keywords enable thermostatting of rotational degrees of freedom in addition to the usual translational degrees of freedom. This can only be done for finite-size particles.

A simulation using atom_style sphere defines an omega for finite-size spheres. A simulation using atom_style ellipsoid defines a finite size and shape for aspherical particles and an angular momentum. The Langevin formulas for thermostatting the rotational degrees of freedom are the same as those above, where force is replaced by torque, m is replaced by the moment of inertia I, and v is replaced by omega (which is derived from the angular momentum in the case of aspherical particles).

The rotational temperature of the particles can be monitored by the compute temp/sphere and compute temp/asphere commands with their rotate options.

For the *omega* keyword there is also a scale factor of 10.0/3.0 that is applied as a multiplier on the Ff (damping) term in the equation above and of sqrt(10.0/3.0) as a multiplier on the Fr term. This does not affect the thermostatting behaviour of the Langevin formalism but insures that the randomized rotational diffusivity of spherical particles is correct.

For the *angmom* keyword a similar scale factor is needed which is 10.0/3.0 for spherical particles, but is anisotropic for aspherical particles (e.g. ellipsoids). Currently LAMMPS only applies an isotropic scale factor, and you can choose its magnitude as the specified value of the *angmom* keyword. If your aspherical particles are (nearly) spherical than a value of 10.0/3.0 = 3.333 is a good choice. If they are highly aspherical, a value of 1.0 is as good a choice as any, since the effects on rotational diffusivity of the particles will be incorrect regardless. Note that for any reasonable scale factor, the thermostatting effect of the *angmom* keyword on the rotational temperature of the aspherical particles should still be valid.

The keyword *scale* allows the damp factor to be scaled up or down by the specified factor for atoms of that type. This can be useful when different atom types have different sizes or masses. It can be used multiple times to adjust damp for several atom types. Note that specifying a ratio of 2 increases the relaxation time which is equivalent to the solvent's viscosity acting on particles with 1/2 the diameter. This is the opposite effect of scale factors used by the fix viscous command, since the damp factor in fix *langevin* is inversely related to the gamma factor in fix *viscous*. Also note that the damping factor in fix *langevin* includes the particle mass in Ff, unlike fix *viscous*. Thus the mass and size of different atom types should be accounted for in the choice of ratio values.

The keyword *tally* enables the calculation of the cumulative energy added/subtracted to the atoms as they are thermostatted. Effectively it is the energy exchanged between the infinite thermal reservoir and the particles. As described below, this energy can then be printed out or added to the potential energy of the system to monitor energy conservation.

NOTE: this accumulated energy does NOT include kinetic energy removed by the *zero* flag. LAMMPS will print a warning when both options are active.

The keyword *zero* can be used to eliminate drift due to the thermostat. Because the random forces on different atoms are independent, they do not sum exactly to zero. As a result, this fix applies a small random force to the entire system, and the center-of-mass of the system undergoes a slow random walk. If the keyword *zero* is set to *yes*, the total random force is set exactly to zero by subtracting off an equal part of it from each atom in the group. As a result, the center-of-mass of a system with zero initial momentum will not drift over time.

The keyword *gjf* can be used to run the Gronbech-Jensen/Farago time-discretization of the Langevin model. As described in the papers cited below, the purpose of this method is to enable longer timesteps to be used (up to the numerical stability limit of the integrator), while still producing the correct Boltzmann distribution of atom positions. It is implemented within LAMMPS, by changing how the the random force is applied so that it is composed of the average of two random forces representing half-contributions from the previous and current time intervals.

In common with all methods based on Verlet integration, the discretized velocities generated by this method in conjunction with velocity-Verlet time integration are not exactly conjugate to the positions. As a result the temperature (computed from the discretized velocities) will be systematically lower than the target temperature, by a small amount which grows with the timestep. Nonetheless, the distribution of atom positions will still be consistent with the target temperature.

As an example of using the *gjf* keyword, for molecules containing C-H bonds, configurational properties generated with dt = 2.5 fs and tdamp = 100 fs are indistinguishable from dt = 0.5 fs. Because the velocity distribution systematically decreases with increasing timestep, the method should not be used to generate properties that depend on the velocity distribution, such as the velocity autocorrelation function (VACF). In this example, the velocity distribution at dt = 2.5fs generates an average temperature of 220 K, instead of 300 K.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior.

The fix_modify *temp* option is supported by this fix. You can use it to assign a temperature compute you have defined to this fix which will be used in its thermostatting procedure, as described above. For consistency, the group used by this fix and by the compute should be the same.

The fix_modify *energy* option is supported by this fix to add the energy change induced by Langevin thermostatting to the system's potential energy as part of thermodynamic output. Note that use of this option requires setting the *tally* keyword to *yes*.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the cummulative energy change due to this fix. The scalar value calculated by this fix is "extensive". Note that calculation of this quantity requires setting the *tally* keyword to *yes*.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

fix nvt, fix temp/rescale, fix viscous, fix nvt, pair_style dpd/tstat

Default:

The option defaults are angmom = no, omega = no, scale = 1.0 for all types, tally = no, zero = no, gjf = no.

(Dunweg) Dunweg and Paul, Int J of Modern Physics C, 2, 817-27 (1991).

(Schneider) Schneider and Stoll, Phys Rev B, 17, 1302 (1978).

(Gronbech-Jensen) Gronbech-Jensen and Farago, Mol Phys, 111, 983 (2013); Gronbech-Jensen, Hayre, and Farago, Comp Phys Comm, 185, 524 (2014)

fix langevin/drude command

Syntax:

```
fix ID group-ID langevin/drude Tcom damp_com seed_com Tdrude damp_drude seed_drude keyword values ..
```

- ID, group-ID are documented in fix command
- langevin/drude = style name of this fix command
- Tcom = desired temperature of the centers of mass (temperature units)
- damp_com = damping parameter for the thermostat on centers of mass (time units)
- seed_com = random number seed to use for white noise of the thermostat on centers of mass (positive integer)
- Tdrude = desired temperature of the Drude oscillators (temperature units)
- damp_drude = damping parameter for the thermostat on Drude oscillators (time units)
- seed_drude = random number seed to use for white noise of the thermostat on Drude oscillators (positive integer)
- zero or more keyword/value pairs may be appended
- keyword = *zero*

```
zero value = no or yes
    no = do not set total random force on centers of mass to zero
    yes = set total random force on centers of mass to zero
```

Examples:

```
fix 3 all langevin/drude 300.0 100.0 19377 1.0 20.0 83451
fix 1 all langevin/drude 298.15 100.0 19377 5.0 10.0 83451 zero yes
```

Description:

Apply two Langevin thermostats as described in (Jiang) for thermalizing the reduced degrees of freedom of Drude oscillators. This link describes how to use the thermalized Drude oscillator model in LAMMPS and polarizable models in LAMMPS are discussed in this Section.

Drude oscillators are a way to simulate polarizables atoms, by splitting them into a core and a Drude particle bound by a harmonic bond. The thermalization works by transforming the particles degrees of freedom by these equations. In these equations upper case denotes atomic or center of mass values and lower case denotes Drude particle or dipole values. Primes denote the transformed (reduced) values, while bare letters denote the original values.

Velocities: \begin{equation} V' = \frac {M\, V + m\, v} {M'} \end{equation} \begin{equation} v' = v - V \end{equation} Masses: \begin{equation} M' = M + m \end{equation} \begin{equation} m' = \frac {M\, m } {M'} \end{equation} The Langevin forces are computed as \begin{equation} F' = - \frac {M'} {\mathtt{damp_com}}\, V' + F_r' \end{equation} \begin{equation} f' = - \frac {m'} {\mathtt{damp_drude}}\, v' + f_r' \end{equation}
\(F_r'\) is a random force proportional to \(\sqrt { \frac {2\, k_B \mathtt{Tcom}\, m'} {\mathrm dt\, \mathtt{damp_com} } } \).
\(f_r'\) is a random force proportional to \(\sqrt { \frac {2\, k_B \mathtt{Tdrude}\, m'} {\mathrm dt\, \mathtt{damp_drude} } } \).

Then the real forces acting on the particles are computed from the inverse transform: \begin{equation} F = \frac M {M'}\, F' - f' \end{equation} \begin{equation} f = \frac m {M'}\, F' + f' \end{equation}

This fix also thermostates non-polarizable atoms in the group at temperature *Tcom*, as if they had a massless Drude partner. The Drude particles themselves need not be in the group. The center of mass and the dipole are thermostated iff the core atom is in the group.

Note that the thermostat effect of this fix is applied to only the translational degrees of freedom of the particles, which is an important consideration if finite-size particles, which have rotational degrees of freedom, are being thermostated. The translational degrees of freedom can also have a bias velocity removed from them before thermostating takes place; see the description below.

NOTE: Like the fix langevin command, this fix does NOT perform time integration. It only modifies forces to effect thermostating. Thus you must use a separate time integration fix, like fix nve or fix nph to actually update the velocities and positions of atoms using the modified forces. Likewise, this fix should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by fix nvt or fix temp/rescale commands.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostating.

This fix requires each atom know whether it is a Drude particle or not. You must therefore use the fix drude command to specify the Drude status of each atom type.

NOTE: only the Drude core atoms need to be in the group specified for this fix. A Drude electron will be transformed together with its cores even if it is not itself in the group. It is safe to include Drude electrons or non-polarizable atoms in the group. The non-polarizable atoms will simply be thermostatted as if they had a massless Drude partner (electron).

NOTE: Ghost atoms need to know their velocity for this fix to act correctly. You must use the comm_modify command to enable this, e.g.

```
comm_modify vel yes
```

Tcom is the target temperature of the centers of mass, which would be used to thermostate the non-polarizable atoms. *Tdrude* is the (normally low) target temperature of the core-Drude particle pairs (dipoles). *Tcom* and *Tdrude* can be specified as an equal-style variable. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the target temperature.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent temperature.

Like other fixes that perform thermostating, this fix can be used with compute commands that remove a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute commands to determine which ones include a bias. In this case, the thermostat works in the following manner: bias is removed from each atom, thermostating is performed on the remaining thermal degrees of freedom, and the bias is added back in. NOTE: this feature has not been tested.

Note: The temperature thermostating the core-Drude particle pairs should be chosen low enough, so as to mimic as closely as possible the self-consistent minimization. It must however be high enough, so that the dipoles can follow the local electric field exerted by the neighbouring atoms. The optimal value probably depends on the temperature of the centers of mass and on the mass of the Drude particles.

damp_com is the characteristic time for reaching thermal equilibrium of the centers of mass. For example, a value of 100.0 means to relax the temperature of the centers of mass in a timespan of (roughly) 100 time units (tau or fmsec or psec - see the units command). *damp_drude* is the characteristic time for reaching thermal equilibrium of the dipoles. It is typically a few timesteps.

The number *seed_com* and *seed_drude* are positive integers. They set the seeds of the Marsaglia random number generators used for generating the random forces on centers of mass and on the dipoles. Each processor uses the input seed to generate its own unique seed and its own stream of random numbers. Thus the dynamics of the system will not be identical on two runs on different numbers of processors.

The keyword *zero* can be used to eliminate drift due to the thermostat on centers of mass. Because the random forces on different centers of mass are independent, they do not sum exactly to zero. As a result, this fix applies a small random force to the entire system, and the momentum of the total center of mass of the system undergoes a slow random walk. If the keyword *zero* is set to *yes*, the total random force on the centers of mass is set exactly to zero by subtracting off an equal part of it from each center of mass in the group. As a result, the total center of mass of a system with zero initial momentum will not drift over time.

The actual temperatures of cores and Drude particles, in center-of-mass and relative coordinates, respectively, can be calculated using the compute temp/drude command.

Usage example for rigid bodies in the NPT ensemble:

```
comm_modify vel yes
fix TEMP all langevin/drude 300. 100. 1256 1. 20. 13977 zero yes
fix NPH ATOMS rigid/nph/small molecule iso 1. 1. 500.
fix NVE DRUDES nve
compute TDRUDE all temp/drude
thermo_style custom step cpu etotal ke pe ebond ecoul elong press vol temp c_TDRUDE[1] c_TDRUDE[2]
```

Comments:

- Drude particles should not be in the rigid group, otherwise the Drude oscillators will be frozen and the system will lose its polarizability.
- *zero yes* avoids a drift of the center of mass of the system, but is a bit slower.
- Use two different random seeds to avoid unphysical correlations.
- Temperature is controlled by the fix *langevin/drude*, so the time-integration fixes do not thermostate. Don't forget to time-integrate both cores and Drude particles.
- Pressure is time-integrated only once by using *nve* for Drude particles and *nph* for atoms/cores (or vice versa). Do not use *nph* for both.
- The temperatures of cores and Drude particles are calculated by compute temp/drude
- Contrary to the alternative thermostating using Nose-Hoover thermostat fix *npt* and fix drude/transform, the *fix_modify* command is not required here, because the fix *nph* computes the global pressure even if its group is *ATOMS*. This is what we want. If we thermostated *ATOMS* using *npt*, the pressure should be the global one, but the temperature should be only that of the cores. That's why the command *fix_modify* should be called in that case.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior.

The fix_modify *temp* option is supported by this fix. You can use it to assign a temperature compute you have defined to this fix which will be used in its thermostating procedure, as described above. For consistency, the group used by the compute should include the group of this fix and the Drude particles.

This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

fix langevin, fix drude, fix drude/transform, compute temp/drude, pair_style thole

Default:

The option defaults are zero = no.

(Jiang) Jiang, Hardy, Phillips, MacKerell, Schulten, and Roux, J Phys Chem Lett, 2, 87-92 (2011).

fix langevin/eff command

Syntax:

```
fix ID group-ID langevin/eff Tstart Tstop damp seed keyword values ...
```

- ID, group-ID are documented in fix command
- langevin/eff = style name of this fix command
- Tstart,Tstop = desired temperature at start/end of run (temperature units)
- damp = damping parameter (time units)
- seed = random number seed to use for white noise (positive integer)
- zero or more keyword/value pairs may be appended

```
keyword = scale or tally or zero
  scale values = type ratio
    type = atom type (1-N)
    ratio = factor by which to scale the damping coefficient
  tally values = no or yes
    no = do not tally the energy added/subtracted to atoms
    yes = do tally the energy added/subtracted to atoms

zero value = no or yes
    no = do not set total random force to zero
    yes = set total random force to zero
```

Examples:

```
fix 3 boundary langevin/eff 1.0 1.0 10.0 699483
fix 1 all langevin/eff 1.0 1.1 10.0 48279 scale 3 1.5
```

Description:

Apply a Langevin thermostat as described in (Schneider) to a group of nuclei and electrons in the electron force field model. Used with fix nve/eff, this command performs Brownian dynamics (BD), since the total force on each atom will have the form:

```
F = Fc + Ff + Fr
Ff = - (m / damp) v
Fr is proportional to sqrt(Kb T m / (dt damp))
```

Fc is the conservative force computed via the usual inter-particle interactions (pair_style).

The Ff and Fr terms are added by this fix on a per-particle basis.

The operation of this fix is exactly like that described by the fix langevin command, except that the thermostatting is also applied to the radial electron velocity for electron particles.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior.

The fix_modify *temp* option is supported by this fix. You can use it to assign a temperature compute you have defined to this fix which will be used in its thermostatting procedure, as described above. For consistency, the group used by this fix and by the compute should be the same.

The fix_modify *energy* option is supported by this fix to add the energy change induced by Langevin thermostatting to the system's potential energy as part of thermodynamic output. Note that use of this option requires setting the *tally* keyword to *yes*.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the cummulative energy change due to this fix. The scalar value calculated by this fix is "extensive". Note that calculation of this quantity requires setting the *tally* keyword to *yes*.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions: none

This fix is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix langevin

Default:

The option defaults are scale = 1.0 for all types and tally = no.

(Dunweg) Dunweg and Paul, Int J of Modern Physics C, 2, 817-27 (1991).

(Schneider) Schneider and Stoll, Phys Rev B, 17, 1302 (1978).

fix lb/fluid command

Syntax:

```
fix ID group-ID lb/fluid nevery LBtype viscosity density keyword values ...
```

- ID, group-ID are documented in fix command
- lb/fluid = style name of this fix command
- nevery = update the lattice-Boltzmann fluid every this many timesteps
- LBtype = 1 to use the standard finite difference LB integrator, 2 to use the LB integrator of Ollila et al.
- viscosity = the fluid viscosity (units of mass/(time*length)).
- density = the fluid density.
- zero or more keyword/value pairs may be appended
- keyword = *setArea* or *setGamma* or *scaleGamma* or *dx* or *dm* or *a0* or *noise* or *calcforce* or *trilinear* or *D3Q19* or *read_restart* or *write_restart* or *zwall_velocity* or *bodyforce* or *printfluid*

```
  setArea values = type node_area
        type = atom type (1-N)
        node_area = portion of the surface area of the composite object associated with the part
  setGamma values = gamma
        gamma = user set value for the force coupling constant.
  scaleGamma values = type gammaFactor
        type = atom type (1-N)
        gammaFactor = factor to scale the setGamma gamma value by, for the specified atom type.
  dx values = dx_LB = the lattice spacing.
  dm values = dm_LB = the lattice-Boltzmann mass unit.
  a0 values = a_0_real = the square of the speed of sound in the fluid.
  noise values = Temperature seed
        Temperature = fluid temperature.
        seed = random number generator seed (positive integer)
  calcforce values = N forcegroup-ID
        N = output the force and torque every N timesteps
        forcegroup-ID = ID of the particle group to calculate the force and torque of
  trilinear values = none (used to switch from the default Peskin interpolation stencil to the
  D3Q19 values = none (used to switch from the default D3Q15, 15 velocity lattice, to the D3Q
  read_restart values = restart file = name of the restart file to use to restart a fluid run
  write_restart values = N = write a restart file every N MD timesteps.
  zwall_velocity values = velocity_bottom velocity_top = velocities along the y-direction of t
  bodyforce values = bodyforcex bodyforcey bodyforcez = the x,y and z components of a constant
  printfluid values = N = print the fluid density and velocity at each grid point every N time
```

Examples:

```
fix 1 all lb/fluid 1 2 1.0 1.0 setGamma 13.0 dx 4.0 dm 10.0 calcforce sphere1
fix 1 all lb/fluid 1 1 1.0 0.0009982071 setArea 1 1.144592082 dx 2.0 dm 0.3 trilinear noise 300.0 89
```

Description:

Implement a lattice-Boltzmann fluid on a uniform mesh covering the LAMMPS simulation domain. The MD particles described by *group-ID* apply a velocity dependent force to the fluid.

The lattice-Boltzmann algorithm solves for the fluid motion governed by the Navier Stokes equations,

$$\partial_t \rho + \partial_\beta \left(\rho u_\beta \right) = 0$$

$$\partial_t \left(\rho u_\alpha \right) + \partial_\beta \left(\rho u_\alpha u_\beta \right) = \partial_\beta \sigma_{\alpha\beta} + F_\alpha + \partial_\beta \left(\eta_{\alpha\beta\gamma\nu} \partial_\gamma u_\nu \right)$$

with,

$$\eta_{\alpha\beta\gamma\nu} = \eta \left[\delta_{\alpha\gamma}\delta_{\beta\nu} + \delta_{\alpha\nu}\delta_{\beta\gamma} - \frac{2}{3}\delta_{\alpha\beta}\delta_{\gamma\nu} \right] + \Lambda \delta_{\alpha\beta}\delta_{\gamma\nu}$$

where rho is the fluid density, u is the local fluid velocity, sigma is the stress tensor, F is a local external force, and eta and Lambda are the shear and bulk viscosities respectively. Here, we have implemented

$$\sigma_{\alpha\beta} = -P_{\alpha\beta} = -\rho a_0 \delta_{\alpha\beta}$$

with a_0 set to 1/3 (dx/dt)^2 by default.

The algorithm involves tracking the time evolution of a set of partial distribution functions which evolve according to a velocity discretized version of the Boltzmann equation,

$$\left(\partial_t + e_{i\alpha}\partial_\alpha \right) f_i = -\frac{1}{\tau} \left(f_i - f_i^{eq} \right) + W_i$$

where the first term on the right hand side represents a single time relaxation towards the equilibrium distribution function, and tau is a parameter physically related to the viscosity. On a technical note, we have implemented a 15 velocity model (D3Q15) as default; however, the user can switch to a 19 velocity model (D3Q19) through the use of the *D3Q19* keyword. This fix provides the user with the choice of two algorithms to solve this equation, through the specification of the keyword *LBtype*. If *LBtype* is set equal to 1, the standard finite difference LB integrator is used. If *LBtype* is set equal to 2, the algorithm of Ollila et al. is used.

Physical variables are then defined in terms of moments of the distribution functions,

$$\rho = \sum_i f_i$$

$$\rho u_\alpha = \sum_i f_i e_{i\alpha}$$

Full details of the lattice-Boltzmann algorithm used can be found in Mackay et al..

The fluid is coupled to the MD particles described by *group-ID* through a velocity dependent force. The contribution to the fluid force on a given lattice mesh site j due to MD particle alpha is calculated as:

$$\mathbf{F}_{j\alpha} = \gamma \left(\mathbf{v}_n - \mathbf{u}_f \right) \zeta_{j\alpha}$$

where v_n is the velocity of the MD particle, u_f is the fluid velocity interpolated to the particle location, and gamma is the force coupling constant. Zeta is a weight assigned to the grid point, obtained by distributing the particle to the nearest lattice sites. For this, the user has the choice between a trilinear stencil, which provides a support of 8 lattice sites, or the immersed boundary method Peskin stencil, which provides a support of 64 lattice sites. While the Peskin stencil is seen to provide more stable results, the trilinear stencil may be better suited for simulation of objects close to walls, due to its smaller support. Therefore, by default, the Peskin stencil is used; however the user may switch to the trilinear stencil by specifying the keyword, *trilinear*.

By default, the force coupling constant, gamma, is calculated according to

$$\gamma = \frac{2 m_u m_v}{m_u + m_v} \left(\frac{1}{\Delta t_{collision}} \right)$$

Here, m_v is the mass of the MD particle, m_u is a representative fluid mass at the particle location, and dt_collision is a collision time, chosen such that tau/dt_collision = 1 (see Mackay and Denniston for full details). In order to calculate m_u, the fluid density is interpolated to the MD particle location, and multiplied by a volume, node_area*dx_lb, where node_area represents the portion of the surface area of the composite object associated with a given MD particle. By default, node_area is set equal to dx_lb*dx_lb; however specific values for given atom types can be set using the *setArea* keyword.

The user also has the option of specifying their own value for the force coupling constant, for all the MD particles associated with the fix, through the use of the *setGamma* keyword. This may be useful when modelling porous particles. See Mackay et al. for a detailed description of the method by which the user can choose an appropriate gamma value.

NOTE: while this fix applies the force of the particles on the fluid, it does not apply the force of the fluid to the particles. When the force coupling constant is set using the default method, there is only one option to include this hydrodynamic force on the particles, and that is through the use of the lb/viscous fix. This fix adds the hydrodynamic force to the total force acting on the particles, after which any of the built-in LAMMPS integrators can be used to integrate the particle motion. However, if the user specifies their own value for the force coupling constant, as mentioned in Mackay et al., the built-in LAMMPS integrators may prove to be unstable. Therefore, we have included our own integrators fix lb/rigid/pc/sphere, and fix lb/pc, to solve for the particle motion in these cases. These integrators should not be used with the lb/viscous fix, as they add hydrodynamic forces to the particles directly. In addition, they can not be used if the force coupling constant has been set the default way.

NOTE: if the force coupling constant is set using the default method, and the lb/viscous fix is NOT used to add the hydrodynamic force to the total force acting on the particles, this physically corresponds to a situation in which an infinitely massive particle is moving through the fluid (since collisions between the particle and the fluid do not act to change the particle's velocity). Therefore, the user should set the mass of the particle to be significantly larger than the mass of the fluid at the particle location, in order to approximate an infinitely massive

particle (see the dragforce test run for an example).

Inside the fix, parameters are scaled by the lattice-Boltzmann timestep, dt, grid spacing, dx, and mass unit, dm. dt is set equal to (nevery*dt_MD), where dt_MD is the MD timestep. By default, dm is set equal to 1.0, and dx is chosen so that tau/(dt) = (3*eta*dt)/(rho*dx^2) is approximately equal to 1. However, the user has the option of specifying their own values for dm, and dx, by using the optional keywords *dm*, and *dx* respectively.

NOTE: Care must be taken when choosing both a value for dx, and a simulation domain size. This fix uses the same subdivision of the simulation domain among processors as the main LAMMPS program. In order to uniformly cover the simulation domain with lattice sites, the lengths of the individual LAMMPS subdomains must all be evenly divisible by dx. If the simulation domain size is cubic, with equal lengths in all dimensions, and the default value for dx is used, this will automatically be satisfied.

Physical parameters describing the fluid are specified through *viscosity*, *density*, and *a0*. If the force coupling constant is set the default way, the surface area associated with the MD particles is specified using the *setArea* keyword. If the user chooses to specify a value for the force coupling constant, this is set using the *setGamma* keyword. These parameters should all be given in terms of the mass, distance, and time units chosen for the main LAMMPS run, as they are scaled by the LB timestep, lattice spacing, and mass unit, inside the fix.

The *setArea* keyword allows the user to associate a surface area with a given atom type. For example if a spherical composite object of radius R is represented as a spherical shell of N evenly distributed MD particles, all of the same type, the surface area per particle associated with that atom type should be set equal to 4*pi*R^2/N. This keyword should only be used if the force coupling constant, gamma, is set the default way.

The *setGamma* keyword allows the user to specify their own value for the force coupling constant, gamma, instead of using the default value.

The *scaleGamma* keyword should be used in conjunction with the *setGamma* keyword, when the user wishes to specify different gamma values for different atom types. This keyword allows the user to scale the *setGamma* gamma value by a factor, gammaFactor, for a given atom type.

The *dx* keyword allows the user to specify a value for the LB grid spacing.

The *dm* keyword allows the user to specify the LB mass unit.

If the *a0* keyword is used, the value specified is used for the square of the speed of sound in the fluid. If this keyword is not present, the speed of sound squared is set equal to (1/3)*(dx/dt)^2. Setting a0 > (dx/dt)^2 is not allowed, as this may lead to instabilities.

If the *noise* keyword is used, followed by a a positive temperature value, and a positive integer random number seed, a thermal lattice-Boltzmann algorithm is used. If *LBtype* is set equal to 1 (i.e. the standard LB integrator is chosen), the thermal LB algorithm of Adhikari et al. is used; however if *LBtype* is set equal to 2 both the LB integrator, and thermal LB algorithm described in Ollila et al. are used.

If the *calcforce* keyword is used, both the fluid force and torque acting on the specified particle group are printed to the screen every N timesteps.

If the keyword *trilinear* is used, the trilinear stencil is used to interpolate the particle nodes onto the fluid mesh. By default, the immersed boundary method, Peskin stencil is used. Both of these interpolation methods are described in Mackay et al..

If the keyword *D3Q19* is used, the 19 velocity (D3Q19) lattice is used by the lattice-Boltzmann algorithm. By default, the 15 velocity (D3Q15) lattice is used.

If the keyword *write_restart* is used, followed by a positive integer, N, a binary restart file is printed every N LB timesteps. This restart file only contains information about the fluid. Therefore, a LAMMPS restart file should also be written in order to print out full details of the simulation.

NOTE: When a large number of lattice grid points are used, the restart files may become quite large.

In order to restart the fluid portion of the simulation, the keyword *read_restart* is specified, followed by the name of the binary lb_fluid restart file to be used.

If the *zwall_velocity* keyword is used y-velocities are assigned to the lower and upper walls. This keyword requires the presence of walls in the z-direction. This is set by assigning fixed boundary conditions in the z-direction. If fixed boundary conditions are present in the z-direction, and this keyword is not used, the walls are assumed to be stationary.

If the *bodyforce* keyword is used, a constant body force is added to the fluid, defined by it's x, y and z components.

If the *printfluid* keyword is used, followed by a positive integer, N, the fluid densities and velocities at each lattice site are printed to the screen every N timesteps.

For further details, as well as descriptions and results of several test runs, see Mackay et al.. Please include a citation to this paper if the lb_fluid fix is used in work contributing to published research.

Restart, fix_modify, output, run start/stop, minimize info:

Due to the large size of the fluid data, this fix writes it's own binary restart files, if requested, independent of the main LAMMPS binary restart files; no information about *lb_fluid* is written to the main LAMMPS binary restart files.

None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the USER-LB package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix can only be used with an orthogonal simulation domain.

Walls have only been implemented in the z-direction. Therefore, the boundary conditions, as specified via the main LAMMPS boundary command must be periodic for x and y, and either fixed or periodic for z. Shrink-wrapped boundary conditions are not permitted with this fix.

This fix must be used before any of fix lb/viscous, fix lb/momentum, fix lb/rigid/pc/sphere, and/ or fix lb/pc , as the fluid needs to be initialized before any of these routines try to access its properties. In addition, in order for the hydrodynamic forces to be added to the particles, this fix must be used in conjunction with the lb/viscous fix if the force coupling constant is set by default, or either the lb/viscous fix or one of the lb/rigid/pc/sphere or lb/pc integrators, if the user chooses to specifiy their own value for the force coupling constant.

Related commands:

fix lb/viscous, fix lb/momentum, fix lb/rigid/pc/sphere, fix lb/pc

Default:

By default, the force coupling constant is set according to

$$\gamma = \frac{2m_u m_v}{m_u + m_v}\left(\frac{1}{\Delta t_{collision}}\right)$$

and an area of dx_lb^2 per node, used to calculate the fluid mass at the particle node location, is assumed.

dx is chosen such that tau/(delta t_LB) = (3 eta dt_LB)/(rho dx_lb^2) is approximately equal to 1. dm is set equal to 1.0. a0 is set equal to (1/3)*(dx_lb/dt_lb)^2. The Peskin stencil is used as the default interpolation method. The D3Q15 lattice is used for the lattice-Boltzmann algorithm. If walls are present, they are assumed to be stationary.

(Ollila et al.) Ollila, S.T.T., Denniston, C., Karttunen, M., and Ala-Nissila, T., Fluctuating lattice-Boltzmann model for complex fluids, J. Chem. Phys. 134 (2011) 064902.

(Mackay et al.) Mackay, F. E., Ollila, S.T.T., and Denniston, C., Hydrodynamic Forces Implemented into LAMMPS through a lattice-Boltzmann fluid, Computer Physics Communications 184 (2013) 2021-2031.

(Mackay and Denniston) Mackay, F. E., and Denniston, C., Coupling MD particles to a lattice-Boltzmann fluid through the use of conservative forces, J. Comput. Phys. 237 (2013) 289-298.

(Adhikari et al.) Adhikari, R., Stratford, K., Cates, M. E., and Wagner, A. J., Fluctuating lattice Boltzmann, Europhys. Lett. 71 (2005) 473-479.

fix lb/momentum command

Syntax:

```
fix ID group-ID lb/momentum nevery keyword values ...
```

- ID, group-ID are documented in the fix command
- lb/momentum = style name of this fix command
- nevery = adjust the momentum every this many timesteps
- zero or more keyword/value pairs may be appended
- keyword = *linear*

```
linear values = xflag yflag zflag
    xflag,yflag,zflag = 0/1 to exclude/include each dimension.
```

Examples:

```
fix 1 sphere lb/momentum
fix 1 all lb/momentum linear 1 1 0
```

Description:

This fix is based on the fix momentum command, and was created to be used in place of that command, when a lattice-Boltzmann fluid is present.

Zero the total linear momentum of the system, including both the atoms specified by group-ID and the lattice-Boltzmann fluid every nevery timesteps. This is accomplished by adjusting the particle velocities and the fluid velocities at each lattice site.

NOTE: This fix only considers the linear momentum of the system.

By default, the subtraction is performed for each dimension. This can be changed by specifying the keyword *linear*, along with a set of three flags set to 0/1 in order to exclude/ include the corresponding dimension.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

Can only be used if a lattice-Boltzmann fluid has been created via the fix lb/fluid command, and must come after this command.

This fix is part of the USER-LB package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix momentum, fix lb/fluid

Default:

Zeros the total system linear momentum in each dimension.

fix lb/pc command

Syntax:

```
fix ID group-ID lb/pc
```

- ID, group-ID are documented in the fix command
- lb/pc = style name of this fix command

Examples:

```
fix 1 all lb/pc
```

Description:

Update the positions and velocities of the individual particles described by *group-ID*, experiencing velocity-dependent hydrodynamic forces, using the integration algorithm described in Mackay et al.. This integration algorithm should only be used if a user-specified value for the force-coupling constant used in fix lb/fluid has been set; do not use this integration algorithm if the force coupling constant has been set by default.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the USER-LB package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Can only be used if a lattice-Boltzmann fluid has been created via the fix lb/fluid command, and must come after this command.

Related commands:

fix lb/fluid fix lb/rigid/pc/sphere

Default: None.

(Mackay et al.) Mackay, F. E., Ollila, S.T.T., and Denniston, C., Hydrodynamic Forces Implemented into LAMMPS through a lattice-Boltzmann fluid, Computer Physics Communications 184 (2013) 2021-2031.

fix lb/rigid/pc/sphere command

Syntax:

```
fix ID group-ID lb/rigid/pc/sphere bodystyle args keyword values ...
```

- ID, group-ID are documented in fix command
- lb/rigid/pc/sphere = style name of this fix command
- bodystyle = *single* or *molecule* or *group*
- *single* args = none *molecule* args = none *group* args = N groupID1 groupID2 ... N = # of groups zero or more keyword/value pairs may be appended
- keyword = *force* or *torque* or *innerNodes*

```
  force values = M xflag yflag zflag
      M = which rigid body from 1-Nbody (see asterisk form below)
      xflag,yflag,zflag = off/on if component of center-of-mass force is active
    torque values = M xflag yflag zflag
      M = which rigid body from 1-Nbody (see asterisk form below)
      xflag,yflag,zflag = off/on if component of center-of-mass torque is active
    innerNodes values = innergroup-ID
      innergroup-ID = ID of the atom group which does not experience a hydrodynamic force from t
```

Examples:

```
fix 1 spheres lb/rigid/pc/sphere
fix 1 all lb/rigid/pc/sphere force 1 0 0 innerNodes ForceAtoms
```

Description:

This fix is based on the fix rigid command, and was created to be used in place of that fix, to integrate the equations of motion of spherical rigid bodies when a lattice-Boltzmann fluid is present with a user-specified value of the force-coupling constant. The fix uses the integration algorithm described in Mackay et al. to update the positions, velocities, and orientations of a set of spherical rigid bodies experiencing velocity dependent hydrodynamic forces. The spherical bodies are assumed to rotate as solid, uniform density spheres, with moments of inertia calculated using the combined sum of the masses of all the constituent particles (which are assumed to be point particles).

By default, all of the atoms that this fix acts on experience a hydrodynamic force due to the presence of the lattice-Boltzmann fluid. However, the *innerNodes* keyword allows the user to specify atoms belonging to a rigid object which do not interact with the lattice-Boltzmann fluid (i.e. these atoms do not feel a hydrodynamic force from the lattice-Boltzmann fluid). This can be used to distinguish between atoms on the surface of a non-porous object, and those on the inside.

This feature can be used, for example, when implementing a hard sphere interaction between two spherical objects. Instead of interactions occurring between the particles on the surfaces of the two spheres, it is desirable simply to place an atom at the center of each sphere, which does not contribute to the hydrodynamic force, and have these central atoms interact with one another.

Apart from the features described above, this fix is very similar to the rigid fix (although it includes fewer optional arguments, and assumes the constituent atoms are point particles); see fix_rigid for a complete documentation.

Restart, fix_modify, output, run start/stop, minimize info:

No information about the *rigid* and *rigid/nve* fixes are written to binary restart files.

Similar to the fix_rigid command: " The rigid fix computes a global scalar which can be accessed by various output commands. The scalar value calculated by these fixes is "intensive". The scalar is the current temperature of the collection of rigid bodies. This is averaged over all rigid bodies and their translational and rotational degrees of freedom. The translational energy of a rigid body is 1/2 m v^2, where m = total mass of the body and v = the velocity of its center of mass. The rotational energy of a rigid body is 1/2 I w^2, where I = the moment of inertia tensor of the body and w = its angular velocity. Degrees of freedom constrained by the *force* and *torque* keywords are removed from this calculation."

"All of these fixes compute a global array of values which can be accessed by various output commands. The number of rows in the array is equal to the number of rigid bodies. The number of columns is 15. Thus for each rigid body, 15 values are stored: the xyz coords of the center of mass (COM), the xyz components of the COM velocity, the xyz components of the force acting on the COM, the xyz components of the torque acting on the COM, and the xyz image flags of the COM, which have the same meaning as image flags for atom positions (see the "dump" command). The force and torque values in the array are not affected by the *force* and *torque* keywords in the fix rigid command; they reflect values before any changes are made by those keywords.

The ordering of the rigid bodies (by row in the array) is as follows. For the *single* keyword there is just one rigid body. For the *molecule* keyword, the bodies are ordered by ascending molecule ID. For the *group* keyword, the list of group IDs determines the ordering of bodies.

The array values calculated by these fixes are "intensive", meaning they are independent of the number of atoms in the simulation.

No parameter of these fixes can be used with the *start/stop* keywords of the run command. These fixes are not invoked during energy minimization. "

Restrictions:

This fix is part of the USER-LB package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Can only be used if a lattice-Boltzmann fluid has been created via the fix lb/fluid command, and must come after this command. Should only be used if the force coupling constant used in fix lb/fluid has been set by the user; this integration fix cannot be used if the force coupling constant is set by default.

Related commands:

fix lb/fluid, fix lb/pc

Default:

The defaults are force * on on on, and torque * on on on.

(Mackay et al.) Mackay, F. E., Ollila, S.T.T., and Denniston, C., Hydrodynamic Forces Implemented into LAMMPS through a lattice-Boltzmann fluid, Computer Physics Communications 184 (2013) 2021-2031.

fix lb/viscous command

Syntax:

```
fix ID group-ID lb/viscous
```

- ID, group-ID are documented in fix command
- lb/viscous = style name of this fix command

Examples:

fix 1 flow lb/viscous

Description:

This fix is similar to the fix viscous command, and is to be used in place of that command when a lattice-Boltzmann fluid is present, and the user wishes to integrate the particle motion using one of the built in LAMMPS integrators.

This fix adds a force, F = - Gamma*(velocity-fluid_velocity), to each atom, where Gamma is the force coupling constant described in the fix lb/fluid command (which applies an equal and opposite force to the fluid).

NOTE: This fix should only be used in conjunction with one of the built in LAMMPS integrators; it should not be used with the fix lb/pc or fix lb/rigid/pc/sphere integrators, which already include the hydrodynamic forces. These latter fixes should only be used if the force coupling constant has been set by the user (instead of using the default value); if the default force coupling value is used, then this fix provides the only method for adding the hydrodynamic forces to the particles.

For further details, as well as descriptions and results of several test runs, see Mackay et al.. Please include a citation to this paper if this fix is used in work contributing to published research.

Restart, fix_modify, output, run start/stop, minimize info:

As described in the fix viscous documentation:

"No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command. This fix should only be used with damped dynamics minimizers that allow for non-conservative forces. See the min_style command for details."

Restrictions:

This fix is part of the USER-LB package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Can only be used if a lattice-Boltzmann fluid has been created via the fix lb/fluid command, and must come after this command.

This fix should not be used if either the fix lb/pc or fix lb/rigid/pc/sphere integrator is used.

Related commands:

fix lb/fluid, fix lb/pc, fix lb/rigid/pc/sphere

Default: none

(Mackay et al.) Mackay, F. E., Ollila, S.T.T., and Denniston, C., Hydrodynamic Forces Implemented into LAMMPS through a lattice-Boltzmann fluid, Computer Physics Communications 184 (2013) 2021-2031.

fix lineforce command

Syntax:

```
fix ID group-ID lineforce x y z
```

- ID, group-ID are documented in fix command
- lineforce = style name of this fix command
- x y z = direction of line as a 3-vector

Examples:

```
fix hold boundary lineforce 0.0 1.0 1.0
```

Description:

Adjust the forces on each atom in the group so that only the component of force along the linear direction specified by the vector (x,y,z) remains. This is done by subtracting out components of force in the plane perpendicular to the line.

If the initial velocity of the atom is 0.0 (or along the line), then it should continue to move along the line thereafter.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command.

Restrictions: none

Related commands:

fix planeforce

Default: none

fix meso command

Syntax:

```
fix ID group-ID meso
```

- ID, group-ID are documented in fix command
- meso = style name of this fix command

Examples:

```
fix 1 all meso
```

Description:

Perform time integration to update position, velocity, internal energy and local density for atoms in the group each timestep. This fix is needed to time-integrate mesoscopic systems where particles carry internal variables such as SPH or DPDE.

See this PDF guide to using SPH in LAMMPS.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

"fix meso/stationary"

Default: none

fix meso/stationary command

Syntax:

```
fix ID group-ID meso/stationary
```

- ID, group-ID are documented in fix command
- meso = style name of this fix command

Examples:

```
fix 1 boundary meso/stationary
```

Description:

Perform time integration to update internal energy and local density, but not position or velocity for atoms in the group each timestep. This fix is needed for SPH simulations to correctly time-integrate fixed boundary particles which constrain a fluid to a given region in space.

See this PDF guide to using SPH in LAMMPS.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

"fix meso"

Default: none

fix_modify command

Syntax:

```
fix_modify fix-ID keyword value ...
```

- fix-ID = ID of the fix to modify
- one or more keyword/value pairs may be appended
- keyword = *temp* or *press* or *energy*

```
  temp value = compute ID that calculates a temperature
    press value = compute ID that calculates a pressure
    energy value = yes or no
```

Examples:

```
fix_modify 3 temp myTemp press myPress
fix_modify 1 energy yes
```

Description:

Modify one or more parameters of a previously defined fix. Only specific fix styles support specific parameters. See the doc pages for individual fix commands for info on which ones support which fix_modify parameters.

The *temp* keyword is used to determine how a fix computes temperature. The specified compute ID must have been previously defined by the user via the compute command and it must be a style of compute that calculates a temperature. All fixes that compute temperatures define their own compute by default, as described in their documentation. Thus this option allows the user to override the default method for computing T.

The *press* keyword is used to determine how a fix computes pressure. The specified compute ID must have been previously defined by the user via the compute command and it must be a style of compute that calculates a pressure. All fixes that compute pressures define their own compute by default, as described in their documentation. Thus this option allows the user to override the default method for computing P.

For fixes that calculate a contribution to the potential energy of the system, the *energy* keyword will include that contribution in thermodynamic output of potential energy. See the thermo_style command for info on how potential energy is output. The contribution by itself can be printed by using the keyword f_ID in the thermo_style custom command, where ID is the fix-ID of the appropriate fix. Note that you must use this setting for a fix if you are using it when performing an energy minimization and if you want the energy and forces it produces to be part of the optimization criteria.

Restrictions: none

Related commands:

fix, compute temp, compute pressure, thermo_style

Default:

The option defaults are temp = ID defined by fix, press = ID defined by fix, energy = no.

fix momentum command

Syntax:

```
fix ID group-ID momentum N keyword values ...
```

- ID, group-ID are documented in fix command
- momentum = style name of this fix command
- N = adjust the momentum every this many timesteps one or more keyword/value pairs may be appended
- keyword = *linear* or *angular* or *rescale*

```
  linear values = xflag yflag zflag
      xflag,yflag,zflag = 0/1 to exclude/include each dimension
    angular values = none

  rescale values = none
```

Examples:

```
fix 1 all momentum 1 linear 1 1 0
fix 1 all momentum 1 linear 1 1 1 rescale
fix 1 all momentum 100 linear 1 1 1 angular
```

Description:

Zero the linear and/or angular momentum of the group of atoms every N timesteps by adjusting the velocities of the atoms. One (or both) of the *linear* or *angular* keywords must be specified.

If the *linear* keyword is used, the linear momentum is zeroed by subtracting the center-of-mass velocity of the group from each atom. This does not change the relative velocity of any pair of atoms. One or more dimensions can be excluded from this operation by setting the corresponding flag to 0.

If the *angular* keyword is used, the angular momentum is zeroed by subtracting a rotational component from each atom.

This command can be used to insure the entire collection of atoms (or a subset of them) does not drift or rotate during the simulation due to random perturbations (e.g. fix langevin thermostatting).

The *rescale* keyword enables conserving the kinetic energy of the group of atoms by rescaling the velocities after the momentum was removed.

Note that the velocity command can be used to create initial velocities with zero aggregate linear and/or angular momentum.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

fix recenter, velocity

Default: none

fix move command

Syntax:

```
fix ID group-ID move style args keyword values ...
```

- ID, group-ID are documented in fix command
- move = style name of this fix command
- style = *linear* or *wiggle* or *rotate* or *variable*

```
  linear args = Vx Vy Vz
      Vx,Vy,Vz = components of velocity vector (velocity units), any component can be specified
    wiggle args = Ax Ay Az period
      Ax,Ay,Az = components of amplitude vector (distance units), any component can be specifie
      period = period of oscillation (time units)
    rotate args = Px Py Pz Rx Ry Rz period
      Px,Py,Pz = origin point of axis of rotation (distance units)
      Rx,Ry,Rz = axis of rotation vector
      period = period of rotation (time units)
    variable args = v_dx v_dy v_dz v_vx v_vy v_vz
      v_dx,v_dy,v_dz = 3 variable names that calculate x,y,z displacement as function of time, a
      v_vx,v_vy,v_vz = 3 variable names that calculate x,y,z velocity as function of time, any c
```

- zero or more keyword/value pairs may be appended
- keyword = *units*

```
  units value = box or lattice
```

Examples:

```
fix 1 boundary move wiggle 3.0 0.0 0.0 1.0 units box
fix 2 boundary move rotate 0.0 0.0 0.0 0.0 0.0 1.0 5.0
fix 2 boundary move variable v_myx v_myy NULL v_VX v_VY NULL
```

Description:

Perform updates of position and velocity for atoms in the group each timestep using the specified settings or formulas, without regard to forces on the atoms. This can be useful for boundary or other atoms, whose movement can influence nearby atoms.

NOTE: The atoms affected by this fix should not normally be time integrated by other fixes (e.g. fix nve, fix nvt), since that will change their positions and velocities twice.

NOTE: As atoms move due to this fix, they will pass thru periodic boundaries and be remapped to the other side of the simulation box, just as they would during normal time integration (e.g. via the fix nve command). It is up to you to decide whether periodic boundaries are appropriate with the kind of atom motion you are prescribing with this fix.

NOTE: As dicsussed below, atoms are moved relative to their initial position at the time the fix is specified. These initial coordinates are stored by the fix in "unwrapped" form, by using the image flags associated with each atom. See the dump custom command for a discussion of "unwrapped" coordinates. See the Atoms section of the read_data command for a discussion of image flags and how they are set for each atom. You can reset the image flags (e.g. to 0) before invoking this fix by using the set image command.

The *linear* style moves atoms at a constant velocity, so that their position X = (x,y,z) as a function of time is given in vector notation as

```
X(t) = X0 + V * delta
```

where *X0* = (x0,y0,z0) is their position at the time the fix is specified, *V* is the specified velocity vector with components (Vx,Vy,Vz), and *delta* is the time elapsed since the fix was specified. This style also sets the velocity of each atom to V = (Vx,Vy,Vz). If any of the velocity components is specified as NULL, then the position and velocity of that component is time integrated the same as the fix nve command would perform, using the corresponding force component on the atom.

Note that the *linear* style is identical to using the *variable* style with an equal-style variable that uses the vdisplace() function. E.g.

```
variable V equal 10.0
variable x equal vdisplace(0.0,$V)
fix 1 boundary move variable v_x NULL NULL v_V NULL NULL
```

The *wiggle* style moves atoms in an oscillatory fashion, so that their position X = (x,y,z) as a function of time is given in vector notation as

```
X(t) = X0 + A sin(omega*delta)
```

where *X0* = (x0,y0,z0) is their position at the time the fix is specified, *A* is the specified amplitude vector with components (Ax,Ay,Az), *omega* is 2 PI / *period*, and *delta* is the time elapsed since the fix was specified. This style also sets the velocity of each atom to the time derivative of this expression. If any of the amplitude components is specified as NULL, then the position and velocity of that component is time integrated the same as the fix nve command would perform, using the corresponding force component on the atom.

Note that the *wiggle* style is identical to using the *variable* style with equal-style variables that use the swiggle() and cwiggle() functions. E.g.

```
variable A equal 10.0
variable T equal 5.0
variable omega equal 2.0*PI/$T
variable x equal swiggle(0.0,$A,$T)
variable v equal v_omega*($A-cwiggle(0.0,$A,$T))
fix 1 boundary move variable v_x NULL NULL v_v NULL NULL
```

The *rotate* style rotates atoms around a rotation axis R = (Rx,Ry,Rz) that goes thru a point P = (Px,Py,Pz). The *period* of the rotation is also specified. The direction of rotation for the atoms around the rotation axis is consistent with the right-hand rule: if your right-hand thumb points along R, then your fingers wrap around the axis in the direction of rotation.

This style also sets the velocity of each atom to (omega cross Rperp) where omega is its angular velocity around the rotation axis and Rperp is a perpendicular vector from the rotation axis to the atom. If the defined atom_style assigns an angular velocity or angular moementum or orientation to each atom (atom styles sphere, ellipsoid, line, tri, body), then those properties are also updated appropriately to correspond to the atom's motion and rotation over time.

The *variable* style allows the position and velocity components of each atom to be set by formulas specified via the variable command. Each of the 6 variables is specified as an argument to the fix as v_name, where name is the variable name that is defined elsewhere in the input script.

Each variable must be of either the *equal* or *atom* style. *Equal*-style variables compute a single numeric quantity, that can be a function of the timestep as well as of other simulation values. *Atom*-style variables compute a numeric quantity for each atom, that can be a function per-atom quantities, such as the atom's position, as well as of the timestep and other simulation values. Note that this fix stores the original coordinates of each atom (see note below) so that per-atom quantity can be used in an atom-style variable formula. See the variable command for details.

The first 3 variables (v_dx,v_dy,v_dz) specified for the *variable* style are used to calculate a displacement from the atom's original position at the time the fix was specified. The second 3 variables (v_vx,v_vy,v_vz) specified are used to compute a velocity for each atom.

Any of the 6 variables can be specified as NULL. If both the displacement and velocity variables for a particular x,y,z component are specified as NULL, then the position and velocity of that component is time integrated the same as the fix nve command would perform, using the corresponding force component on the atom. If only the velocity variable for a component is specified as NULL, then the displacement variable will be used to set the position of the atom, and its velocity component will not be changed. If only the displacement variable for a component is specified as NULL, then the velocity variable will be used to set the velocity of the atom, and the position of the atom will be time integrated using that velocity.

The *units* keyword determines the meaning of the distance units used to define the *linear* velocity and *wiggle* amplitude and *rotate* origin. This setting is ignored for the *variable* style. A *box* value selects standard units as defined by the units command, e.g. velocity in Angstroms/fmsec and amplitude and position in Angstroms for units = real. A *lattice* value means the velocity units are in lattice spacings per time and the amplitude and position are in lattice spacings. The lattice command must have been previously used to define the lattice spacing. Each of these 3 quantities may be dependent on the x,y,z dimension, since the lattice spacings can be different in x,y,z.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the original coordinates of moving atoms to binary restart files, as well as the initial timestep, so that the motion can be continuous in a restarted simulation. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

NOTE: Because the move positions are a function of the current timestep and the initial timestep, you cannot reset the timestep to a different value after reading a restart file, if you expect a fix move command to work in an uninterrupted fashion.

None of the fix_modify options are relevant to this fix.

This fix produces a per-atom array which can be accessed by various output commands. The number of columns for each atom is 3, and the columns store the original unwrapped x,y,z coords of each atom. The per-atom values can be accessed on any timestep.

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

For rRESPA time integration, this fix adjusts the position and velocity of atoms on the outermost rRESPA level.

Restrictions: none

Related commands:

fix nve, displace_atoms

Default: none

The option default is units = lattice.

fix msst command

Syntax:

```
fix ID group-ID msst dir shockvel keyword value ...
```

- ID, group-ID are documented in fix command
- msst = style name of this fix
- dir = *x* or *y* or *z*
- shockvel = shock velocity (strictly positive, distance/time units)
- zero or more keyword value pairs may be appended
- keyword = *q* or *mu* or *p0* or *v0* or *e0* or *tscale*

```
  q value = cell mass-like parameter (mass^2/distance^4 units)
    mu value = artificial viscosity (mass/length/time units)
    p0 value = initial pressure in the shock equations (pressure units)
    v0 value = initial simulation cell volume in the shock equations (distance^3 units)
    e0 value = initial total energy (energy units)
    tscale value = reduction in initial temperature (unitless fraction between 0.0 and 1.0)
```

Examples:

```
fix 1 all msst y 100.0 q 1.0e5 mu 1.0e5
fix 2 all msst z 50.0 q 1.0e4 mu 1.0e4  v0 4.3419e+03 p0 3.7797e+03 e0 -9.72360e+02 tscale 0.01
```

Description:

This command performs the Multi-Scale Shock Technique (MSST) integration to update positions and velocities each timestep to mimic a compressive shock wave passing over the system. See (Reed) for a detailed description of this method. The MSST varies the cell volume and temperature in such a way as to restrain the system to the shock Hugoniot and the Rayleigh line. These restraints correspond to the macroscopic conservation laws dictated by a shock front. *shockvel* determines the steady shock velocity that will be simulated.

To perform a simulation, choose a value of *q* that provides volume compression on the timescale of 100 fs to 1 ps. If the volume is not compressing, either the shock speed is chosen to be below the material sound speed or *p0* has been chosen inaccurately. Volume compression at the start can be sped up by using a non-zero value of *tscale*. Use the smallest value of *tscale* that results in compression.

Under some special high-symmetry conditions, the pressure (volume) and/or temperature of the system may oscillate for many cycles even with an appropriate choice of mass-like parameter *q*. Such oscillations have physical significance in some cases. The optional *mu* keyword adds an artificial viscosity that helps break the system symmetry to equilibrate to the shock Hugoniot and Rayleigh line more rapidly in such cases.

tscale is a factor between 0 and 1 that determines what fraction of thermal kinetic energy is converted to compressive strain kinetic energy at the start of the simulation. Setting this parameter to a non-zero value may assist in compression at the start of simulations where it is slow to occur.

If keywords *e0*, *p0*,or *v0* are not supplied, these quantities will be calculated on the first step, after the energy specified by *tscale* is removed. The value of *e0* is not used in the dynamical equations, but is used in calculating the deviation from the Hugoniot.

Values of shockvel less than a critical value determined by the material response will not have compressive solutions. This will be reflected in lack of significant change of the volume in the MSST.

For all pressure styles, the simulation box stays orthogonal in shape. Parrinello-Rahman boundary conditions (tilted box) are supported by LAMMPS, but are not implemented for MSST.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp group-ID temp
compute fix-ID_press group-ID pressure fix-ID_temp
```

See the compute temp and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press". The group for the new computes is "all".

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of all internal variables to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The progress of the MSST can be monitored by printing the global scalar and global vector quantities computed by the fix.

The scalar is the cumulative energy change due to the fix. This is also the energy added to the potential energy by the fix_modify *energy* command. With this command, the thermo keyword *etotal* prints the conserved quantity of the MSST dynamic equations. This can be used to test if the MD timestep is sufficiently small for accurate integration of the dynamic equations. See also thermo_style command.

The global vector contains four values in this order:

[*dhugoniot*, *drayleigh*, *lagrangian_speed*, *lagrangian_position*]

1. *dhugoniot* is the departure from the Hugoniot (temperature units).
2. *drayleigh* is the departure from the Rayleigh line (pressure units).
3. *lagrangian_speed* is the laboratory-frame Lagrangian speed (particle velocity) of the computational cell (velocity units).
4. *lagrangian_position* is the computational cell position in the reference frame moving at the shock speed. This is usually a good estimate of distance of the computational cell behind the shock front.

To print these quantities to the log file with descriptive column headers, the following LAMMPS commands are suggested:

```
fix             msst all msst z
fix_modify      msst energy yes
variable dhug   equal f_msst[1]
variable dray   equal f_msst[2]
variable lgr_vel equal f_msst[3]
variable lgr_pos equal f_msst[4]
thermo_style    custom step temp ke pe lz pzz etotal v_dhug v_dray v_lgr_vel v_lgr_pos f_msst
```

These fixes compute a global scalar and a global vector of 4 quantities, which can be accessed by various output commands. The scalar values calculated by this fix are "extensive"; the vector values are "intensive".

Restrictions:

This fix style is part of the SHOCK package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

All cell dimensions must be periodic. This fix can not be used with a triclinic cell. The MSST fix has been tested only for the group-ID all.

Related commands:

fix nphug, fix deform

Default:

The keyword defaults are q = 10, mu = 0, tscale = 0.01. p0, v0, and e0 are calculated on the first step.

(Reed) Reed, Fried, and Joannopoulos, Phys. Rev. Lett., 90, 235503 (2003).

fix neb command

Syntax:

```
fix ID group-ID neb Kspring
```

- ID, group-ID are documented in fix command
- neb = style name of this fix command
- Kspring = inter-replica spring constant (force/distance units)

Examples:

```
fix 1 active neb 10.0
```

Description:

Add inter-replica forces to atoms in the group for a multi-replica simulation run via the neb command to perform a nudged elastic band (NEB) calculation for transition state finding. Hi-level explanations of NEB are given with the neb command and in Section_howto 5 of the manual. The fix neb command must be used with the "neb" command to define how inter-replica forces are computed.

Only the N atoms in the fix group experience inter-replica forces. Atoms in the two end-point replicas do not experience these forces, but those in intermediate replicas do. During the initial stage of NEB, the 3N-length vector of interatomic forces Fi = -Grad(V) acting on the atoms of each intermediate replica I is altered, as described in the (Henkelman1) paper, to become:

```
Fi = -Grad(V) + (Grad(V) dot That) That + Kspring (|Ri+i - Ri| - |Ri - Ri-1|) That
```

Ri are the atomic coordinates of replica I; Ri-1 and Ri+1 are the coordinates of its neighbor replicas. That (t with a hat over it) is the unit "tangent" vector for replica I which is a function of Ri, Ri-1, Ri+1, and the potential energy of the 3 replicas; it points roughly in the direction of (Ri+i - Ri-1); see the (Henkelman1) paper for details.

The first two terms in the above equation are the component of the interatomic forces perpendicular to the tangent vector. The last term is a spring force between replica I and its neighbors, parallel to the tangent vector direction with the specified spring constant *Kspring*.

The effect of the first two terms is to push the atoms of each replica toward the minimum energy path (MEP) of conformational states that transition over the energy barrier. The MEP for an energy barrier is defined as a sequence of 3N-dimensional states which cross the barrier at its saddle point, each of which has a potential energy gradient parallel to the MEP itself.

The effect of the last term is to push each replica away from its two neighbors in a direction along the MEP, so that the final set of states are equidistant from each other.

During the second stage of NEB, the forces on the N atoms in the replica nearest the top of the energy barrier are altered so that it climbs to the top of the barrier and finds the saddle point. The forces on atoms in this replica are described in the (Henkelman2) paper, and become:

```
Fi = -Grad(V) + 2 (Grad(V) dot That) That
```

The inter-replica forces for the other replicas are unchanged from the first equation.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, as invoked by the minimize command via the neb command.

Restrictions:

This command can only be used if LAMMPS was built with the REPLICA package. See the Making LAMMPS section for more info on packages.

Related commands:

neb

Default: none

(Henkelman1) Henkelman and Jonsson, J Chem Phys, 113, 9978-9985 (2000).

(Henkelman2) Henkelman, Uberuaga, Jonsson, J Chem Phys, 113, 9901-9904 (2000).

fix nvt command

fix nvt/cuda command

fix nvt/intel command

fix nvt/kk command

fix nvt/omp command

fix npt command

fix npt/cuda command

fix npt/intel command

fix npt/kk command

fix npt/omp command

fix nph command

fix nph/kk command

fix nph/omp command

Syntax:

```
fix ID group-ID style_name keyword value ...
```

- ID, group-ID are documented in fix command
- style_name = *nvt* or *npt* or *nph*
- one or more keyword/value pairs may be appended

```
keyword = temp or iso or aniso or tri or x or y or z or xy or yz or xz or couple or tchain or
  temp values = Tstart Tstop Tdamp
    Tstart,Tstop = external temperature at start/end of run
    Tdamp = temperature damping parameter (time units)
  iso or aniso or tri values = Pstart Pstop Pdamp
    Pstart,Pstop = scalar external pressure at start/end of run (pressure units)
    Pdamp = pressure damping parameter (time units)
  x or y or z or xy or yz or xz values = Pstart Pstop Pdamp
    Pstart,Pstop = external stress tensor component at start/end of run (pressure units)
    Pdamp = stress damping parameter (time units)
  couple = none or xyz or xy or yz or xz
  tchain value = N
    N = length of thermostat chain (1 = single thermostat)
  pchain values = N
    N length of thermostat chain on barostat (0 = no thermostat)
  mtk value = yes or no = add in MTK adjustment term or not
```

```
tloop value = M
  M = number of sub-cycles to perform on thermostat
ploop value = M
  M = number of sub-cycles to perform on barostat thermostat
nreset value = reset reference cell every this many timesteps
drag value = Df
  Df = drag factor added to barostat/thermostat (0.0 = no drag)
dilate value = dilate-group-ID
  dilate-group-ID = only dilate atoms in this group due to barostat volume changes
scalexy value = yes or no = scale xy with ly
scaleyz value = yes or no = scale yz with lz
scalexz value = yes or no = scale xz with lz
flip value = yes or no = allow or disallow box flips when it becomes highly skewed
fixedpoint values = x y z
  x,y,z = perform barostat dilation/contraction around this point (distance units)
update value = dipole update dipole orientation (only for sphere variants)
```

Examples:

```
fix 1 all nvt temp 300.0 300.0 100.0
fix 1 water npt temp 300.0 300.0 100.0 iso 0.0 0.0 1000.0
fix 2 jello npt temp 300.0 300.0 100.0 tri 5.0 5.0 1000.0
fix 2 ice nph x 1.0 1.0 0.5 y 2.0 2.0 0.5 z 3.0 3.0 0.5 yz 0.1 0.1 0.5 xz 0.2 0.2 0.5 xy 0.3 0.3 0.5
```

Description:

These commands perform time integration on Nose-Hoover style non-Hamiltonian equations of motion which are designed to generate positions and velocities sampled from the canonical (nvt), isothermal-isobaric (npt), and isenthalpic (nph) ensembles. This updates the position and velocity for atoms in the group each timestep.

The thermostatting and barostatting is achieved by adding some dynamic variables which are coupled to the particle velocities (thermostatting) and simulation domain dimensions (barostatting). In addition to basic thermostatting and barostatting, these fixes can also create a chain of thermostats coupled to the particle thermostat, and another chain of thermostats coupled to the barostat variables. The barostat can be coupled to the overall box volume, or to individual dimensions, including the *xy*, *xz* and *yz* tilt dimensions. The external pressure of the barostat can be specified as either a scalar pressure (isobaric ensemble) or as components of a symmetric stress tensor (constant stress ensemble). When used correctly, the time-averaged temperature and stress tensor of the particles will match the target values specified by Tstart/Tstop and Pstart/Pstop.

The equations of motion used are those of Shinoda et al in (Shinoda), which combine the hydrostatic equations of Martyna, Tobias and Klein in (Martyna) with the strain energy proposed by Parrinello and Rahman in (Parrinello). The time integration schemes closely follow the time-reversible measure-preserving Verlet and rRESPA integrators derived by Tuckerman et al in (Tuckerman).

The thermostat parameters for fix styles *nvt* and *npt* is specified using the *temp* keyword. Other thermostat-related keywords are *tchain*, *tloop* and *drag*, which are discussed below.

The thermostat is applied to only the translational degrees of freedom for the particles. The translational degrees of freedom can also have a bias velocity removed before thermostatting takes place; see the description below. The desired temperature at each timestep is a ramped value during the run from *Tstart* to *Tstop*. The *Tdamp* parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 10.0 means to relax the temperature in a timespan of (roughly) 10 time units (e.g. tau or fmsec or psec - see the units command). The atoms in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the integration.

NOTE: A Nose-Hoover thermostat will not work well for arbitrary values of *Tdamp*. If *Tdamp* is too small, the temperature can fluctuate wildly; if it is too large, the temperature will take a very long time to equilibrate. A good choice for many models is a *Tdamp* of around 100 timesteps. Note that this is NOT the same as 100 time units for most units settings.

The barostat parameters for fix styles *npt* and *nph* is specified using one or more of the *iso*, *aniso*, *tri*, *x*, *y*, *z*, *xy*, *xz*, *yz*, and *couple* keywords. These keywords give you the ability to specify all 6 components of an external stress tensor, and to couple various of these components together so that the dimensions they represent are varied together during a constant-pressure simulation.

Other barostat-related keywords are *pchain*, *mtk*, *ploop*, *nreset*, *drag*, and *dilate*, which are discussed below.

Orthogonal simulation boxes have 3 adjustable dimensions (x,y,z). Triclinic (non-orthogonal) simulation boxes have 6 adjustable dimensions (x,y,z,xy,xz,yz). The create_box, read data, and read_restart commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the xy,xz,yz tilt factors.

The target pressures for each of the 6 components of the stress tensor can be specified independently via the *x*, *y*, *z*, *xy*, *xz*, *yz* keywords, which correspond to the 6 simulation box dimensions. For each component, the external pressure or tensor component at each timestep is a ramped value during the run from *Pstart* to *Pstop*. If a target pressure is specified for a component, then the corresponding box dimension will change during a simulation. For example, if the *y* keyword is used, the y-box length will change. If the *xy* keyword is used, the xy tilt factor will change. A box dimension will not change if that component is not specified, although you have the option to change that dimension via the fix deform command.

Note that in order to use the *xy*, *xz*, or *yz* keywords, the simulation box must be triclinic, even if its initial tilt factors are 0.0.

For all barostat keywords, the *Pdamp* parameter operates like the *Tdamp* parameter, determining the time scale on which pressure is relaxed. For example, a value of 10.0 means to relax the pressure in a timespan of (roughly) 10 time units (e.g. tau or fmsec or psec - see the units command).

NOTE: A Nose-Hoover barostat will not work well for arbitrary values of *Pdamp*. If *Pdamp* is too small, the pressure and volume can fluctuate wildly; if it is too large, the pressure will take a very long time to equilibrate. A good choice for many models is a *Pdamp* of around 1000 timesteps. Note that this is NOT the same as 1000 time units for most units settings.

Regardless of what atoms are in the fix group (the only atoms which are time integrated), a global pressure or stress tensor is computed for all atoms. Similarly, when the size of the simulation box is changed, all atoms are re-scaled to new positions, unless the keyword *dilate* is specified with a *dilate-group-ID* for a group that represents a subset of the atoms. This can be useful, for example, to leave the coordinates of atoms in a solid substrate unchanged and controlling the pressure of a surrounding fluid. This option should be used with care, since it can be unphysical to dilate some atoms and not others, because it can introduce large, instantaneous displacements between a pair of atoms (one dilated, one not) that are far from the dilation origin. Also note that for atoms not in the fix group, a separate time integration fix like fix nve or fix nvt can be used on them, independent of whether they are dilated or not.

The *couple* keyword allows two or three of the diagonal components of the pressure tensor to be "coupled" together. The value specified with the keyword determines which are coupled. For example, *xz* means the *Pxx* and *Pzz* components of the stress tensor are coupled. *Xyz* means all 3 diagonal components are coupled. Coupling means two things: the instantaneous stress will be computed as an average of the corresponding diagonal components, and the coupled box dimensions will be changed together in lockstep, meaning coupled dimensions

will be dilated or contracted by the same percentage every timestep. The *Pstart*, *Pstop*, *Pdamp* parameters for any coupled dimensions must be identical. *Couple xyz* can be used for a 2d simulation; the *z* dimension is simply ignored.

The *iso*, *aniso*, and *tri* keywords are simply shortcuts that are equivalent to specifying several other keywords together.

The keyword *iso* means couple all 3 diagonal components together when pressure is computed (hydrostatic pressure), and dilate/contract the dimensions together. Using "iso Pstart Pstop Pdamp" is the same as specifying these 4 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple xyz
```

The keyword *aniso* means *x*, *y*, and *z* dimensions are controlled independently using the *Pxx*, *Pyy*, and *Pzz* components of the stress tensor as the driving forces, and the specified scalar external pressure. Using "aniso Pstart Pstop Pdamp" is the same as specifying these 4 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple none
```

The keyword *tri* means *x*, *y*, *z*, *xy*, *xz*, and *yz* dimensions are controlled independently using their individual stress components as the driving forces, and the specified scalar pressure as the external normal stress. Using "tri Pstart Pstop Pdamp" is the same as specifying these 7 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
xy 0.0 0.0 Pdamp
yz 0.0 0.0 Pdamp
xz 0.0 0.0 Pdamp
couple none
```

In some cases (e.g. for solids) the pressure (volume) and/or temperature of the system can oscillate undesirably when a Nose/Hoover barostat and thermostat is applied. The optional *drag* keyword will damp these oscillations, although it alters the Nose/Hoover equations. A value of 0.0 (no drag) leaves the Nose/Hoover formalism unchanged. A non-zero value adds a drag term; the larger the value specified, the greater the damping effect. Performing a short run and monitoring the pressure and temperature is the best way to determine if the drag term is working. Typically a value between 0.2 to 2.0 is sufficient to damp oscillations after a few periods. Note that use of the drag keyword will interfere with energy conservation and will also change the distribution of positions and velocities so that they do not correspond to the nominal NVT, NPT, or NPH ensembles.

An alternative way to control initial oscillations is to use chain thermostats. The keyword *tchain* determines the number of thermostats in the particle thermostat. A value of 1 corresponds to the original Nose-Hoover thermostat. The keyword *pchain* specifies the number of thermostats in the chain thermostatting the barostat degrees of freedom. A value of 0 corresponds to no thermostatting of the barostat variables.

The *mtk* keyword controls whether or not the correction terms due to Martyna, Tuckerman, and Klein are included in the equations of motion (Martyna). Specifying *no* reproduces the original Hoover barostat, whose volume probability distribution function differs from the true NPT and NPH ensembles by a factor of 1/V. Hence using *yes* is more correct, but in many cases the difference is negligible.

The keyword *tloop* can be used to improve the accuracy of integration scheme at little extra cost. The initial and final updates of the thermostat variables are broken up into *tloop* substeps, each of length *dt*/*tloop*. This corresponds to using a first-order Suzuki-Yoshida scheme (Tuckerman). The keyword *ploop* does the same thing for the barostat thermostat.

The keyword *nreset* controls how often the reference dimensions used to define the strain energy are reset. If this keyword is not used, or is given a value of zero, then the reference dimensions are set to those of the initial simulation domain and are never changed. If the simulation domain changes significantly during the simulation, then the final average pressure tensor will differ significantly from the specified values of the external stress tensor. A value of *nstep* means that every *nstep* timesteps, the reference dimensions are set to those of the current simulation domain.

The *scaleyz*, *scalexz*, and *scalexy* keywords control whether or not the corresponding tilt factors are scaled with the associated box dimensions when barostatting triclinic periodic cells. The default values *yes* will turn on scaling, which corresponds to adjusting the linear dimensions of the cell while preserving its shape. Choosing *no* ensures that the tilt factors are not scaled with the box dimensions. See below for restrictions and default values in different situations. In older versions of LAMMPS, scaling of tilt factors was not performed. The old behavior can be recovered by setting all three scale keywords to *no*.

The *flip* keyword allows the tilt factors for a triclinic box to exceed half the distance of the parallel box length, as discussed below. If the *flip* value is set to *yes*, the bound is enforced by flipping the box when it is exceeded. If the *flip* value is set to *no*, the tilt will continue to change without flipping. Note that if applied stress induces large deformations (e.g. in a liquid), this means the box shape can tilt dramatically and LAMMPS will run less efficiently, due to the large volume of communication needed to acquire ghost atoms around a processor's irregular-shaped sub-domain. For extreme values of tilt, LAMMPS may also lose atoms and generate an error.

The *fixedpoint* keyword specifies the fixed point for barostat volume changes. By default, it is the center of the box. Whatever point is chosen will not move during the simulation. For example, if the lower periodic boundaries pass through (0,0,0), and this point is provided to *fixedpoint*, then the lower periodic boundaries will remain at (0,0,0), while the upper periodic boundaries will move twice as far. In all cases, the particle trajectories are unaffected by the chosen value, except for a time-dependent constant translation of positions.

If the *update* keyword is used with the *dipole* value, then the orientation of the dipole moment of each particle is also updated during the time integration. This option should be used for models where a dipole moment is assigned to finite-size particles, e.g. spheroids via use of the atom_style hybrid sphere dipole command.

NOTE: Using a barostat coupled to tilt dimensions *xy*, *xz*, *yz* can sometimes result in arbitrarily large values of the tilt dimensions, i.e. a dramatically deformed simulation box. LAMMPS allows the tilt factors to grow a small amount beyond the normal limit of half the box length (0.6 times the box length), and then performs a box "flip" to an equivalent periodic cell. See the discussion of the *flip* keyword above, to allow this bound to be exceeded, if desired.

The flip operation is described in more detail in the doc page for fix deform. Both the barostat dynamics and the atom trajectories are unaffected by this operation. However, if a tilt factor is incremented by a large amount (1.5 times the box length) on a single timestep, LAMMPS can not accomodate this event and will terminate the simulation with an error. This error typically indicates that there is something badly wrong with how the simulation was constructed, such as specifying values of *Pstart* that are too far from the current stress value, or specifying a timestep that is too large. Triclinic barostatting should be used with care. This also is true for other barostat styles, although they tend to be more forgiving of insults. In particular, it is important to recognize that equilibrium liquids can not support a shear stress and that equilibrium solids can not support shear stresses that exceed the yield stress.

One exception to this rule is if the 1st dimension in the tilt factor (x for xy) is non-periodic. In that case, the limits on the tilt factor are not enforced, since flipping the box in that dimension does not change the atom positions due to non-periodicity. In this mode, if you tilt the system to extreme angles, the simulation will simply become inefficient due to the highly skewed simulation box.

NOTE: Unlike the fix temp/berendsen command which performs thermostatting but NO time integration, these fixes perform thermostatting/barostatting AND time integration. Thus you should not use any other time integration fix, such as fix nve on atoms to which this fix is applied. Likewise, fix nvt and fix npt should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by fix langevin or fix temp/rescale commands.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting and barostatting.

These fixes compute a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp" and "pressure", as if one of these two sets of commands had been issued:

```
compute fix-ID_temp group-ID temp
compute fix-ID_press group-ID pressure fix-ID_temp

compute fix-ID_temp all temp
compute fix-ID_press all pressure fix-ID_temp
```

See the compute temp and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press". For fix nvt, the group for the new computes is the same as the fix group. For fix nph and fix npt, the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the compute_modify command or print this temperature or pressure during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Like other fixes that perform thermostatting, fix nvt and fix npt can be used with compute commands that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute commands to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

These fixes can be used with either the *verlet* or *respa* integrators. When using one of the barostat fixes with *respa*, LAMMPS uses an integrator constructed according to the following factorization of the Liouville propagator (for two rRESPA levels):

$$\begin{aligned}\exp\left(\mathrm{i}L\Delta t\right) = & \exp\left(\mathrm{i}L_{\text{T-baro}}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_{\text{T-part}}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_{\epsilon,2}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_2^{(2)}\frac{\Delta t}{2}\right) \\ & \times\left[\exp\left(\mathrm{i}L_2^{(1)}\frac{\Delta t}{2n}\right)\exp\left(\mathrm{i}L_{\epsilon,1}\frac{\Delta t}{n}\right)\exp\left(\mathrm{i}L_1\frac{\Delta t}{n}\right)\exp\left(\mathrm{i}L_2^{(1)}\frac{\Delta t}{2n}\right)\right]^n \\ & \times\exp\left(\mathrm{i}L_2^{(2)}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_{\epsilon,2}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_{\text{T-part}}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_{\text{T-baro}}\frac{\Delta t}{2}\right) \\ & +\mathcal{O}\left(\Delta t^3\right)\end{aligned}$$

This factorization differs somewhat from that of Tuckerman et al, in that the barostat is only updated at the outermost rRESPA level, whereas Tuckerman's factorization requires splitting the pressure into pieces corresponding to the forces computed at each rRESPA level. In theory, the latter method will exhibit better numerical stability. In practice, because Pdamp is normally chosen to be a large multiple of the outermost rRESPA timestep, the barostat dynamics are not the limiting factor for numerical stability. Both factorizations are time-reversible and can be shown to preserve the phase space measure of the underlying non-Hamiltonian equations of motion.

NOTE: This implementation has been shown to conserve linear momentum up to machine precision under NVT dynamics. Under NPT dynamics, for a system with zero initial total linear momentum, the total momentum fluctuates close to zero. It may occasionally undergo brief excursions to non-negligible values, before returning close to zero. Over long simulations, this has the effect of causing the center-of-mass to undergo a slow random walk. This can be mitigated by resetting the momentum at infrequent intervals using the fix momentum command.

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The fix npt and fix nph commands can be used with rigid bodies or mixtures of rigid bodies and non-rigid particles (e.g. solvent). But there are also fix rigid/npt and fix rigid/nph commands, which are typically a more natural choice. See the doc page for those commands for more discussion of the various ways to do this.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

These fixes writes the state of all the thermostat and barostat variables to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify *temp* and *press* options are supported by these fixes. You can use them to assign a compute you have defined to this fix which will be used in its thermostatting or barostatting procedure, as described above. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

NOTE: If both the *temp* and *press* keywords are used in a single thermo_modify command (or in two separate commands), then the order in which the keywords are specified is important. Note that a pressure compute defines its own temperature compute as an argument when it is specified. The *temp* keyword will override this (for the pressure compute being used by fix npt), but only if the *temp* keyword comes after the *press* keyword. If the *temp* keyword comes before the *press* keyword, then the new pressure compute specified by the *press* keyword will be unaffected by the *temp* setting.

The fix_modify *energy* option is supported by these fixes to add the energy change induced by Nose/Hoover thermostatting and barostatting to the system's potential energy as part of thermodynamic output.

These fixes compute a global scalar and a global vector of quantities, which can be accessed by various output commands. The scalar value calculated by these fixes is "extensive"; the vector values are "intensive".

The scalar is the cumulative energy change due to the fix.

The vector stores internal Nose/Hoover thermostat and barostat variables. The number and meaning of the vector values depends on which fix is used and the settings for keywords *tchain* and *pchain*, which specify the number of Nose/Hoover chains for the thermostat and barostat. If no thermostatting is done, then *tchain* is 0. If no barostatting is done, then *pchain* is 0. In the following list, "ndof" is 0, 1, 3, or 6, and is the number of degrees of freedom in the barostat. Its value is 0 if no barostat is used, else its value is 6 if any off-diagonal stress tensor component is barostatted, else its value is 1 if *couple xyz* is used or *couple xy* for a 2d simulation, otherwise its value is 3.

The order of values in the global vector and their meaning is as follows. The notation means there are tchain values for eta, followed by tchain for eta_dot, followed by ndof for omega, etc:

- eta[tchain] = particle thermostat displacements (unitless)
- eta_dot[tchain] = particle thermostat velocities (1/time units)
- omega[ndof] = barostat displacements (unitless)
- omega_dot[ndof] = barostat velocities (1/time units)
- etap[pchain] = barostat thermostat displacements (unitless)
- etap_dot[pchain] = barostat thermostat velocities (1/time units)
- PE_eta[tchain] = potential energy of each particle thermostat displacement (energy units)
- KE_eta_dot[tchain] = kinetic energy of each particle thermostat velocity (energy units)
- PE_omega[ndof] = potential energy of each barostat displacement (energy units)
- KE_omega_dot[ndof] = kinetic energy of each barostat velocity (energy units)
- PE_etap[pchain] = potential energy of each barostat thermostat displacement (energy units)
- KE_etap_dot[pchain] = kinetic energy of each barostat thermostat velocity (energy units)

- PE_strain[1] = scalar strain energy (energy units)

These fixes can ramp their external temperature and pressure over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

These fixes are not invoked during energy minimization.

Restrictions:

X, *y*, *z* cannot be barostatted if the associated dimension is not periodic. *Xy*, *xz*, and *yz* can only be barostatted if the simulation domain is triclinic and the 2nd dimension in the keyword (*y* dimension in *xy*) is periodic. *Z*, *xz*, and *yz*, cannot be barostatted for 2D simulations. The create_box, read data, and read_restart commands specify whether the simulation box is orthogonal or non-orthogonal (triclinic) and explain the meaning of the xy,xz,yz tilt factors.

For the *temp* keyword, the final Tstop cannot be 0.0 since it would make the external T = 0.0 at some timestep during the simulation which is not allowed in the Nose/Hoover formulation.

The *scaleyz yes* and *scalexz yes* keyword/value pairs can not be used for 2D simulations. *scaleyz yes*, *scalexz yes*, and *scalexy yes* options can only be used if the 2nd dimension in the keyword is periodic, and if the tilt factor is not coupled to the barostat via keywords *tri*, *yz*, *xz*, and *xy*.

These fixes can be used with dynamic groups as defined by the group command. Likewise they can be used with groups to which atoms are added or deleted over time, e.g. a deposition simulation. However, the conservation properties of the thermostat and barostat are defined for systems with a static set of atoms. You may observe odd behavior if the atoms in a group vary dramatically over time or the atom count becomes very small.

Related commands:

fix nve, fix_modify, run_style

Default:

The keyword defaults are tchain = 3, pchain = 3, mtk = yes, tloop = ploop = 1, nreset = 0, drag = 0.0, dilate = all, couple = none, scaleyz = scalexz = scalexy = yes if periodic in 2nd dimension and not coupled to barostat, otherwise no.

(Martyna) Martyna, Tobias and Klein, J Chem Phys, 101, 4177 (1994).

(Parrinello) Parrinello and Rahman, J Appl Phys, 52, 7182 (1981).

(Tuckerman) Tuckerman, Alejandre, Lopez-Rendon, Jochim, and Martyna, J Phys A: Math Gen, 39, 5629 (2006).

(Shinoda) Shinoda, Shiga, and Mikami, Phys Rev B, 69, 134103 (2004).

fix nvt/eff command

fix npt/eff command

fix nph/eff command

Syntax:

```
fix ID group-ID style_name keyword value ...
```

- ID, group-ID are documented in fix command
- style_name = *nvt/eff* or *npt/eff* or *nph/eff*

```
one or more keyword value pairs may be appended
keyword = temp or iso or aniso or tri or x or y or z or xy or yz or xz or couple or tchain or
  temp values = Tstart Tstop Tdamp
    Tstart,Tstop = external temperature at start/end of run
    Tdamp = temperature damping parameter (time units)
  iso or aniso or tri values = Pstart Pstop Pdamp
    Pstart,Pstop = scalar external pressure at start/end of run (pressure units)
    Pdamp = pressure damping parameter (time units)
  x or y or z or xy or yz or xz values = Pstart Pstop Pdamp
    Pstart,Pstop = external stress tensor component at start/end of run (pressure units)
    Pdamp = stress damping parameter (time units)
  couple = none or xyz or xy or yz or xz
  tchain value = length of thermostat chain (1 = single thermostat)
  pchain values = length of thermostat chain on barostat (0 = no thermostat)
  mtk value = yes or no = add in MTK adjustment term or not
  tloop value = number of sub-cycles to perform on thermostat
  ploop value = number of sub-cycles to perform on barostat thermostat
  nreset value = reset reference cell every this many timesteps
  drag value = drag factor added to barostat/thermostat (0.0 = no drag)
  dilate value = all or partial
```

Examples:

```
fix 1 all nvt/eff temp 300.0 300.0 0.1
fix 1 part npt/eff temp 300.0 300.0 0.1 iso 0.0 0.0 1.0
fix 2 part npt/eff temp 300.0 300.0 0.1 tri 5.0 5.0 1.0
fix 2 ice nph/eff x 1.0 1.0 0.5 y 2.0 2.0 0.5 z 3.0 3.0 0.5 yz 0.1 0.1 0.5 xz 0.2 0.2 0.5 xy 0.3 0.3
```

Description:

These commands perform time integration on Nose-Hoover style non-Hamiltonian equations of motion for nuclei and electrons in the group for the electron force field model. The fixes are designed to generate positions and velocities sampled from the canonical (nvt), isothermal-isobaric (npt), and isenthalpic (nph) ensembles. This is achieved by adding some dynamic variables which are coupled to the particle velocities (thermostatting) and simulation domain dimensions (barostatting). In addition to basic thermostatting and barostatting, these fixes can also create a chain of thermostats coupled to the particle thermostat, and another chain of thermostats coupled to the barostat variables. The barostat can be coupled to the overall box volume, or to individual dimensions, including the *xy*, *xz* and *yz* tilt dimensions. The external pressure of the barostat can be specified as either a scalar pressure (isobaric ensemble) or as components of a symmetric stress tensor (constant stress ensemble). When used correctly, the time-averaged temperature and stress tensor of the particles will match the target values specified by Tstart/Tstop and Pstart/Pstop.

The operation of these fixes is exactly like that described by the fix nvt, npt, and nph commands, except that the radius and radial velocity of electrons are also updated. Likewise the temperature and pressure calculated by the fix, using the computes it creates (as discussed in the fix nvt, npt, and nph doc page), are performed with computes that include the eFF contribution to the temperature or kinetic energy from the electron radial velocity.

NOTE: there are two different pressures that can be reported for eFF when defining the pair_style (see pair eff/cut to understand these settings), one (default) that considers electrons do not contribute radial virial components (i.e. electrons treated as incompressible 'rigid' spheres) and one that does. The radial electronic contributions to the virials are only tallied if the flexible pressure option is set, and this will affect both global and per-atom quantities. In principle, the true pressure of a system is somewhere in between the rigid and the flexible eFF pressures, but, for most cases, the difference between these two pressures will not be significant over long-term averaged runs (i.e. even though the energy partitioning changes, the total energy remains similar).

NOTE: currently, there is no available option for the user to set or create temperature distributions that include the radial electronic degrees of freedom with the velocity command, so the the user must allow for these degrees of freedom to equilibrate (i.e. equi-partitioning of energy) through time integration.

Restart, fix_modify, output, run start/stop, minimize info:

See the doc page for the fix nvt, npt, and nph commands for details.

Restrictions:

This fix is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Other restriction discussed on the doc page for the fix nvt, npt, and nph commands also apply.

NOTE: The temperature for systems (regions or groups) with only electrons and no nuclei is 0.0 (i.e. not defined) in the current temperature calculations, a practical example would be a uniform electron gas or a very hot plasma, where electrons remain delocalized from the nuclei. This is because, even though electron virials are included in the temperature calculation, these are averaged over the nuclear degrees of freedom only. In such cases a corrective term must be added to the pressure to get the correct kinetic contribution.

Related commands:

fix nvt, fix nph, fix npt, fix_modify, run_style

Default:

The keyword defaults are tchain = 3, pchain = 3, mtk = yes, tloop = ploop = 1, nreset = 0, drag = 0.0, dilate = all, and couple = none.

(Martyna) Martyna, Tobias and Klein, J Chem Phys, 101, 4177 (1994).

(Parrinello) Parrinello and Rahman, J Appl Phys, 52, 7182 (1981).

(Tuckerman) Tuckerman, Alejandre, Lopez-Rendon, Jochim, and Martyna, J Phys A: Math Gen, 39, 5629 (2006).

(Shinoda) Shinoda, Shiga, and Mikami, Phys Rev B, 69, 134103 (2004).

fix nph/asphere command

fix nph/asphere/omp command

Syntax:

```
fix ID group-ID nph/asphere args keyword value ...
```

- ID, group-ID are documented in fix command
- nph/asphere = style name of this fix command
- additional barostat related keyword/value pairs from the fix nph command can be appended

Examples:

```
fix 1 all nph/asphere iso 0.0 0.0 1000.0
fix 2 all nph/asphere x 5.0 5.0 1000.0
fix 2 all nph/asphere x 5.0 5.0 1000.0 drag 0.2
fix 2 water nph/asphere aniso 0.0 0.0 1000.0 dilate partial
```

Description:

Perform constant NPH integration to update position, velocity, orientation, and angular velocity each timestep for aspherical or ellipsoidal particles in the group using a Nose/Hoover pressure barostat. P is pressure; H is enthalpy. This creates a system trajectory consistent with the isenthalpic ensemble.

This fix differs from the fix nph command, which assumes point particles and only updates their position and velocity.

Additional parameters affecting the barostat are specified by keywords and values documented with the fix nph command. See, for example, discussion of the *aniso*, and *dilate* keywords.

The particles in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the NPH integration.

Regardless of what particles are in the fix group, a global pressure is computed for all particles. Similarly, when the size of the simulation box is changed, all particles are re-scaled to new positions, unless the keyword *dilate* is specified with a value of *partial*, in which case only the particles in the fix group are re-scaled. The latter can be useful for leaving the coordinates of particles in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp/asphere" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp all temp/asphere
compute fix-ID_press all pressure fix-ID_temp
```

See the compute temp/asphere and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the compute_modify command or print this temperature or pressure during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover barostat to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify *temp* and *press* options are supported by this fix. You can use them to assign a compute you have defined to this fix which will be used in its thermostatting or barostatting procedure. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The fix_modify *energy* option is supported by this fix to add the energy change induced by Nose/Hoover barostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the fix nph command.

This fix can ramp its target pressure over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that atoms store torque and angular momementum and a quaternion as defined by the atom_style ellipsoid command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

Related commands:

fix nph, fix nve_asphere, fix nvt_asphere, fix npt_asphere, fix_modify

Default: none

fix nph/body command

Syntax:

```
fix ID group-ID nph/body args keyword value ...
```

- ID, group-ID are documented in fix command
- nph/body = style name of this fix command
- additional barostat related keyword/value pairs from the fix nph command can be appended

Examples:

```
fix 1 all nph/body iso 0.0 0.0 1000.0
fix 2 all nph/body x 5.0 5.0 1000.0
fix 2 all nph/body x 5.0 5.0 1000.0 drag 0.2
fix 2 water nph/body aniso 0.0 0.0 1000.0 dilate partial
```

Description:

Perform constant NPH integration to update position, velocity, orientation, and angular velocity each timestep for body particles in the group using a Nose/Hoover pressure barostat. P is pressure; H is enthalpy. This creates a system trajectory consistent with the isenthalpic ensemble.

This fix differs from the fix nph command, which assumes point particles and only updates their position and velocity.

Additional parameters affecting the barostat are specified by keywords and values documented with the fix nph command. See, for example, discussion of the *aniso*, and *dilate* keywords.

The particles in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the NPH integration.

Regardless of what particles are in the fix group, a global pressure is computed for all particles. Similarly, when the size of the simulation box is changed, all particles are re-scaled to new positions, unless the keyword *dilate* is specified with a value of *partial*, in which case only the particles in the fix group are re-scaled. The latter can be useful for leaving the coordinates of particles in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp/body" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp all temp/body
compute fix-ID_press all pressure fix-ID_temp
```

See the compute temp/body and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the compute_modify command or print this temperature or pressure during thermodynamic output via the

thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover barostat to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify *temp* and *press* options are supported by this fix. You can use them to assign a compute you have defined to this fix which will be used in its thermostatting or barostatting procedure. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The fix_modify *energy* option is supported by this fix to add the energy change induced by Nose/Hoover barostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the fix nph command.

This fix can ramp its target pressure over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the BODY package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that atoms store torque and angular momementum and a quaternion as defined by the atom_style body command.

Related commands:

fix nph, fix nve_body, fix nvt_body, fix npt_body, fix_modify

Default: none

fix nph/sphere command

fix nph/sphere/omp command

Syntax:

```
fix ID group-ID nph/sphere args keyword value ...
```

- ID, group-ID are documented in fix command
- nph/sphere = style name of this fix command
- additional barostat related keyword/value pairs from the fix nph command can be appended

Examples:

```
fix 1 all nph/sphere iso 0.0 0.0 1000.0
fix 2 all nph/sphere x 5.0 5.0 1000.0
fix 2 all nph/sphere x 5.0 5.0 1000.0 drag 0.2
fix 2 water nph/sphere aniso 0.0 0.0 1000.0 dilate partial
```

Description:

Perform constant NPH integration to update position, velocity, and angular velocity each timestep for finite-size spherical particles in the group using a Nose/Hoover pressure barostat. P is pressure; H is enthalpy. This creates a system trajectory consistent with the isenthalpic ensemble.

This fix differs from the fix nph command, which assumes point particles and only updates their position and velocity.

Additional parameters affecting the barostat are specified by keywords and values documented with the fix nph command. See, for example, discussion of the *aniso*, and *dilate* keywords.

The particles in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the NPH integration.

Regardless of what particles are in the fix group, a global pressure is computed for all particles. Similarly, when the size of the simulation box is changed, all particles are re-scaled to new positions, unless the keyword *dilate* is specified with a value of *partial*, in which case only the particles in the fix group are re-scaled. The latter can be useful for leaving the coordinates of particles in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp/sphere" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp all temp/sphere
compute fix-ID_press all pressure fix-ID_temp
```

See the compute temp/sphere and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the compute_modify command or print this temperature or pressure during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover barostat to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify *temp* and *press* options are supported by this fix. You can use them to assign a compute you have defined to this fix which will be used in its thermostatting or barostatting procedure. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The fix_modify *energy* option is supported by this fix to add the energy change induced by Nose/Hoover barostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the fix nph command.

This fix can ramp its target pressure over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

This fix requires that atoms store torque and angular velocity (omega) and a radius as defined by the atom_style sphere command.

All particles in the group must be finite-size spheres. They cannot be point particles.

Related commands:

fix nph, fix nve_sphere, fix nvt_sphere, fix npt_sphere, fix_modify

Default: none

fix nphug command

fix nphug/omp command

Syntax:

```
fix ID group-ID nphug keyword value ...
```

- ID, group-ID are documented in fix command

```
one or more keyword value pairs may be appended
keyword = temp or iso or aniso or tri or x or y or z or couple or tchain or pchain or mtk or
  temp values = Value1 Value2 Tdamp
    Value1, Value2 = Nose-Hoover target temperatures, ignored by Hugoniostat
    Tdamp = temperature damping parameter (time units)
  iso or aniso or tri values = Pstart Pstop Pdamp
    Pstart,Pstop = scalar external pressures, must be equal (pressure units)
    Pdamp = pressure damping parameter (time units)
  x or y or z or xy or yz or xz values = Pstart Pstop Pdamp
    Pstart,Pstop = external stress tensor components, must be equal (pressure units)
    Pdamp = stress damping parameter (time units)
  couple = none or xyz or xy or yz or xz
  tchain value = length of thermostat chain (1 = single thermostat)
  pchain values = length of thermostat chain on barostat (0 = no thermostat)
  mtk value = yes or no = add in MTK adjustment term or not
  tloop value = number of sub-cycles to perform on thermostat
  ploop value = number of sub-cycles to perform on barostat thermostat
  nreset value = reset reference cell every this many timesteps
  drag value = drag factor added to barostat/thermostat (0.0 = no drag)
  dilate value = all or partial
  scaleyz value = yes or no = scale yz with lz
  scalexz value = yes or no = scale xz with lz
  scalexy value = yes or no = scale xy with ly
```

Examples:

```
fix myhug all nphug temp 1.0 1.0 10.0 z 40.0 40.0 70.0
fix myhug all nphug temp 1.0 1.0 10.0 iso 40.0 40.0 70.0 drag 200.0 tchain 1 pchain 0
```

Description:

This command is a variant of the Nose-Hoover fix npt fix style. It performs time integration of the Hugoniostat equations of motion developed by Ravelo et al. (Ravelo). These equations compress the system to a state with average axial stress or pressure equal to the specified target value and that satisfies the Rankine-Hugoniot (RH) jump conditions for steady shocks.

The compression can be performed either hydrostatically (using keyword *iso*, *aniso*, or *tri*) or uniaxially (using keywords *x*, *y*, or *z*). In the hydrostatic case, the cell dimensions change dynamically so that the average axial stress in all three directions converges towards the specified target value. In the uniaxial case, the chosen cell dimension changes dynamically so that the average axial stress in that direction converges towards the target value. The other two cell dimensions are kept fixed (zero lateral strain).

This leads to the following additional restrictions on the keywords:

- One and only one of the following keywords should be used: *iso*, *aniso*, *tri*, *x*, *y*, *z*
- The specified initial and final target pressures must be the same.
- The keywords *xy*, *xz*, *yz* may not be used.
- The only admissible value for the couple keyword is *xyz*, which has the same effect as keyword *iso*
- The *temp* keyword must be used to specify the time constant for kinetic energy relaxation, but initial and final target temperature values are ignored.

Essentially, a Hugoniostat simulation is an NPT simulation in which the user-specified target temperature is replaced with a time-dependent target temperature Tt obtained from the following equation:

$$T_t - T = \frac{\left(\frac{1}{2}\left(P + P_0\right)\left(V_0 - V\right) + E_0 - E\right)}{N_{dof} k_B} = Delta$$

where T and Tt are the instantaneous and target temperatures, P and P0 are the instantaneous and reference pressures or axial stresses, depending on whether hydrostatic or uniaxial compression is being performed, V and V0 are the instantaneous and reference volumes, E and E0 are the instantaneous and reference internal energy (potential plus kinetic), Ndof is the number of degrees of freedom used in the definition of temperature, and kB is the Boltzmann constant. Delta is the negative deviation of the instantaneous temperature from the target temperature. When the system reaches a stable equilibrium, the value of Delta should fluctuate about zero.

The values of E0, V0, and P0 are the instantaneous values at the start of the simulation. These can be overridden using the fix_modify keywords *e0*, *v0*, and *p0* described below.

NOTE: Unlike the fix temp/berendsen command which performs thermostatting but NO time integration, this fix performs thermostatting/barostatting AND time integration. Thus you should not use any other time integration fix, such as fix nve on atoms to which this fix is applied. Likewise, this fix should not be used on atoms that have their temperature controlled by another fix - e.g. by fix langevin or fix temp/rescale commands.

This fix computes a temperature and pressure at each timestep. To do this, the fix creates its own computes of style "temp" and "pressure", as if one of these two sets of commands had been issued:

```
compute fix-ID_temp group-ID temp
compute fix-ID_press group-ID pressure fix-ID_temp

compute fix-ID_temp all temp
compute fix-ID_press all pressure fix-ID_temp
```

See the compute temp and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press". The group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the compute_modify command or print this temperature or pressure during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in

Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the values of E0, V0, and P0, as well as the state of all the thermostat and barostat variables to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify *e0*, *v0* and *p0* keywords can be used to define the values of E0, V0, and P0. Note the the values for *e0* and *v0* are extensive, and so must correspond to the total energy and volume of the entire system, not energy and volume per atom. If any of these quantities are not specified, then the instantaneous value in the system at the start of the simulation is used.

The fix_modify *temp* and *press* options are supported by these fixes. You can use them to assign a compute you have defined to this fix which will be used in its thermostatting or barostatting procedure, as described above. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The fix_modify *energy* option is supported by these fixes to add the energy change induced by Nose/Hoover thermostatting and barostatting to the system's potential energy as part of thermodynamic output. Either way, this energy is *not* included in the definition of internal energy E when calculating the value of Delta in the above equation.

These fixes compute a global scalar and a global vector of quantities, which can be accessed by various output commands. The scalar value calculated by these fixes is "extensive"; the vector values are "intensive".

The scalar is the cumulative energy change due to the fix.

The vector stores three quantities unique to this fix (Delta, Us, and up), followed by all the internal Nose/Hoover thermostat and barostat variables defined for fix_style npt. Delta is the deviation of the temperature from the target temperature, given by the above equation. Us and up are the shock and particle velocity corresponding to a steady shock calculated from the RH conditions. They have units of distance/time.

Restrictions:

This fix style is part of the SHOCK package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

All the usual restrictions for fix_style npt apply, plus the additional ones mentioned above.

Related commands:

fix msst, fix npt, fix_modify

Default:

The keyword defaults are the same as those for fix npt

(Ravelo) Ravelo, Holian, Germann and Lomdahl, Phys Rev B, 70, 014103 (2004).

fix npt/asphere command

fix npt/asphere/omp command

Syntax:

```
fix ID group-ID npt/asphere keyword value ...
```

- ID, group-ID are documented in fix command
- npt/asphere = style name of this fix command
- additional thermostat and barostat related keyword/value pairs from the fix npt command can be appended

Examples:

```
fix 1 all npt/asphere temp 300.0 300.0 100.0 iso 0.0 0.0 1000.0
fix 2 all npt/asphere temp 300.0 300.0 100.0 x 5.0 5.0 1000.0
fix 2 all npt/asphere temp 300.0 300.0 100.0 x 5.0 5.0 1000.0 drag 0.2
fix 2 water npt/asphere temp 300.0 300.0 100.0 aniso 0.0 0.0 1000.0 dilate partial
```

Description:

Perform constant NPT integration to update position, velocity, orientation, and angular velocity each timestep for aspherical or ellipsoidal particles in the group using a Nose/Hoover temperature thermostat and Nose/Hoover pressure barostat. P is pressure; T is temperature. This creates a system trajectory consistent with the isothermal-isobaric ensemble.

This fix differs from the fix npt command, which assumes point particles and only updates their position and velocity.

The thermostat is applied to both the translational and rotational degrees of freedom for the aspherical particles, assuming a compute is used which calculates a temperature that includes the rotational degrees of freedom (see below). The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

Additional parameters affecting the thermostat and barostat are specified by keywords and values documented with the fix npt command. See, for example, discussion of the *temp*, *iso*, *aniso*, and *dilate* keywords.

The particles in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the NPT integration.

Regardless of what particles are in the fix group, a global pressure is computed for all particles. Similarly, when the size of the simulation box is changed, all particles are re-scaled to new positions, unless the keyword *dilate* is specified with a value of *partial*, in which case only the particles in the fix group are re-scaled. The latter can be useful for leaving the coordinates of particles in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp/asphere" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp all temp/asphere
```

```
compute fix-ID_press all pressure fix-ID_temp
```

See the compute temp/asphere and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the compute_modify command or print this temperature or pressure during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with compute commands that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute commands to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat and barostat to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify *temp* and *press* options are supported by this fix. You can use them to assign a compute you have defined to this fix which will be used in its thermostatting or barostatting procedure. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The fix_modify *energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting and barostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the fix npt command.

This fix can ramp its target temperature and pressure over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that atoms store torque and angular momementum and a quaternion as defined by the atom_style ellipsoid command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

Related commands:

fix npt, fix nve_asphere, fix nvt_asphere, fix_modify

Default: none

fix npt/body command

Syntax:

```
fix ID group-ID npt/body keyword value ...
```

- ID, group-ID are documented in fix command
- npt/body = style name of this fix command
- additional thermostat and barostat related keyword/value pairs from the fix npt command can be appended

Examples:

```
fix 1 all npt/body temp 300.0 300.0 100.0 iso 0.0 0.0 1000.0
fix 2 all npt/body temp 300.0 300.0 100.0 x 5.0 5.0 1000.0
fix 2 all npt/body temp 300.0 300.0 100.0 x 5.0 5.0 1000.0 drag 0.2
fix 2 water npt/body temp 300.0 300.0 100.0 aniso 0.0 0.0 1000.0 dilate partial
```

Description:

Perform constant NPT integration to update position, velocity, orientation, and angular velocity each timestep for body particles in the group using a Nose/Hoover temperature thermostat and Nose/Hoover pressure barostat. P is pressure; T is temperature. This creates a system trajectory consistent with the isothermal-isobaric ensemble.

This fix differs from the fix npt command, which assumes point particles and only updates their position and velocity.

The thermostat is applied to both the translational and rotational degrees of freedom for the body particles, assuming a compute is used which calculates a temperature that includes the rotational degrees of freedom (see below). The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

Additional parameters affecting the thermostat and barostat are specified by keywords and values documented with the fix npt command. See, for example, discussion of the *temp*, *iso*, *aniso*, and *dilate* keywords.

The particles in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the NPT integration.

Regardless of what particles are in the fix group, a global pressure is computed for all particles. Similarly, when the size of the simulation box is changed, all particles are re-scaled to new positions, unless the keyword *dilate* is specified with a value of *partial*, in which case only the particles in the fix group are re-scaled. The latter can be useful for leaving the coordinates of particles in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp/body" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp all temp/body
compute fix-ID_press all pressure fix-ID_temp
```

See the compute temp/body and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the compute_modify command or print this temperature or pressure during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with compute commands that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute commands to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat and barostat to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify *temp* and *press* options are supported by this fix. You can use them to assign a compute you have defined to this fix which will be used in its thermostatting or barostatting procedure. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The fix_modify *energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting and barostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the fix npt command.

This fix can ramp its target temperature and pressure over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the BODY package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that atoms store torque and angular momementum and a quaternion as defined by the atom_style body command.

Related commands:

fix npt, fix nve_body, fix nvt_body, fix_modify

Default: none

fix npt/sphere command

fix npt/sphere/omp command

Syntax:

```
fix ID group-ID npt/sphere keyword value ...
```

- ID, group-ID are documented in fix command
- npt/sphere = style name of this fix command
- additional thermostat and barostat related keyword/value pairs from the fix npt command can be appended

Examples:

```
fix 1 all npt/sphere temp 300.0 300.0 100.0 iso 0.0 0.0 1000.0
fix 2 all npt/sphere temp 300.0 300.0 100.0 x 5.0 5.0 1000.0
fix 2 all npt/sphere temp 300.0 300.0 100.0 x 5.0 5.0 1000.0 drag 0.2
fix 2 water npt/sphere temp 300.0 300.0 100.0 aniso 0.0 0.0 1000.0 dilate partial
```

Description:

Perform constant NPT integration to update position, velocity, and angular velocity each timestep for finite-sizex spherical particles in the group using a Nose/Hoover temperature thermostat and Nose/Hoover pressure barostat. P is pressure; T is temperature. This creates a system trajectory consistent with the isothermal-isobaric ensemble.

This fix differs from the fix npt command, which assumes point particles and only updates their position and velocity.

The thermostat is applied to both the translational and rotational degrees of freedom for the spherical particles, assuming a compute is used which calculates a temperature that includes the rotational degrees of freedom (see below). The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

Additional parameters affecting the thermostat and barostat are specified by keywords and values documented with the fix npt command. See, for example, discussion of the *temp*, *iso*, *aniso*, and *dilate* keywords.

The particles in the fix group are the only ones whose velocities and positions are updated by the velocity/position update portion of the NPT integration.

Regardless of what particles are in the fix group, a global pressure is computed for all particles. Similarly, when the size of the simulation box is changed, all particles are re-scaled to new positions, unless the keyword *dilate* is specified with a value of *partial*, in which case only the particles in the fix group are re-scaled. The latter can be useful for leaving the coordinates of particles in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style "temp/sphere" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp all temp/sphere
compute fix-ID_press all pressure fix-ID_temp
```

See the compute temp/sphere and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is "all" since pressure is computed for the entire system.

Note that these are NOT the computes used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the compute_modify command or print this temperature or pressure during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with compute commands that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute commands to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat and barostat to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify *temp* and *press* options are supported by this fix. You can use them to assign a compute you have defined to this fix which will be used in its thermostatting or barostatting procedure. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

The fix_modify *energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting and barostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the fix npt command.

This fix can ramp its target temperature and pressure over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

This fix requires that atoms store torque and angular velocity (omega) and a radius as defined by the atom_style sphere command.

All particles in the group must be finite-size spheres. They cannot be point particles.

Related commands:

fix npt, fix nve_sphere, fix nvt_sphere, fix npt_asphere, fix_modify

Default: none

fix nve command

fix nve/cuda command

fix nve/intel command

fix nve/kk command

fix nve/omp command

Syntax:

```
fix ID group-ID nve
```

- ID, group-ID are documented in fix command
- nve = style name of this fix command

Examples:

```
fix 1 all nve
```

Description:

Perform constant NVE integration to update position and velocity for atoms in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

fix nvt, fix npt

Default: none

fix nve/asphere command

fix nve/asphere/intel command

Syntax:

```
fix ID group-ID nve/asphere
```

- ID, group-ID are documented in fix command
- nve/asphere = style name of this fix command

Examples:

```
fix 1 all nve/asphere
```

Description:

Perform constant NVE integration to update position, velocity, orientation, and angular velocity for aspherical particles in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble.

This fix differs from the fix nve command, which assumes point particles and only updates their position and velocity.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that atoms store torque and angular momementum and a quaternion as defined by the atom_style ellipsoid command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

Related commands:

fix nve, fix nve/sphere

Default: none

fix nve/asphere/noforce command

Syntax:

```
fix ID group-ID nve/asphere/noforce
```

- ID, group-ID are documented in fix command
- nve/asphere/noforce = style name of this fix command

Examples:

fix 1 all nve/asphere/noforce

Description:

Perform updates of position and orientation, but not velocity or angular momentum for atoms in the group each timestep. In other words, the force and torque on the atoms is ignored and their velocity and angular momentum are not updated. The atom velocities and angularm momenta are used to update their positions and orientation.

This is useful as an implicit time integrator for Fast Lubrication Dynamics, since the velocity and angular momentum are updated by the pair_style lubricuteU command.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that atoms store torque and angular momementum and a quaternion as defined by the atom_style ellipsoid command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

Related commands:

fix nve/noforce, fix nve/asphere

Default: none

fix nve/body command

Syntax:

```
fix ID group-ID nve/body
```

- ID, group-ID are documented in fix command
- nve/body = style name of this fix command

Examples:

```
fix 1 all nve/body
```

Description:

Perform constant NVE integration to update position, velocity, orientation, and angular velocity for body particles in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble. See Section_howto 14 of the manual and the body doc page for more details on using body particles.

This fix differs from the fix nve command, which assumes point particles and only updates their position and velocity.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the BODY package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that atoms store torque and angular momementum and a quaternion as defined by the atom_style body command.

All particles in the group must be body particles. They cannot be point particles.

Related commands:

fix nve, fix nve/sphere, fix nve/asphere

Default: none

fix nve/eff command

Syntax:

```
fix ID group-ID nve/eff
```

- ID, group-ID are documented in fix command
- nve/eff = style name of this fix command

Examples:

```
fix 1 all nve/eff
```

Description:

Perform constant NVE integration to update position and velocity for nuclei and electrons in the group for the electron force field model. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble.

The operation of this fix is exactly like that described by the fix nve command, except that the radius and radial velocity of electrons are also updated.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix nve, fix nvt/eff, fix npt/eff

Default: none

fix nve/limit command

Syntax:

```
fix ID group-ID nve/limit xmax
```

- ID, group-ID are documented in fix command
- nve = style name of this fix command
- xmax = maximum distance an atom can move in one timestep (distance units)

Examples:

```
fix 1 all nve/limit 0.1
```

Description:

Perform constant NVE updates of position and velocity for atoms in the group each timestep. A limit is imposed on the maximum distance an atom can move in one timestep. This is useful when starting a simulation with a configuration containing highly overlapped atoms. Normally this would generate huge forces which would blow atoms out of the simulation box, causing LAMMPS to stop with an error.

Using this fix can overcome that problem. Forces on atoms must still be computable (which typically means 2 atoms must have a separation distance > 0.0). But large velocities generated by large forces are reset to a value that corresponds to a displacement of length *xmax* in a single timestep. *Xmax* is specified in distance units; see the units command for details. The value of *xmax* should be consistent with the neighbor skin distance and the frequency of neighbor list re-building, so that pairwise interactions are not missed on successive timesteps as atoms move. See the neighbor and neigh_modify commands for details.

Note that if a velocity reset occurs the integrator will not conserve energy. On steps where no velocity resets occur, this integrator is exactly like the fix nve command. Since forces are unaltered, pressures computed by thermodynamic output will still be very large for overlapped configurations.

NOTE: You should not use fix shake in conjunction with this fix. That is because fix shake applies contraint forces based on the predicted postitions of atoms after the next timestep. It has no way of knowing the timestep may change due to this fix, which will cause the constraint forces to be invalid. A better strategy is to turn off fix shake when performing initial dynamics that need this fix, then turn fix shake on when doing normal dynamics with a fixed-size timestep.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the count of how many updates of atom's velocity/position were limited by the maximum distance criterion. This should be roughly the number of atoms so affected, except that updates occur at both the beginning and end of a timestep in a velocity Verlet timestepping algorithm. This is a cumulative quantity for the current run, but is re-initialized to zero each time a run is performed. The scalar value calculated by this fix is "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

fix nve, fix nve/noforce, pair_style soft

Default: none

fix nve/line command

Syntax:

```
fix ID group-ID nve/line
```

- ID, group-ID are documented in fix command
- nve/line = style name of this fix command

Examples:

```
fix 1 all nve/line
```

Description:

Perform constant NVE integration to update position, velocity, orientation, and angular velocity for line segment particles in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble. See Section_howto 14 of the manual for an overview of using line segment particles.

This fix differs from the fix nve command, which assumes point particles and only updates their position and velocity.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that particles be line segments as defined by the atom_style line command.

Related commands:

fix nve, fix nve/asphere

Default: none

fix nve/noforce command

Syntax:

```
fix ID group-ID nve
```

- ID, group-ID are documented in fix command
- nve/noforce = style name of this fix command

Examples:

```
fix 3 wall nve/noforce
```

Description:

Perform updates of position, but not velocity for atoms in the group each timestep. In other words, the force on the atoms is ignored and their velocity is not updated. The atom velocities are used to update their positions.

This can be useful for wall atoms, when you set their velocities, and want the wall to move (or stay stationary) in a prescribed fashion.

This can also be accomplished via the fix setforce command, but with fix nve/noforce, the forces on the wall atoms are unchanged, and can thus be printed by the dump command or queried with an equal-style variable that uses the fcm() group function to compute the total force on the group of atoms.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

fix nve

Default: none

fix nve/sphere command

fix nve/sphere/omp command

Syntax:

```
fix ID group-ID nve/sphere
```

- ID, group-ID are documented in fix command
- nve/sphere = style name of this fix command
- zero or more keyword/value pairs may be appended
- keyword = *update*

```
update value = dipole
    dipole = update orientation of dipole moment during integration
```

Examples:

```
fix 1 all nve/sphere
fix 1 all nve/sphere update dipole
```

Description:

Perform constant NVE integration to update position, velocity, and angular velocity for finite-size spherical particles in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble.

This fix differs from the fix nve command, which assumes point particles and only updates their position and velocity.

If the *update* keyword is used with the *dipole* value, then the orientation of the dipole moment of each particle is also updated during the time integration. This option should be used for models where a dipole moment is assigned to finite-size particles, e.g. spheroids via use of the atom_style hybrid sphere dipole command.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix requires that atoms store torque and angular velocity (omega) and a radius as defined by the atom_style sphere command. If the *dipole* keyword is used, then they must also store a dipole moment as defined by the atom_style dipole command.

All particles in the group must be finite-size spheres. They cannot be point particles.

Related commands:

fix nve, fix nve/asphere

Default: none

fix nve/tri command

Syntax:

```
fix ID group-ID nve/tri
```

- ID, group-ID are documented in fix command
- nve/tri = style name of this fix command

Examples:

```
fix 1 all nve/tri
```

Description:

Perform constant NVE integration to update position, velocity, orientation, and angular momentum for triangular particles in the group each timestep. V is volume; E is energy. This creates a system trajectory consistent with the microcanonical ensemble. See Section_howto 14 of the manual for an overview of using triangular particles.

This fix differs from the fix nve command, which assumes point particles and only updates their position and velocity.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that particles be triangles as defined by the atom_style tri command.

Related commands:

fix nve, fix nve/asphere

Default: none

fix nvt/asphere command

fix nvt/asphere/omp command

Syntax:

```
fix ID group-ID nvt/asphere keyword value ...
```

- ID, group-ID are documented in fix command
- nvt/asphere = style name of this fix command
- additional thermostat related keyword/value pairs from the fix nvt command can be appended

Examples:

```
fix 1 all nvt/asphere temp 300.0 300.0 100.0
fix 1 all nvt/asphere temp 300.0 300.0 100.0 drag 0.2
```

Description:

Perform constant NVT integration to update position, velocity, orientation, and angular velocity each timestep for aspherical or ellipsoidal particles in the group using a Nose/Hoover temperature thermostat. V is volume; T is temperature. This creates a system trajectory consistent with the canonical ensemble.

This fix differs from the fix nvt command, which assumes point particles and only updates their position and velocity.

The thermostat is applied to both the translational and rotational degrees of freedom for the aspherical particles, assuming a compute is used which calculates a temperature that includes the rotational degrees of freedom (see below). The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

Additional parameters affecting the thermostat are specified by keywords and values documented with the fix nvt command. See, for example, discussion of the *temp* and *drag* keywords.

This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp/asphere", as if this command had been issued:

```
compute fix-ID_temp group-ID temp/asphere
```

See the compute temp/asphere command for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp*. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the compute_modify command or print this temperature during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with compute commands that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a

group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute commands to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify *temp* option is supported by this fix. You can use it to assign a compute you have defined to this fix which will be used in its thermostatting procedure.

The fix_modify *energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the fix nvt command.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that atoms store torque and angular momementum and a quaternion as defined by the atom_style ellipsoid command.

All particles in the group must be finite-size. They cannot be point particles, but they can be aspherical or spherical as defined by their shape attribute.

Related commands:

fix nvt, fix nve_asphere, fix npt_asphere, fix_modify

Default: none

fix nvt/body command

Syntax:

```
fix ID group-ID nvt/body keyword value ...
```

- ID, group-ID are documented in fix command
- nvt/body = style name of this fix command
- additional thermostat related keyword/value pairs from the fix nvt command can be appended

Examples:

```
fix 1 all nvt/body temp 300.0 300.0 100.0
fix 1 all nvt/body temp 300.0 300.0 100.0 drag 0.2
```

Description:

Perform constant NVT integration to update position, velocity, orientation, and angular velocity each timestep for body particles in the group using a Nose/Hoover temperature thermostat. V is volume; T is temperature. This creates a system trajectory consistent with the canonical ensemble.

This fix differs from the fix nvt command, which assumes point particles and only updates their position and velocity.

The thermostat is applied to both the translational and rotational degrees of freedom for the body particles, assuming a compute is used which calculates a temperature that includes the rotational degrees of freedom (see below). The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

Additional parameters affecting the thermostat are specified by keywords and values documented with the fix nvt command. See, for example, discussion of the *temp* and *drag* keywords.

This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp/body", as if this command had been issued:

```
compute fix-ID_temp group-ID temp/body
```

See the compute temp/body command for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp*. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the compute_modify command or print this temperature during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with compute commands that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute

commands to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify *temp* option is supported by this fix. You can use it to assign a compute you have defined to this fix which will be used in its thermostatting procedure.

The fix_modify *energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the fix nvt command.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the BODY package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires that atoms store torque and angular momementum and a quaternion as defined by the atom_style body command.

Related commands:

fix nvt, fix nve_body, fix npt_body, fix_modify

Default: none

fix nvt/sllod command

fix nvt/sllod/intel command

fix nvt/sllod/omp command

Syntax:

```
fix ID group-ID nvt/sllod keyword value ...
```

- ID, group-ID are documented in fix command
- nvt/sllod = style name of this fix command
- additional thermostat related keyword/value pairs from the fix nvt command can be appended

Examples:

```
fix 1 all nvt/sllod temp 300.0 300.0 100.0
fix 1 all nvt/sllod temp 300.0 300.0 100.0 drag 0.2
```

Description:

Perform constant NVT integration to update positions and velocities each timestep for atoms in the group using a Nose/Hoover temperature thermostat. V is volume; T is temperature. This creates a system trajectory consistent with the canonical ensemble.

This thermostat is used for a simulation box that is changing size and/or shape, for example in a non-equilibrium MD (NEMD) simulation. The size/shape change is induced by use of the fix deform command, so each point in the simulation box can be thought of as having a "streaming" velocity. This position-dependent streaming velocity is subtracted from each atom's actual velocity to yield a thermal velocity which is used for temperature computation and thermostatting. For example, if the box is being sheared in x, relative to y, then points at the bottom of the box (low y) have a small x velocity, while points at the top of the box (hi y) have a large x velocity. These velocities do not contribute to the thermal "temperature" of the atom.

NOTE: Fix deform has an option for remapping either atom coordinates or velocities to the changing simulation box. To use fix nvt/sllod, fix deform should NOT remap atom positions, because fix nvt/sllod adjusts the atom positions and velocities to create a velocity profile that matches the changing box size/shape. Fix deform SHOULD remap atom velocities when atoms cross periodic boundaries since that is consistent with maintaining the velocity profile created by fix nvt/sllod. LAMMPS will give an error if this setting is not consistent.

The SLLOD equations of motion, originally proposed by Hoover and Ladd (see (Evans and Morriss)), were proven to be equivalent to Newton's equations of motion for shear flow by (Evans and Morriss). They were later shown to generate the desired velocity gradient and the correct production of work by stresses for all forms of homogeneous flow by (Daivis and Todd). As implemented in LAMMPS, they are coupled to a Nose/Hoover chain thermostat in a velocity Verlet formulation, closely following the implementation used for the fix nvt command.

Additional parameters affecting the thermostat are specified by keywords and values documented with the fix nvt command. See, for example, discussion of the *temp* and *drag* keywords.

This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp/deform", as if this command had been issued:

```
compute fix-ID_temp group-ID temp/deform
```

See the compute temp/deform command for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp*. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the compute_modify command or print this temperature during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with compute commands that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute commands to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify *temp* option is supported by this fix. You can use it to assign a compute you have defined to this fix which will be used in its thermostatting procedure.

The fix_modify *energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the fix nvt command.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

This fix works best without Nose-Hoover chain thermostats, i.e. using tchain = 1. Setting tchain to larger values can result in poor equilibration.

Related commands:

fix nve, fix nvt, fix temp/rescale, fix langevin, fix_modify, compute temp/deform

Default:

Same as fix nvt, except tchain = 1.

(Evans and Morriss) Evans and Morriss, Phys Rev A, 30, 1528 (1984).

(Daivis and Todd) Daivis and Todd, J Chem Phys, 124, 194103 (2006).

fix nvt/sllod/eff command

Syntax:

```
fix ID group-ID nvt/sllod/eff keyword value ...
```

- ID, group-ID are documented in fix command
- nvt/sllod/eff = style name of this fix command
- additional thermostat related keyword/value pairs from the fix nvt/eff command can be appended

Examples:

```
fix 1 all nvt/sllod/eff temp 300.0 300.0 0.1
fix 1 all nvt/sllod/eff temp 300.0 300.0 0.1 drag 0.2
```

Description:

Perform constant NVT integration to update positions and velocities each timestep for nuclei and electrons in the group for the electron force field model, using a Nose/Hoover temperature thermostat. V is volume; T is temperature. This creates a system trajectory consistent with the canonical ensemble.

The operation of this fix is exactly like that described by the fix nvt/sllod command, except that the radius and radial velocity of electrons are also updated and thermostatted. Likewise the temperature calculated by the fix, using the compute it creates (as discussed in the fix nvt, npt, and nph doc page), is performed with a compute temp/deform/eff commmand that includes the eFF contribution to the temperature from the electron radial velocity.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify *temp* option is supported by this fix. You can use it to assign a compute you have defined to this fix which will be used in its thermostatting procedure.

The fix_modify *energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the fix nvt/eff command.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix works best without Nose-Hoover chain thermostats, i.e. using tchain = 1. Setting tchain to larger values can result in poor equilibration.

Related commands:

fix nve/eff, fix nvt/eff, fix langevin/eff, fix nvt/sllod, fix_modify, compute temp/deform/eff

Default:

Same as fix nvt/eff, except tchain = 1.

(Tuckerman) Tuckerman, Mundy, Balasubramanian, Klein, J Chem Phys, 106, 5615 (1997).

fix nvt/sphere command

fix nvt/sphere/omp command

Syntax:

```
fix ID group-ID nvt/sphere keyword value ...
```

- ID, group-ID are documented in fix command
- nvt/sphere = style name of this fix command
- additional thermostat related keyword/value pairs from the fix nvt command can be appended

Examples:

```
fix 1 all nvt/sphere temp 300.0 300.0 100.0
fix 1 all nvt/sphere temp 300.0 300.0 100.0 drag 0.2
```

Description:

Perform constant NVT integration to update position, velocity, and angular velocity each timestep for finite-size spherical particles in the group using a Nose/Hoover temperature thermostat. V is volume; T is temperature. This creates a system trajectory consistent with the canonical ensemble.

This fix differs from the fix nvt command, which assumes point particles and only updates their position and velocity.

The thermostat is applied to both the translational and rotational degrees of freedom for the spherical particles, assuming a compute is used which calculates a temperature that includes the rotational degrees of freedom (see below). The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

Additional parameters affecting the thermostat are specified by keywords and values documented with the fix nvt command. See, for example, discussion of the *temp* and *drag* keywords.

This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp/sphere", as if this command had been issued:

```
compute fix-ID_temp group-ID temp/sphere
```

See the compute temp/sphere command for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp*. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the compute_modify command or print this temperature during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with compute commands that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a

group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute commands to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the state of the Nose/Hoover thermostat to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify *temp* option is supported by this fix. You can use it to assign a compute you have defined to this fix which will be used in its thermostatting procedure.

The fix_modify *energy* option is supported by this fix to add the energy change induced by Nose/Hoover thermostatting to the system's potential energy as part of thermodynamic output.

This fix computes the same global scalar and global vector of quantities as does the fix nvt command.

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

This fix requires that atoms store torque and angular velocity (omega) and a radius as defined by the atom_style sphere command.

All particles in the group must be finite-size spheres. They cannot be point particles.

Related commands:

fix nvt, fix nve_sphere, fix nvt_asphere, fix npt_sphere, fix_modify

Default: none

fix oneway command

Syntax:

```
fix ID group-ID oneway N region-ID direction
```

- ID, group-ID are documented in fix command
- oneway = style name of this fix command
- N = apply this fix every this many timesteps
- region-ID = ID of region where fix is active
- direction = *x* or *-x* or *y* or *-y* or *z* or *-z* = coordinate and direction of the oneway constraint

Examples:

```
fix ions oneway 10 semi -x
fix all oneway 1 left -z
fix all oneway 1 right z
```

Description:

Enforce that particles in the group and in a given region can only move in one direction. This is done by reversing a particle's velocity component, if it has the wrong sign in the specified dimension. The effect is that the particle moves in one direction only.

This can be used, for example, as a simple model of a semi-permeable membrane, or as an implementation of Maxwell's demon.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

fix wall/reflect command

Default: none

---

fix orient/fcc command

```
fix ID group-ID orient/fcc nstats dir alat dE cutlo cuthi file0 file1
```

- ID, group-ID are documented in fix command
- nstats = print stats every this many steps, 0 = never
- dir = 0/1 for which crystal is used as reference
- alat = fcc cubic lattice constant (distance units)
- dE = energy added to each atom (energy units)
- cutlo,cuthi = values between 0.0 and 1.0, cutlo < cuthi
- file0,file1 = files that specify orientation of each grain

Examples:

```
fix gb all orient/fcc 0 1 4.032008 0.001 0.25 0.75 xi.vec chi.vec
```

Description:

The fix applies an orientation-dependent force to atoms near a planar grain boundary which can be used to induce grain boundary migration (in the direction perpendicular to the grain boundary plane). The motivation and explanation of this force and its application are described in (Janssens). The force is only applied to atoms in the fix group.

The basic idea is that atoms in one grain (on one side of the boundary) have a potential energy dE added to them. Atoms in the other grain have 0.0 potential energy added. Atoms near the boundary (whose neighbor environment is intermediate between the two grain orientations) have an energy between 0.0 and dE added. This creates an effective driving force to reduce the potential energy of atoms near the boundary by pushing them towards one of the grain orientations. For dir = 1 and dE > 0, the boundary will thus move so that the grain described by file0 grows and the grain described by file1 shrinks. Thus this fix is designed for simulations of two-grain systems, either with one grain boundary and free surfaces parallel to the boundary, or a system with periodic boundary conditions and two equal and opposite grain boundaries. In either case, the entire system can displace during the simulation, and such motion should be accounted for in measuring the grain boundary velocity.

The potential energy added to atom I is given by these formulas

$$\xi_i = \sum_{j=1}^{12} \left| \mathbf{r}_j - \mathbf{r}_j^{\mathrm{I}} \right| \tag{1}$$

$$\xi_{\mathrm{IJ}} = \sum_{j=1}^{12} \left| \mathbf{r}_j^{\mathrm{J}} - \mathbf{r}_j^{\mathrm{I}} \right| \tag{2}$$

$$\xi_{\mathrm{low}} = \mathrm{cutlo}\, \xi_{\mathrm{IJ}} \tag{3}$$

$$\xi_{\mathrm{high}} = \mathrm{cuthi}\, \xi_{\mathrm{IJ}} \tag{4}$$

$$\omega_i = \frac{\pi}{2} \frac{\xi_i - \xi_{\mathrm{low}}}{\xi_{\mathrm{high}} - \xi_{\mathrm{low}}} \tag{5}$$

$$\begin{aligned} u_i &= 0 && \text{for } \xi_i < \xi_{\mathrm{low}} \\ &= \mathrm{dE}\, \frac{1 - \cos(2\omega_i)}{2} && \text{for } \xi_{\mathrm{low}} < \xi_i < \xi_{\mathrm{high}} \\ &= \mathrm{dE} && \text{for } \xi_{\mathrm{high}} < \xi_i \end{aligned} \tag{6}$$

which are fully explained in (Janssens). The order parameter Xi for atom I in equation (1) is a sum over the 12 nearest neighbors of atom I. Rj is the vector from atom I to its neighbor J, and RIj is a vector in the reference (perfect) crystal. That is, if dir = 0/1, then RIj is a vector to an atom coord from file 0/1. Equation (2) gives the expected value of the order parameter XiIJ in the other grain. Hi and lo cutoffs are defined in equations (3) and (4), using the input parameters *cutlo* and *cuthi* as thresholds to avoid adding grain boundary energy when the deviation in the order parameter from 0 or 1 is small (e.g. due to thermal fluctuations in a perfect crystal). The added potential energy Ui for atom I is given in equation (6) where it is interpolated between 0 and dE using the two threshold Xi values and the Wi value of equation (5).

The derivative of this energy expression gives the force on each atom which thus depends on the orientation of its neighbors relative to the 2 grain orientations. Only atoms near the grain boundary feel a net force which tends to drive them to one of the two grain orientations.

In equation (1), the reference vector used for each neighbor is the reference vector closest to the actual neighbor position. This means it is possible two different neighbors will use the same reference vector. In such cases, the atom in question is far from a perfect orientation and will likely receive the full dE addition, so the effect of duplicate reference vector usage is small.

The *dir* parameter determines which grain wants to grow at the expense of the other. A value of 0 means the first grain will shrink; a value of 1 means it will grow. This assumes that *dE* is positive. The reverse will be true if *dE* is negative.

The *alat* parameter is the cubic lattice constant for the fcc material and is only used to compute a cutoff distance of 1.57 * alat / sqrt(2) for finding the 12 nearest neighbors of each atom (which should be valid for an fcc crystal). A longer/shorter cutoff can be imposed by adjusting *alat*. If a particular atom has less than 12 neighbors within the cutoff, the order parameter of equation (1) is effectively multiplied by 12 divided by the actual number of neighbors within the cutoff.

The *dE* parameter is the maximum amount of additional energy added to each atom in the grain which wants to shrink.

The *cutlo* and *cuthi* parameters are used to reduce the force added to bulk atoms in each grain far away from the boundary. An atom in the bulk surrounded by neighbors at the ideal grain orientation would compute an order parameter of 0 or 1 and have no force added. However, thermal vibrations in the solid will cause the order parameters to be greater than 0 or less than 1. The cutoff parameters mask this effect, allowing forces to only be added to atoms with order-parameters between the cutoff values.

File0 and *file1* are filenames for the two grains which each contain 6 vectors (6 lines with 3 values per line) which specify the grain orientations. Each vector is a displacement from a central atom (0,0,0) to a nearest neighbor atom in an fcc lattice at the proper orientation. The vector lengths should all be identical since an fcc lattice has a coordination number of 12. Only 6 are listed due to symmetry, so the list must include one from each pair of equal-and-opposite neighbors. A pair of orientation files for a Sigma=5 tilt boundary are show below.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *energy* option is supported by this fix to add the potential energy of atom interactions with the grain boundary driving force to the system's potential energy as part of thermodynamic output.

This fix calculates a global scalar which can be accessed by various output commands. The scalar is the potential energy change due to this fix. The scalar value calculated by this fix is "extensive".

This fix also calculates a per-atom array which can be accessed by various output commands. The array stores the order parameter Xi and normalized order parameter (0 to 1) for each atom. The per-atom values can be accessed on any timestep.

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix should only be used with fcc lattices.

Related commands:

fix_modify

Default: none

(Janssens) Janssens, Olmsted, Holm, Foiles, Plimpton, Derlet, Nature Materials, 5, 124-127 (2006).

For illustration purposes, here are example files that specify a Sigma=5 tilt boundary. This is for a lattice constant of 3.5706 Angs.

file0:

```
 0.798410432046075    1.785300000000000    1.596820864092150
-0.798410432046075    1.785300000000000   -1.596820864092150
 2.395231296138225    0.000000000000000    0.798410432046075
 0.798410432046075    0.000000000000000   -2.395231296138225
 1.596820864092150    1.785300000000000   -0.798410432046075
 1.596820864092150   -1.785300000000000   -0.798410432046075
```

file1:

```
-0.798410432046075    1.785300000000000    1.596820864092150
 0.798410432046075    1.785300000000000   -1.596820864092150
 0.798410432046075    0.000000000000000    2.395231296138225
 2.395231296138225    0.000000000000000   -0.798410432046075
 1.596820864092150    1.785300000000000    0.798410432046075
 1.596820864092150   -1.785300000000000    0.798410432046075
```

fix phonon command

Syntax:

```
fix ID group-ID phonon N Noutput Nwait map_file prefix keyword values ...
```

- ID, group-ID are documented in fix command
- phonon = style name of this fix command
- N = measure the Green's function every this many timesteps
- Noutput = output the dynamical matrix every this many measurements
- Nwait = wait this many timesteps before measuring
- map_file = *file* or *GAMMA*

```
  file is the file that contains the mapping info between atom ID and the lattice indices.

  GAMMA flags to treate the whole simulation box as a unit cell, so that the mapping
    info can be generated internally. In this case, dynamical matrix at only the gamma-point
    will/can be evaluated.
```

- prefix = prefix for output files
- one or none keyword/value pairs may be appended
- keyword = *sysdim* or *nasr*

```
  sysdim value = d
      d = dimension of the system, usually the same as the MD model dimension
    nasr value = n
      n = number of iterations to enforce the acoustic sum rule
```

Examples:

```
fix 1 all phonon 20 5000 200000 map.in LJ1D sysdim 1
fix 1 all phonon 20 5000 200000 map.in EAM3D
fix 1 all phonon 10 5000 500000 GAMMA EAM0D nasr 100
```

Description:

Calculate the dynamical matrix from molecular dynamics simulations based on fluctuation-dissipation theory for a group of atoms.

Consider a crystal with N unit cells in three dimensions labelled $l = (l_1,l_2,l_3)$ where l_i are integers. Each unit cell is defined by three linearly independent vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ forming a parallelipiped, containing K basis atoms labelled k.

Based on fluctuation-dissipation theory, the force constant coefficients of the system in reciprocal space are given by (Campañá , Kong)

$$_{k\ ,k'}\ (\mathbf{q}) = k_B T\ \mathbf{G}^{-1}{}_{k\ ,k'}\ (\mathbf{q}),$$

where **G** is the Green's functions coefficients given by

$$\mathbf{G}_{k\ ,k'}\ (\mathbf{q}) = <\mathbf{u}_k\ (\mathbf{q})\ \ \mathbf{u}_{k'}{}^{*}(\mathbf{q})>,$$

where denotes the ensemble average, and

$$\mathbf{u}_k\ (\mathbf{q}) = \sum_l \mathbf{u}_{lk}\ \ \exp(i\mathbf{q}\mathbf{r}_l)$$

is the component of the atomic displacement for the *k*th atom in the unit cell in reciprocal space at **q**. In practice, the Green's functions coefficients can also be measured according to the following formula,

$$\mathbf{G}_{k\ ,k'}\ (\mathbf{q}) = <\mathbf{R}_k\ (\mathbf{q})\ \ \mathbf{R}^*_{k'}\ (\mathbf{q})> - <\mathbf{R}>_k\ (\mathbf{q})\ \ <\mathbf{R}>^*_{k'}\ (\mathbf{q}),$$

where **R** is the instantaneous positions of atoms, and **<R>** is the averaged atomic positions. It gives essentially the same results as the displacement method and is easier to implement in an MD code.

Once the force constant matrix is known, the dynamical matrix **D** can then be obtained by

$$\mathbf{D}_{k\ ,k'}\ (\mathbf{q}) = (m_k m_{k'})^{-1/2}\ \ \ _{k\ ,k'}\ (\mathbf{q})$$

whose eigenvalues are exactly the phonon frequencies at **q**.

This fix uses positions of atoms in the specified group and calculates two-point correlations. To achieve this. the positions of the atoms are examined every *Nevery* steps and are Fourier-transformed into reciprocal space, where the averaging process and correlation computation is then done. After every *Noutput* measurements, the matrix **G**(**q**) is calculated and inverted to obtain the elastic stiffness coefficients. The dynamical matrices are then constructed and written to *prefix*.bin.timestep files in binary format and to the file *prefix*.log for each wavevector **q**.

A detailed description of this method can be found in (Kong2011).

The *sysdim* keyword is optional. If specified with a value smaller than the dimensionality of the LAMMPS simulation, its value is used for the dynamical matrix calculation. For example, using LAMMPS ot model a 2D or 3D system, the phonon dispersion of a 1D atomic chain can be computed using *sysdim* = 1.

The *nasr* keyword is optional. An iterative procedure is employed to enforce the acoustic sum rule on at , and the number provided by keyword *nasr* gives the total number of iterations. For a system whose unit cell has only one atom, *nasr* = 1 is sufficient; for other systems, *nasr* = 10 is typically sufficient.

The *map_file* contains the mapping information between the lattice indices and the atom IDs, which tells the code which atom sits at which lattice point; the lattice indices start from 0. An auxiliary code, latgen, can be employed to generate the compatible map file for various crystals.

In case one simulates an aperiodic system, where the whole simulation box is treated as a unit cell, one can set *map_file* as *GAMMA*, so that the mapping info will be generated internally and a file is not needed. In this case, the dynamical matrix at only the gamma-point will/can be evaluated. Please keep in mind that fix-phonon is designed for cyrstals, it will be inefficient and even degrade the performance of lammps in case the unit cell is too large.

The calculated dynamical matrix elements are written out in energy/distance^2/mass units. The coordinates for *q* points in the log file is in the units of the basis vectors of the corresponding reciprocal lattice.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *temp* option is supported by this fix. You can use it to change the temperature compute from thermo_temp to the one that reflects the true temperature of atoms in the group.

No global scalar or vector or per-atom quantities are stored by this fix for access by various output commands.

Instead, this fix outputs its initialization information (including mapping information) and the calculated dynamical matrices to the file *prefix*.log, with the specified *prefix*. The dynamical matrices are also written to files *prefix*.bin.timestep in binary format. These can be read by the post-processing tool in tools/phonon to compute the phonon density of states and/or phonon dispersion curves.

No parameter of this fix can be used with the *start/stop* keywords of the run command.

This fix is not invoked during energy minimization.

Restrictions:

This fix assumes a crystalline system with periodical lattice. The temperature of the system should not exceed the melting temperature to keep the system in its solid state.

This fix is part of the USER-PHONON package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix requires LAMMPS be built with an FFT library. See the Making LAMMPS section for more info.

Related commands:

compute msd

Default:

The option defaults are sysdim = the same dimemsion as specified by the dimension command, and nasr = 20.

(Campañá) C. Campañá and M. H. Müser, *Practical Green's function approach to the simulation of elastic semi-infinite solids*, Phys. Rev. B [74], 075420 (2006)

(Kong) L.T. Kong, G. Bartels, C. Campañá, C. Denniston, and Martin H. Müser, *Implementation of Green's function molecular dynamics: An extension to LAMMPS*, Computer Physics Communications [180](6):1004-1010 (2009).

L.T. Kong, C. Denniston, and Martin H. Müser, *An improved version of the Green's function molecular dynamics method*, Computer Physics Communications [182](2):540-541 (2011).

(Kong2011) L.T. Kong, *Phonon dispersion measured directly from molecular dynamics simulations*, Computer Physics Communications [182](10):2201-2207, (2011).

fix pimd command

Syntax:

```
fix ID group-ID pimd keyword value ...
```

- ID, group-ID are documented in fix command
- pimd = style name of this fix command
- zero or more keyword/value pairs may be appended
- keyword = *method* or *fmass* or *sp* or *temp* or *nhc*

```
method value = pimd or nmpimd or cmd
  fmass value = scaling factor on mass
  sp value = scaling factor on Planck constant
  temp value = temperature (temperarate units)
  nhc value = Nc = number of chains in Nose-Hoover thermostat
```

Examples:

```
fix 1 all pimd method nmpimd fmass 1.0 sp 2.0 temp 300.0 nhc 4
```

Description:

This command performs quantum molecular dynamics simulations based on the Feynman path integral to include effects of tunneling and zero-point motion. In this formalism, the isomorphism of a quantum partition function for the original system to a classical partition function for a ring-polymer system is exploited, to efficiently sample configurations from the canonical ensemble (Feynman). The classical partition function and its components are given by the following equations:

$$Z = \int d\mathbf{q} d\mathbf{p} \cdot \exp[-\beta H_{eff}]$$

$$H_{eff} = \left(\sum_{i=1}^{P} \frac{p_i^2}{2m_i} \right) + V_{eff}$$

$$V_{eff} = \sum_{i=1}^{P} \left[\frac{mP}{2\beta^2\hbar^2}(q_i - q_{i+1})^2 + \frac{1}{P}V(q_i) \right]$$

The interested user is referred to any of the numerous references on this methodology, but briefly, each quantum particle in a path integral simulation is represented by a ring-polymer of P quasi-beads, labeled from 1 to P. During the simulation, each quasi-bead interacts with beads on the other ring-polymers with the same imaginary time index (the second term in the effective potential above). The quasi-beads also interact with the two neighboring quasi-beads through the spring potential in imaginary-time space (first term in effective potential). To sample the canonical ensemble, a Nose-Hoover massive chain thermostat is applied (Tuckerman). With the massive chain algorithm, a chain of NH thermostats is coupled to each degree of freedom for each quasi-bead.

The keyword *temp* sets the target temperature for the system and the keyword *nhc* sets the number *Nc* of thermostats in each chain. For example, for a simulation of N particles with P beads in each ring-polymer, the total number of NH thermostats would be 3 x N x P x Nc.

NOTE: This fix implements a complete velocity-verlet integrator combined with NH massive chain thermostat, so no other time integration fix should be used.

The *method* keyword determines what style of PIMD is performed. A value of *pimd* is standard PIMD. A value of *nmpimd* is for normal-mode PIMD. A value of *cmd* is for centroid molecular dynamics (CMD). The difference between the styles is as follows.

In standard PIMD, the value used for a bead's fictitious mass is arbitrary. A common choice is to use Mi = m/P, which results in the mass of the entire ring-polymer being equal to the real quantum particle. But it can be difficult to efficiently integrate the equations of motion for the stiff harmonic interactions in the ring polymers.

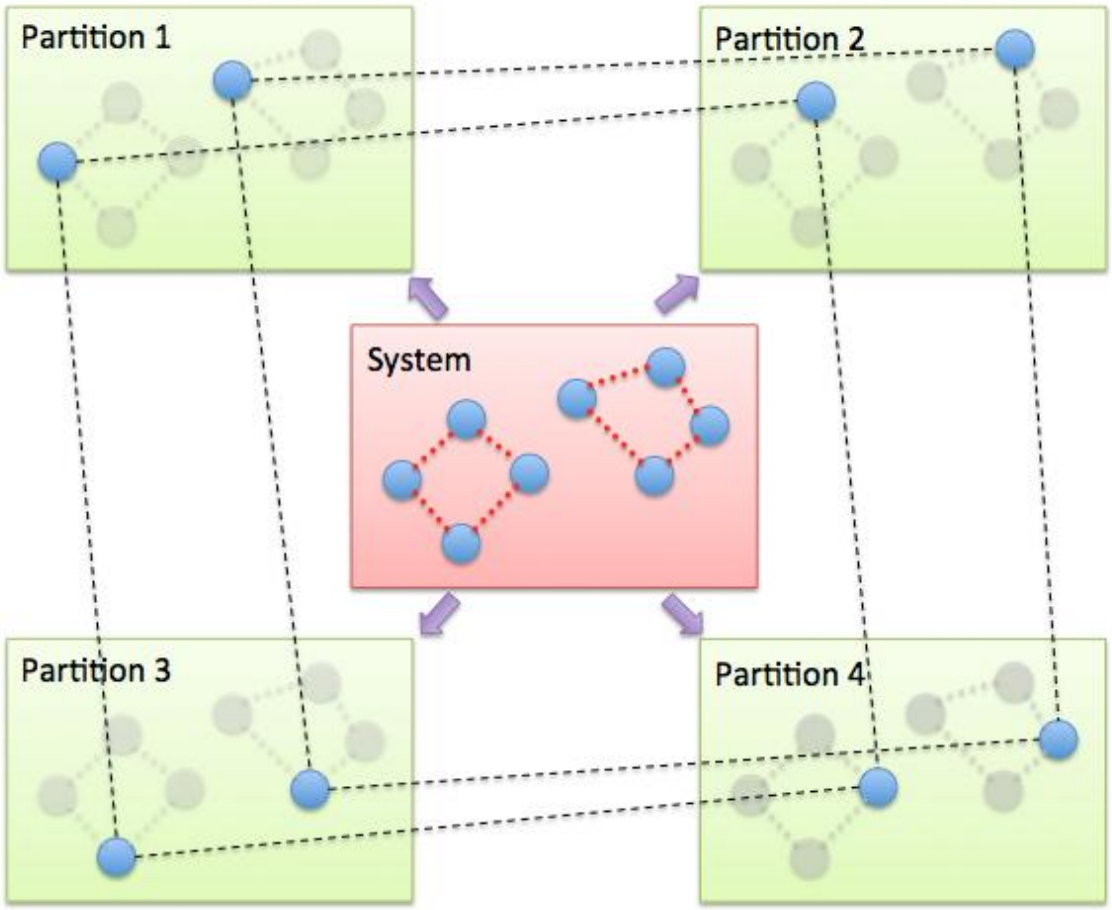
A useful way to resolve this issue is to integrate the equations of motion in a normal mode representation, using Normal Mode Path-Integral Molecular Dynamics (NMPIMD) (Cao1). In NMPIMD, the NH chains are attached to each normal mode of the ring-polymer and the fictitious mass of each mode is chosen as Mk = the eigenvalue of the Kth normal mode for k > 0. The k = 0 mode, referred to as the zero-frequency mode or centroid, corresponds to overall translation of the ring-polymer and is assigned the mass of the real particle.

Motion of the centroid can be effectively uncoupled from the other normal modes by scaling the fictitious masses to achieve a partial adiabatic separation. This is called a Centroid Molecular Dynamics (CMD) approximation (Cao2). The time-evolution (and resulting dynamics) of the quantum particles can be used to obtain centroid time correlation functions, which can be further used to obtain the true quantum correlation function for the original system. The CMD method also uses normal modes to evolve the system, except only the k > 0 modes are thermostatted, not the centroid degrees of freedom.

The keyword *fmass* sets a further scaling factor for the fictitious masses of beads, which can be used for the Partial Adiabatic CMD (Hone), or to be set as P, which results in the fictitious masses to be equal to the real particle masses.

The keyword *sp* is a scaling factor on Planck's constant, which can be useful for debugging or other purposes. The default value of 1.0 is appropriate for most situations.

The PIMD algorithm in LAMMPS is implemented as a hyper-parallel scheme as described in (Calhoun). In LAMMPS this is done by using multi-replica feature in LAMMPS, where each quasi-particle system is stored and simulated on a separate partition of processors. The following diagram illustrates this approach. The original system with 2 ring polymers is shown in red. Since each ring has 4 quasi-beads (imaginary time slices), there are 4 replicas of the system, each running on one of the 4 partitions of processors. Each replica (shown in green) owns one quasi-bead in each ring.



To run a PIMD simulation with M quasi-beads in each ring polymer using N MPI tasks for each partition's domain-decomposition, you would use P = MxN processors (cores) and run the simulation as follows:

```
mpirun -np P lmp_mpi -partition MxN -in script
```

Note that in the LAMMPS input script for a multi-partition simulation, it is often very useful to define a uloop-style variable such as

```
variable ibead uloop M pad
```

where M is the number of quasi-beads (partitions) used in the calculation. The uloop variable can then be used to manage I/O related tasks for each of the partitions, e.g.

```
dump dcd all dcd 10 system_${ibead}.dcd
restart 1000 system_${ibead}.restart1 system_${ibead}.restart2
read_restart system_${ibead}.restart2
```

Restrictions:

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

A PIMD simulation can be initialized with a single data file read via the read_data command. However, this means all quasi-beads in a ring polymer will have identical positions and velocities, resulting in identical trajectories for all quasi-beads. To avoid this, users can simply initialize velocities with different random number

seeds assigned to each partition, as defined by the uloop variable, e.g.

```
velocity all create 300.0 1234${ibead} rot yes dist gaussian
```

Default:

The keyword defaults are method = pimd, fmass = 1.0, sp = 1.0, temp = 300.0, and nhc = 2.

(Feynman) R. Feynman and A. Hibbs, Chapter 7, Quantum Mechanics and Path Integrals, McGraw-Hill, New York (1965).

(Tuckerman) M. Tuckerman and B. Berne, J Chem Phys, 99, 2796 (1993).

(Cao1) J. Cao and B. Berne, J Chem Phys, 99, 2902 (1993).

(Cao2) J. Cao and G. Voth, J Chem Phys, 100, 5093 (1994).

(Hone) T. Hone, P. Rossky, G. Voth, J Chem Phys, 124, 154103 (2006).

(Calhoun) A. Calhoun, M. Pavese, G. Voth, Chem Phys Letters, 262, 415 (1996).

fix planeforce command

Syntax:

```
fix ID group-ID planeforce x y z
```

- ID, group-ID are documented in fix command
- planeforce = style name of this fix command
- x y z = 3-vector that is normal to the plane

Examples:

```
fix hold boundary planeforce 1.0 0.0 0.0
```

Description:

Adjust the forces on each atom in the group so that only the components of force in the plane specified by the normal vector (x,y,z) remain. This is done by subtracting out the component of force perpendicular to the plane.

If the initial velocity of the atom is 0.0 (or in the plane), then it should continue to move in the plane thereafter.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command.

Restrictions: none

Related commands:

fix lineforce

Default: none

fix poems

Syntax:

```
fix ID group-ID poems keyword values
```

- ID, group-ID are documented in fix command
- poems = style name of this fix command
- keyword = *group* or *file* or *molecule*

```
  group values = list of group IDs
    molecule values = none
    file values = filename
```

Examples:

```
fix 3 fluid poems group clump1 clump2 clump3
fix 3 fluid poems file cluster.list
```

Description:

Treats one or more sets of atoms as coupled rigid bodies. This means that each timestep the total force and torque on each rigid body is computed and the coordinates and velocities of the atoms are updated so that the collection of bodies move as a coupled set. This can be useful for treating a large biomolecule as a collection of connected, coarse-grained particles.

The coupling, associated motion constraints, and time integration is performed by the software package Parallelizable Open source Efficient Multibody Software (POEMS) which computes the constrained rigid-body motion of articulated (jointed) multibody systems (Anderson). POEMS was written and is distributed by Prof Kurt Anderson, his graduate student Rudranarayan Mukherjee, and other members of his group at Rensselaer Polytechnic Institute (RPI). Rudranarayan developed the LAMMPS/POEMS interface. For copyright information on POEMS and other details, please refer to the documents in the poems directory distributed with LAMMPS.

This fix updates the positions and velocities of the rigid atoms with a constant-energy time integration, so you should not update the same atoms via other fixes (e.g. nve, nvt, npt, temp/rescale, langevin).

Each body must have a non-degenerate inertia tensor, which means if must contain at least 3 non-collinear atoms. Which atoms are in which bodies can be defined via several options.

For option *group*, each of the listed groups is treated as a rigid body. Note that only atoms that are also in the fix group are included in each rigid body.

For option *molecule*, each set of atoms in the group with a different molecule ID is treated as a rigid body.

For option *file*, sets of atoms are read from the specified file and each set is treated as a rigid body. Each line of the file specifies a rigid body in the following format:

ID type atom1-ID atom2-ID atom3-ID ...

ID as an integer from 1 to M (the number of rigid bodies). Type is any integer; it is not used by the fix poems command. The remaining arguments are IDs of atoms in the rigid body, each typically from 1 to N (the number of

atoms in the system). Only atoms that are also in the fix group are included in each rigid body. Blank lines and lines that begin with '#' are skipped.

A connection between a pair of rigid bodies is inferred if one atom is common to both bodies. The POEMS solver treats that atom as a spherical joint with 3 degrees of freedom. Currently, a collection of bodies can only be connected by joints as a linear chain. The entire collection of rigid bodies can represent one or more chains. Other connection topologies (tree, ring) are not allowed, but will be added later. Note that if no joints exist, it is more efficient to use the fix rigid command to simulate the system.

When the poems fix is defined, it will print out statistics on the total # of clusters, bodies, joints, atoms involved. A cluster in this context means a set of rigid bodies connected by joints.

For computational efficiency, you should turn off pairwise and bond interactions within each rigid body, as they no longer contribute to the motion. The "neigh_modify exclude" and "delete_bonds" commands can be used to do this if each rigid body is a group.

For computational efficiency, you should only define one fix poems which includes all the desired rigid bodies. LAMMPS will allow multiple poems fixes to be defined, but it is more expensive.

The degrees-of-freedom removed by coupled rigid bodies are accounted for in temperature and pressure computations. Similarly, the rigid body contribution to the pressure virial is also accounted for. The latter is only correct if forces within the bodies have been turned off, and there is only a single fix poems defined.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the POEMS package. It is only enabled if LAMMPS was built with that package, which also requires the POEMS library be built and linked with LAMMPS. See the Making LAMMPS section for more info.

Related commands:

fix rigid, delete_bonds, neigh_modify exclude

Default: none

(Anderson) Anderson, Mukherjee, Critchley, Ziegler, and Lipton "POEMS: Parallelizable Open-source Efficient Multibody Software ", Engineering With Computers (2006). (link to paper)

fix pour command

Syntax:

```
fix ID group-ID pour N type seed keyword values ...
```

- ID, group-ID are documented in fix command
- pour = style name of this fix command
- N = # of particles to insert
- type = atom type to assign to inserted particles (offset for molecule insertion)
- seed = random # seed (positive integer)
- one or more keyword/value pairs may be appended to args
- keyword = *region* or *diam* or *vol* or *rate* or *dens* or *vel* or *mol* or *rigid* or *shake* or *ignore*

```
  region value = region-ID
      region-ID = ID of region to use as insertion volume
    diam values = dstyle args
      dstyle = one or range or poly
        one args = D
          D = single diameter for inserted particles (distance units)
        range args = Dlo Dhi
          Dlo,Dhi = range of diameters for inserted particles (distance units)
        poly args = Npoly D1 P1 D2 P2 ...
          Npoly = # of (D,P) pairs
          D1,D2,... = diameter for subset of inserted particles (distance units)
          P1,P2,... = percentage of inserted particles with this diameter (0-1)
    id values = idflag
      idflag = max or next = how to choose IDs for inserted particles and molecules
    vol values = fraction Nattempt
      fraction = desired volume fraction for filling insertion volume
      Nattempt = max # of insertion attempts per particle
    rate value = V
      V = z velocity (3d) or y velocity (2d) at which
          insertion volume moves (velocity units)
    dens values = Rholo Rhohi
      Rholo,Rhohi = range of densities for inserted particles (mass/volume units)
    vel values (3d) = vxlo vxhi vylo vyhi vz
    vel values (2d) = vxlo vxhi vy
      vxlo,vxhi = range of x velocities for inserted particles (velocity units)
      vylo,vyhi = range of y velocities for inserted particles (velocity units)
      vz = z velocity (3d) assigned to inserted particles (velocity units)
      vy = y velocity (2d) assigned to inserted particles (velocity units)
    mol value = template-ID
      template-ID = ID of molecule template specified in a separate molecule command
    molfrac values = f1 f2 ... fN
      f1 to fN = relative probability of creating each of N molecules in template-ID
    rigid value = fix-ID
      fix-ID = ID of fix rigid/small command
    shake value = fix-ID
      fix-ID = ID of fix shake command
    ignore value = none
      skip any line or triangle particles when detecting possible
        overlaps with inserted particles
```

Examples:

```
fix 3 all pour 1000 2 29494 region myblock
fix 2 all pour 10000 1 19985583 region disk vol 0.33 100 rate 1.0 diam range 0.9 1.1
```

```
fix 2 all pour 10000 1 19985583 region disk diam poly 2 0.7 0.4 1.5 0.6
fix ins all pour 500 1 4767548 vol 0.8 10 region slab mol object rigid myRigid
```

Description:

Insert finite-size particles or molecules into the simulation box every few timesteps within a specified region until N particles or molecules have been inserted. This is typically used to model the pouring of granular particles into a container under the influence of gravity. For the remainder of this doc page, a single inserted atom or molecule is referred to as a "particle".

If inserted particles are individual atoms, they are assigned the specified atom type. If they are molecules, the type of each atom in the inserted molecule is specified in the file read by the molecule command, and those values are added to the specified atom type. E.g. if the file specifies atom types 1,2,3, and those are the atom types you want for inserted molecules, then specify *type* = 0. If you specify *type* = 2, the in the inserted molecule will have atom types 3,4,5.

All atoms in the inserted particle are assigned to two groups: the default group "all" and the group specified in the fix pour command (which can also be "all").

This command must use the *region* keyword to define an insertion volume. The specified region must have been previously defined with a region command. It must be of type *block* or a z-axis *cylinder* and must be defined with side = *in*. The cylinder style of region can only be used with 3d simulations.

Individual atoms are inserted, unless the *mol* keyword is used. It specifies a *template-ID* previously defined using the molecule command, which reads a file that defines the molecule. The coordinates, atom types, center-of-mass, moments of inertia, etc, as well as any bond/angle/etc and special neighbor information for the molecule can be specified in the molecule file. See the molecule command for details. The only settings required to be in this file are the coordinates and types of atoms in the molecule.

If the molecule template contains more than one molecule, the relative probability of depositing each molecule can be specified by the *molfrac* keyword. N relative probablities, each from 0.0 to 1.0, are specified, where N is the number of molecules in the template. Each time a molecule is inserted, a random number is used to sample from the list of relative probabilities. The N values must sum to 1.0.

If you wish to insert molecules via the *mol* keyword, that will be treated as rigid bodies, use the *rigid* keyword, specifying as its value the ID of a separate fix rigid/small command which also appears in your input script.

If you wish to insert molecules via the *mol* keyword, that will have their bonds or angles constrained via SHAKE, use the *shake* keyword, specifying as its value the ID of a separate fix shake command which also appears in your input script.

Each timestep particles are inserted, they are placed randomly inside the insertion volume so as to mimic a stream of poured particles. If they are molecules they are also oriented randomly. Each atom in the particle is tested for overlaps with existing particles, including effects due to periodic boundary conditions if applicable. If an overlap is detected, another random insertion attempt is made; see the *vol* keyword discussion below. The larger the volume of the insertion region, the more particles that can be inserted at any one timestep. Particles are inserted again after enough time has elapsed that the previously inserted particles fall out of the insertion volume under the influence of gravity. Insertions continue every so many timesteps until the desired # of particles has been inserted.

NOTE: If you are monitoring the temperature of a system where the particle count is changing due to adding particles, you typically should use the compute_modify dynamic yes command for the temperature compute you are using.

All other keywords are optional with defaults as shown below.

The *diam* option is only used when inserting atoms and specifes the diameters of inserted particles. There are 3 styles: *one*, *range*, or *poly*. For *one*, all particles will have diameter *D*. For *range*, the diameter of each particle will be chosen randomly and uniformly between the specified *Dlo* and *Dhi* bounds. For *poly*, a series of *Npoly* diameters is specified. For each diameter a percentage value from 0.0 to 1.0 is also specified. The *Npoly* percentages must sum to 1.0. For the example shown above with "diam 2 0.7 0.4 1.5 0.6", all inserted particles will have a diameter of 0.7 or 1.5. 40% of the particles will be small; 60% will be large.

Note that for molecule insertion, the diameters of individual atoms in the molecule can be specified in the file read by the molecule command. If not specified, the diameter of each atom in the molecule has a default diameter of 1.0.

The *id* option has two settings which are used to determine the atom or molecule IDs to assign to inserted particles/molecules. In both cases a check is done of the current system to find the maximum current atom and molecule ID of any existing particle. Newly inserted particles and molecules are assigned IDs that increment those max values. For the *max* setting, which is the default, this check is done at every insertion step, which allows for particles to leave the system, and their IDs to potentially be re-used. For the *next* setting this check is done only once when the fix is specified, which can be more efficient if you are sure particles will not be added in some other way.

The *vol* option specifies what volume fraction of the insertion volume will be filled with particles. For particles with a size specified by the *diam range* keyword, they are assumed to all be of maximum diamter *Dhi* for purposes of computing their contribution to the volume fraction.

The higher the volume fraction value, the more particles are inserted each timestep. Since inserted particles cannot overlap, the maximum volume fraction should be no higher than about 0.6. Each timestep particles are inserted, LAMMPS will make up to a total of M tries to insert the new particles without overlaps, where M = # of inserted particles * Nattempt. If LAMMPS is unsuccessful at completing all insertions, it prints a warning.

The *dens* and *vel* options enable inserted particles to have a range of densities or xy velocities. The specific values for a particular inserted particle will be chosen randomly and uniformly between the specified bounds. Internally, the density value for a particle is converted to a mass, based on the radius (volume) of the particle. The *vz* or *vy* value for option *vel* assigns a z-velocity (3d) or y-velocity (2d) to each inserted particle.

The *rate* option moves the insertion volume in the z direction (3d) or y direction (2d). This enables pouring particles from a successively higher height over time.

The *ignore* option is useful when running a simulation that used line segment (2d) or triangle (3d) particles, typically to define boundaries for spherical granular particles to interact with. See the atom_style line or tri command for details. Lines and triangles store their size, and if the size is large it may overlap (in a spherical sense) with the insertion region, even if the line/triangle is oriented such that there is no actual overlap. This can prevent particles from being inserted. The *ignore* keyword causes the overlap check to skip any line or triangle particles. Obviously you should only use it if there is in fact no overlap of the line or triangle particles with the insertion region.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. This means you must be careful when restarting a pouring simulation, when the restart file was written in the middle of the pouring operation. Specifically, you should use a new fix pour command in the input script for the restarted simulation that continues the operation. You will need to adjust the arguments of the original fix pour command to do this.

Also note that because the state of the random number generator is not saved in restart files, you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior if you adjust the fix pour parameters appropriately.

None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the GRANULAR package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

For 3d simulations, a gravity fix in the -z direction must be defined for use in conjunction with this fix. For 2d simulations, gravity must be defined in the -y direction.

The specified insertion region cannot be a "dynamic" region, as defined by the region command.

Related commands:

fix_deposit, fix_gravity, region

Default:

Insertions are performed for individual particles, i.e. no *mol* setting is defined. If the *mol* keyword is used, the default for *molfrac* is an equal probabilities for all molecules in the template. Additional option defaults are diam = one 1.0, dens = 1.0 1.0, vol = 0.25 50, rate = 0.0, vel = 0.0 0.0 0.0 0.0 0.0 (for 3d), vel = 0.0 0.0 0.0 (for 2d), and id = max.

fix press/berendsen command

Syntax:

```
fix ID group-ID press/berendsen keyword value ...
```

- ID, group-ID are documented in fix command
- press/berendsen = style name of this fix command

```
one or more keyword value pairs may be appended
keyword = iso or aniso or x or y or z or couple or dilate or modulus
  iso or aniso values = Pstart Pstop Pdamp
    Pstart,Pstop = scalar external pressure at start/end of run (pressure units)
    Pdamp = pressure damping parameter (time units)
  x or y or z values = Pstart Pstop Pdamp
    Pstart,Pstop = external stress tensor component at start/end of run (pressure units)
    Pdamp = stress damping parameter (time units)
  couple = none or xyz or xy or yz or xz
  modulus value = bulk modulus of system (pressure units)
  dilate value = all or partial
```

Examples:

```
fix 1 all press/berendsen iso 0.0 0.0 1000.0
fix 2 all press/berendsen aniso 0.0 0.0 1000.0 dilate partial
```

Description:

Reset the pressure of the system by using a Berendsen barostat (Berendsen), which rescales the system volume and (optionally) the atoms coordinates within the simulation box every timestep.

Regardless of what atoms are in the fix group, a global pressure is computed for all atoms. Similarly, when the size of the simulation box is changed, all atoms are re-scaled to new positions, unless the keyword *dilate* is specified with a value of *partial*, in which case only the atoms in the fix group are re-scaled. The latter can be useful for leaving the coordinates of atoms in a solid substrate unchanged and controlling the pressure of a surrounding fluid.

NOTE: Unlike the fix npt or fix nph commands which perform Nose/Hoover barostatting AND time integration, this fix does NOT perform time integration. It only modifies the box size and atom coordinates to effect barostatting. Thus you must use a separate time integration fix, like fix nve or fix nvt to actually update the positions and velocities of atoms. This fix can be used in conjunction with thermostatting fixes to control the temperature, such as fix nvt or fix langevin or fix temp/berendsen.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting and barostatting.

The barostat is specified using one or more of the *iso*, *aniso*, *x*, *y*, *z*, and *couple* keywords. These keywords give you the ability to specify the 3 diagonal components of an external stress tensor, and to couple various of these components together so that the dimensions they represent are varied together during a constant-pressure simulation. Unlike the fix npt and fix nph commands, this fix cannot be used with triclinic (non-orthogonal) simulation boxes to control all 6 components of the general pressure tensor.

The target pressures for each of the 3 diagonal components of the stress tensor can be specified independently via the *x*, *y*, *z*, keywords, which correspond to the 3 simulation box dimensions. For each component, the external pressure or tensor component at each timestep is a ramped value during the run from *Pstart* to *Pstop*. If a target pressure is specified for a component, then the corresponding box dimension will change during a simulation. For example, if the *y* keyword is used, the y-box length will change. A box dimension will not change if that component is not specified, although you have the option to change that dimension via the fix deform command.

For all barostat keywords, the *Pdamp* parameter determines the time scale on which pressure is relaxed. For example, a value of 1000.0 means to relax the pressure in a timespan of (roughly) 1000 time units (tau or fmsec or psec - see the units command).

NOTE: The relaxation time is actually also a function of the bulk modulus of the system (inverse of isothermal compressibility). The bulk modulus has units of pressure and is the amount of pressure that would need to be applied (isotropically) to reduce the volume of the system by a factor of 2 (assuming the bulk modulus was a constant, independent of density, which it's not). The bulk modulus can be set via the keyword *modulus*. The *Pdamp* parameter is effectively multiplied by the bulk modulus, so if the pressure is relaxing faster than expected or desired, increasing the bulk modulus has the same effect as increasing *Pdamp*. The converse is also true. LAMMPS does not attempt to guess a correct value of the bulk modulus; it just uses 10.0 as a default value which gives reasonable relaxation for a Lennard-Jones liquid, but will be way off for other materials and way too small for solids. Thus you should experiment to find appropriate values of *Pdamp* and/or the *modulus* when using this fix.

The *couple* keyword allows two or three of the diagonal components of the pressure tensor to be "coupled" together. The value specified with the keyword determines which are coupled. For example, *xz* means the *Pxx* and *Pzz* components of the stress tensor are coupled. *Xyz* means all 3 diagonal components are coupled. Coupling means two things: the instantaneous stress will be computed as an average of the corresponding diagonal components, and the coupled box dimensions will be changed together in lockstep, meaning coupled dimensions will be dilated or contracted by the same percentage every timestep. The *Pstart*, *Pstop*, *Pdamp* parameters for any coupled dimensions must be identical. *Couple xyz* can be used for a 2d simulation; the *z* dimension is simply ignored.

The *iso* and *aniso* keywords are simply shortcuts that are equivalent to specifying several other keywords together.

The keyword *iso* means couple all 3 diagonal components together when pressure is computed (hydrostatic pressure), and dilate/contract the dimensions together. Using "iso Pstart Pstop Pdamp" is the same as specifying these 4 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple xyz
```

The keyword *aniso* means *x*, *y*, and *z* dimensions are controlled independently using the *Pxx*, *Pyy*, and *Pzz* components of the stress tensor as the driving forces, and the specified scalar external pressure. Using "aniso Pstart Pstop Pdamp" is the same as specifying these 4 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple none
```

This fix computes a temperature and pressure each timestep. To do this, the fix creates its own computes of style

"temp" and "pressure", as if these commands had been issued:

```
compute fix-ID_temp group-ID temp
compute fix-ID_press group-ID pressure fix-ID_temp
```

See the compute temp and compute pressure commands for details. Note that the IDs of the new computes are the fix-ID + underscore + "temp" or fix_ID + underscore + "press", and the group for the new computes is the same as the fix group.

Note that these are NOT the computes used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp* and *thermo_press*. This means you can change the attributes of this fix's temperature or pressure via the compute_modify command or print this temperature or pressure during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* or *thermo_press* will have no effect on this fix.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *temp* and *press* options are supported by this fix. You can use them to assign a compute you have defined to this fix which will be used in its temperature and pressure calculations. If you do this, note that the kinetic energy derived from the compute temperature should be consistent with the virial term computed using all atoms for the pressure. LAMMPS will warn you if you choose to compute temperature on a subset of atoms.

No global or per-atom quantities are stored by this fix for access by various output commands.

This fix can ramp its target pressure over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

Any dimension being adjusted by this fix must be periodic.

Related commands:

fix nve, fix nph, fix npt, fix temp/berendsen, fix_modify

Default:

The keyword defaults are dilate = all, modulus = 10.0 in units of pressure for whatever units are defined.

(Berendsen) Berendsen, Postma, van Gunsteren, DiNola, Haak, J Chem Phys, 81, 3684 (1984).

fix print command

Syntax:

```
fix ID group-ID print N string keyword value ...
```

- ID, group-ID are documented in fix command
- print = style name of this fix command
- N = print every N steps
- string = text string to print with optional variable names
- zero or more keyword/value pairs may be appended
- keyword = *file* or *append* or *screen* or *title*

```
  file value = filename
    append value = filename
    screen value = yes or no
    title value = string
      string =  text to print as 1st line of output file
```

Examples:

```
fix extra all print 100 "Coords of marker atom = $x $y $z"
fix extra all print 100 "Coords of marker atom = $x $y $z" file coord.txt
```

Description:

Print a text string every N steps during a simulation run. This can be used for diagnostic purposes or as a debugging tool to monitor some quantity during a run. The text string must be a single argument, so it should be enclosed in double quotes if it is more than one word. If it contains variables it must be enclosed in double quotes to insure they are not evaluated when the input script line is read, but will instead be evaluated each time the string is printed.

The specified group-ID is ignored by this fix.

See the variable command for a description of *equal* style variables which are the most useful ones to use with the fix print command, since they are evaluated afresh each timestep that the fix print line is output. Equal-style variables calculate formulas involving mathematical operations, atom properties, group properties, thermodynamic properties, global values calculated by a compute or fix, or references to other variables.

If the *file* or *append* keyword is used, a filename is specified to which the output generated by this fix will be written. If *file* is used, then the filename is overwritten if it already exists. If *append* is used, then the filename is appended to if it already exists, or created if it does not exist.

If the *screen* keyword is used, output by this fix to the screen and logfile can be turned on or off as desired.

The *title* keyword allow specification of the string that will be printed as the first line of the output file, assuming the *file* keyword was used. By default, the title line is as follows:

```
# Fix print output for fix ID
```

where ID is replaced with the fix-ID.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

variable, print

Default:

The option defaults are no file output, screen = yes, and title string as described above.

fix property/atom command

Syntax:

```
fix ID group-ID property/atom vec1 vec2 ... keyword value ...
```

- ID, group-ID are documented in fix command
- property/atom = style name of this fix command
- vec1,vec2,... = *mol* or *q* or *i_name* or *d_name*

```
  mol = molecule IDs
    q = charge
    i_name = new integer vector referenced by name
    d_name = new floating-point vector referenced by name
```

- zero of more keyword/value pairs may be appended
- keyword = *ghost*

```
  ghost value = no or yes for whether ghost atom info in communicated
```

Examples:

```
fix 1 all property/atom mol
fix 1 all property/atom i_myflag1 i_myflag2
fix 1 all property/atom d_sx d_sy d_sz
```

Description:

Create one or more additional per-atom vectors to store information about atoms and to use during a simulation. The specified *group-ID* is ignored by this fix.

The atom style used for a simulation defines a set of per-atom properties, as explained on the atom_style and read_data doc pages. The latter command allows these properties to be defined for each atom in the system when a data file is read. This fix will augment the set of properties with new custom ones.

This can be useful in at least two scenarios.

If the atom style does not define molecule IDs or per-atom charge, they can be added using the *mol* or *q* keywords. This can be useful, e.g, to define "molecules" to use as rigid bodies with the fix rigid command, or just to carry around an extra flag with the atoms (stored as a molecule ID). An alternative is to use an atom style that does define molecule IDs or charge or to use a hybrid atom style that combines two styles to allow for molecule IDs or charge, but that has 2 practical drawbacks. First it typically necessitates changing the format of the data file. And it may define additional properties that aren't needed such as bond lists, which has some overhead when there are no bonds.

In the future, we may add additional per-atom properties similar to *mol* or *q*, which "turn-on" specific properties defined by some atom styles, so they can be used by atom styles that don't define them.

More generally, the *i_name* and *d_name* vectors allow one or more new custom per-atom properties to be defined. Each name must be unique and can use alphanumeric or underscore characters. These vectors can store whatever values you decide are useful in your simulation. As explained below there are several ways to initialize and access and output these values, both via input script commands and in new code that you add to LAMMPS.

This is effectively a simple way to add per-atom properties to a model without needing to write code for a new atom style that defines the properties. Note however that implementing a new atom style allows new atom properties to be more tightly and seamlessly integrated with the rest of the code.

The new atom properties encode values that migrate with atoms to new processors and are written to restart files. If you want the new properties to also be defined for ghost atoms, then use the *ghost* keyword with a value of *yes*. This will invoke extra communication when ghost atoms are created (at every re-neighboring) to insure the new properties are also defined for the ghost atoms.

NOTE: If you use this command with the *mol* or *charge* vectors than you most likely want to set *ghost* yes, since these properties are stored with ghost atoms if you use an atom_style that defines them, and many LAMMPS operations that use molecule IDs or charge, such as neighbor lists and pair styles, will expect ghost atoms to have these valuse. LAMMPS will issue a warning it you define those vectors but do not set *ghost* yes.

NOTE: The properties for ghost atoms are not updated every timestep, but only once every few steps when neighbor lists are re-built. Thus the *ghost* keyword is suitable for static properties, like molecule IDs, but not for dynamic properties that change every step. For the latter, the code you add to LAMMPS to change the properties will also need to communicate their new values to/from ghost atoms, an operation that can be invoked from within a pair style or fix or compute that you write.

This fix is one of a small number that can be defined in an input script before the simulation box is created or atoms are defined. This is so it can be used with the read_data command as described below.

Per-atom properties that are defined by the atom style are initialized when atoms are created, e.g. by the read_data or create_atoms commands. The per-atom properaties defined by this fix are not. So you need to initialize them explicitly. This can be done by the read_data command, using its *fix* keyword and passing it the fix-ID of this fix.

Thus these commands:

```
fix prop all property/atom mol d_flag
read_data data.txt fix prop NULL Molecules
```

would allow a data file to have a section like this:

```
Molecules

1 4 1.5
2 4 3.0
3 10 1.0
4 10 1.0
5 10 1.0
...
N 763 4.5
```

where N is the number of atoms, and the first field on each line is the atom-ID, followed by a molecule-ID and a floating point value that will be stored in a new property called "flag". Note that the list of per-atom properties can be in any order.

Another way of initializing the new properties is via the set command. For example, if you wanted molecules defined for every set of 10 atoms, based on their atom-IDs, these commands could be used:

```
fix prop all property/atom mol
variable cluster atom ((id-1)/10)+1
set id * mol v_cluster
```

The atom-style variable will create values for atoms with IDs 31,32,33,...40 that are 4.0,4.1,4.2,...,4.9. When the set commands assigns them to the molecule ID for each atom, they will be truncated to an integer value, so atoms 31-40 will all be assigned a molecule ID of 4.

Note that atomfile-style variables can also be used in place of atom-style variables, which means in this case that the molecule IDs could be read-in from a separate file and assinged by the set command. This allows you to initialize new per-atom properties in a completely general fashion.

For new atom properties specified as *i_name* or *d_name*, the compute property/atom command can access their values. This means that the values can be output via the dump custom command, accessed by fixes like fix ave/atom, accessed by other computes like compute reduce, or used in atom-style variables.

For example, these commands will output two new properties to a custom dump file:

```
fix prop all property/atom i_flag1 d_flag2
compute 1 all property/atom i_flag1 d_flag2
dump 1 all custom 100 tmp.dump id x y z c_1[1] c_1[2]
```

If you wish to add new pair styles, fixes, or computes that use the per-atom properties defined by this fix, see Section modify of the manual which has some details on how the properties can be accessed from added classes.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the per-atom values it stores to binary restart files, so that the values can be restored when a simulation is restarted. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

read_data, set, compute property/atom

Default:

The default keyword values are ghost = no.

fix qbmsst command

Syntax:

```
fix ID group-ID qbmsst dir shockvel keyword value ...
```

- ID, group-ID are documented in fix command
- qbmsst = style name of this fix
- dir = *x* or *y* or *z*
- shockvel = shock velocity (strictly positive, velocity units)
- zero or more keyword/value pairs may be appended
- keyword = *q* or *mu* or *p0* or *v0* or *e0* or *tscale* or *damp* or *seed*or *f_max* or *N_f* or *eta* or *beta* or *T_init*

```
  q value = cell mass-like parameter (mass^2/distance^4 units)
    mu value = artificial viscosity (mass/distance/time units)
    p0 value = initial pressure in the shock equations (pressure units)
    v0 value = initial simulation cell volume in the shock equations (distance^3 units)
    e0 value = initial total energy (energy units)
    tscale value = reduction in initial temperature (unitless fraction between 0.0 and 1.0)
    damp value = damping parameter (time units) inverse of friction
    seed value = random number seed (positive integer)
    f_max value = upper cutoff frequency of the vibration spectrum (1/time units)
    N_f value = number of frequency bins (positive integer)
    eta value = coupling constant between the shock system and the quantum thermal bath (positiv
    beta value = the quantum temperature is updated every beta time steps (positive integer)
    T_init value = quantum temperature for the initial state (temperature units)
```

Examples:

```
fix 1 all qbmsst z 0.122 q 25 mu 0.9 tscale 0.01 damp 200 seed 35082 f_max 0.3 N_f 100 eta 1 beta 40
fix 2 all qbmsst z 72 q 40 tscale 0.05 damp 1 seed 47508 f_max 120.0 N_f 100 eta 1.0 beta 500 T_init
```

Two example input scripts are given, including shocked alpha quartz and shocked liquid methane. The input script first equilibrate an initial state with the quantum thermal bath at the target temperature and then apply the qbmsst to simulate shock compression with quantum nuclear correction. The following two figures plot related quantities for shocked alpha quartz.

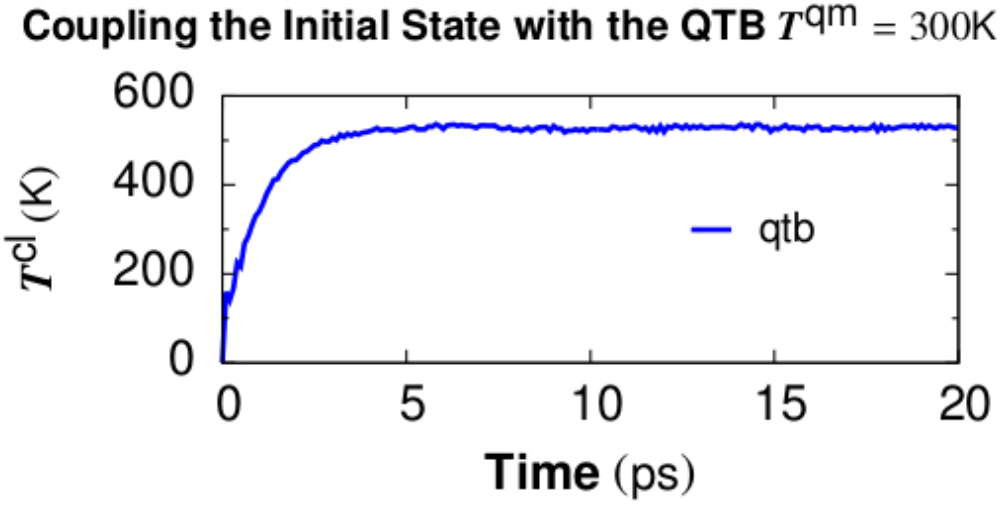


Figure 1. Classical temperature $T^{cl} = \sum m_i v_i^2 / 3Nk_B$ vs. time for coupling the alpha quartz initial state with the quantum thermal bath at target quantum temperature T^{qm} = 300 K. The NpH ensemble is used for time integration while QTB provides the colored random force. T^{cl} converges at the timescale of *damp* which is set to be 1 ps.

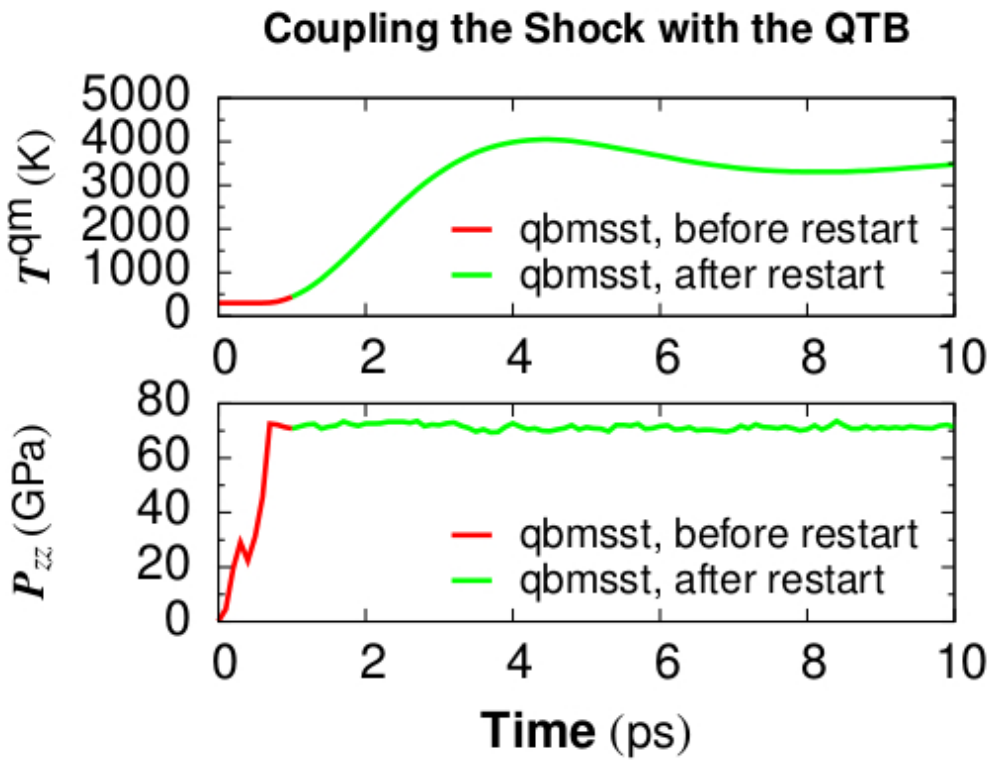


Figure 2. Quantum temperature and pressure vs. time for simulating shocked alpha quartz with the QBMSST. The shock propagates along the z direction. Restart of the QBMSST command is demonstrated in the example input script. Thermodynamic quantities stay continuous before and after the restart.

Description:

This command performs the Quantum-Bath coupled Multi-Scale Shock Technique (QBMSST) integration. See (Qi) for a detailed description of this method. The QBMSST provides description of the thermodynamics and kinetics of shock processes while incorporating quantum nuclear effects. The *shockvel* setting determines the steady shock velocity that will be simulated along direction *dir*.

Quantum nuclear effects (fix qtb) can be crucial especially when the temperature of the initial state is below the classical limit or there is a great change in the zero point energies between the initial and final states. Theoretical post processing quantum corrections of shock compressed water and methane have been reported as much as 30% of the temperatures (Goldman). A self-consistent method that couples the shock to a quantum thermal bath described by a colored noise Langevin thermostat has been developed by Qi et al (Qi) and applied to shocked methane. The onset of chemistry is reported to be at a pressure on the shock Hugoniot that is 40% lower than observed with classical molecular dynamics.

It is highly recommended that the system be already in an equilibrium state with a quantum thermal bath at temperature of *T_init*. The fix command fix qtb at constant temperature *T_init* could be used before applying this command to introduce self-consistent quantum nuclear effects into the initial state.

The parameters *q*, *mu*, *e0*, *p0*, *v0* and *tscale* are described in the command fix msst. The values of *e0*, *p0*, or *v0* will be calculated on the first step if not specified. The parameter of *damp*, *f_max*, and *N_f* are described in the

command fix qtb.

The fix qbmsst command couples the shock system to a quantum thermal bath with a rate that is proportional to the change of the total energy of the shock system, *etot* - $etot_0$. Here *etot* consists of both the system energy and a thermal term, see (Qi), and $etot_0$ = *e0* is the initial total energy.

The *eta* ( ) parameter is a unitless coupling constant between the shock system and the quantum thermal bath. A small *eta* value cannot adjust the quantum temperature fast enough during the temperature ramping period of shock compression while large *eta* leads to big temperature oscillation. A value of *eta* between 0.3 and 1 is usually appropriate for simulating most systems under shock compression. We observe that different values of *eta* lead to almost the same final thermodynamic state behind the shock, as expected.

The quantum temperature is updated every *beta* ( ) steps with an integration time interval *beta* times longer than the simulation time step. In that case, *etot* is taken as its average over the past *beta* steps. The temperature of the quantum thermal bath T^{qm} changes dynamically according to the following equation where Δt is the MD time step and is the friction constant which is equal to the inverse of the *damp* parameter.

$$dT^{qm}/dt = \sum_{l=1}[etot(t-l\Delta t)-etot_0]/3 \; Nk_B$$

The parameter *T_init* is the initial temperature of the quantum thermal bath and the system before shock loading.

For all pressure styles, the simulation box stays orthorhombic in shape. Parrinello-Rahman boundary conditions (tilted box) are supported by LAMMPS, but are not implemented for QBMSST.

Restart, fix_modify, output, run start/stop, minimize info:

Because the state of the random number generator is not written to binary restart files, this fix cannot be restarted "exactly" in an uninterrupted fashion. However, in a statistical sense, a restarted simulation should produce similar behaviors of the system as if it is not interrupted. To achieve such a restart, one should write explicitly the same value for *q*, *mu*, *damp*, *f_max*, *N_f*, *eta*, and *beta* and set *tscale* = 0 if the system is compressed during the first run.

The progress of the QBMSST can be monitored by printing the global scalar and global vector quantities computed by the fix. The global vector contains five values in this order:

[*dhugoniot*, *drayleigh*, *lagrangian_speed*, *lagrangian_position*, *quantum_temperature*]

1. *dhugoniot* is the departure from the Hugoniot (temperature units).
2. *drayleigh* is the departure from the Rayleigh line (pressure units).
3. *lagrangian_speed* is the laboratory-frame Lagrangian speed (particle velocity) of the computational cell (velocity units).
4. *lagrangian_position* is the computational cell position in the reference frame moving at the shock speed. This is the distance of the computational cell behind the shock front.
5. *quantum_temperature* is the temperature of the quantum thermal bath T^{qm}.

To print these quantities to the log file with descriptive column headers, the following LAMMPS commands are suggested. Here the fix_modify energy command is also enabled to allow the thermo keyword *etotal* to print the quantity *etot*. See also the thermo_style command.

```
fix             fix_id all msst z
fix_modify      fix_id energy yes
variable        dhug    equal f_fix_id[1]
variable        dray    equal f_fix_id[2]
```

```
variable        lgr_vel equal f_fix_id[3]
variable        lgr_pos equal f_fix_id[4]
variable        T_qm    equal f_fix_id[5]
thermo_style    custom  step temp ke pe lz pzz etotal v_dhug v_dray v_lgr_vel v_lgr_pos v_T_qm f_fix
```

The global scalar under the entry f_fix_id is the quantity of thermo energy as an extra part of *etot*. This global scalar and the vector of 5 quantities can be accessed by various output commands. It is worth noting that the temp keyword under the thermo_style command print the instantaneous classical temperature T^{cl} as described in the command fix qtb.

Restrictions:

This fix style is part of the USER-QTB package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

All cell dimensions must be periodic. This fix can not be used with a triclinic cell. The QBMSST fix has been tested only for the group-ID all.

Related commands:

fix qtb, fix msst

Default:

The keyword defaults are q = 10, mu = 0, tscale = 0.01, damp = 1, seed = 880302, f_max = 200.0, N_f = 100, eta = 1.0, beta = 100, and T_init=300.0. e0, p0, and v0 are calculated on the first step.

(Goldman) Goldman, Reed and Fried, J. Chem. Phys. 131, 204103 (2009)

(Qi) Qi and Reed, J. Phys. Chem. A 116, 10451 (2012).

fix qeq/point command

fix qeq/shielded command

fix qeq/slater command

fix qeq/dynamic command

fix qeq/fire command

Syntax:

```
fix ID group-ID style Nevery cutoff tolerance maxiter qfile keyword ...
```

- ID, group-ID are documented in fix command
- style = *qeq/point* or *qeq/shielded* or *qeq/slater* or *qeq/dynamic* or *qeq/fire*
- Nevery = perform charge equilibration every this many steps
- cutoff = global cutoff for charge-charge interactions (distance unit)
- tolerance = precision to which charges will be equilibrated
- maxiter = maximum iterations to perform charge equilibration
- qfile = a filename with QEq parameters
- zero or more keyword/value pairs may be appended
- keyword = *alpha* or *qdamp* or *qstep*

```
  alpha value = Slater type orbital exponent (qeq/slater only)
    qdamp value = damping factor for damped dynamics charge solver (qeq/dynamic and qeq/fire onl
    qstep value = time step size for damped dynamics charge solver (qeq/dynamic and qeq/fire onl
```

Examples:

```
fix 1 all qeq/point 1 10 1.0e-6 200 param.qeq1
fix 1 qeq qeq/shielded 1 8 1.0e-6 100 param.qeq2
fix 1 all qeq/slater 5 10 1.0e-6 100 params alpha 0.2
fix 1 qeq qeq/dynamic 1 12 1.0e-3 100 my_qeq
fix 1 all qeq/fire 1 10 1.0e-3 100 my_qeq qdamp 0.2 qstep 0.1
```

Description:

Perform the charge equilibration (QEq) method as described in (Rappe and Goddard) and formulated in (Nakano) (also known as the matrix inversion method) and in (Rick and Stuart) (also known as the extended Lagrangian method) based on the electronegativity equilization principle.

These fixes can be used with any pair style in LAMMPS, so long as per-atom charges are defined. The most typical use-case is in conjunction with a pair style that performs charge equilibration periodically (e.g. every timestep), such as the ReaxFF or Streitz-Mintmire potential. But these fixes can also be used with potentials that normally assume per-atom charges are fixed, e.g. a Buckingham or LJ/Coulombic potential.

Because the charge equilibration calculation is effectively independent of the pair style, these fixes can also be used to perform a one-time assignment of charges to atoms. For example, you could define the QEq fix, perform a zero-timestep run via the run command without any pair style defined which would set per-atom charges (based

on the current atom configuration), then remove the fix via the unfix command before performing further dynamics.

NOTE: Computing and using charge values different from published values defined for a fixed-charge potential like Buckingham or CHARMM or AMBER, can have a strong effect on energies and forces, and produces a different model than the published versions.

NOTE: The fix qeq/comb command must still be used to perform charge equliibration with the COMB potential. The fix qeq/reax command can be used to perform charge equilibration with the ReaxFF force field, although fix qeq/shielded yields the same results as fix qeq/reax if *Nevery*, *cutoff*, and *tolerance* are the same. Eventually the fix qeq/reax command will be deprecated.

The QEq method minimizes the electrostatic energy of the system (or equalizes the derivative of energy with respect to charge of all the atoms) by adjusting the partial charge on individual atoms based on interactions with their neighbors within *cutoff*. It reqires a few parameters, in *metal* units, for each atom type which provided in a file specified by *qfile*. The file has the following format

```
1 chi eta gamma zeta qcore
2 chi eta gamma zeta qcore
...
Ntype chi eta gamma zeta qcore
```

There is one line per atom type with the following parameters. Only a subset of the parameters is used by each QEq style as descibed below, thus the others can be set to 0.0 if desired.

- *chi* = electronegativity in energy units
- *eta* = self-Coulomb potential in energy units
- *gamma* = shielded Coulomb constant defined by ReaxFF force field in distance units
- *zeta* = Slater type orbital exponent defined by the Streitz-Mintmire potential in reverse distance units
- *qcore* = charge of the nucleus defined by the Streitz-Mintmire potential potential in charge units

The *qeq/point* style describes partial charges on atoms as point charges. Interaction between a pair of charged particles is 1/r, which is the simplest description of the interaction between charges. Only the *chi* and *eta* parameters from the *qfile* file are used. Note that Coulomb catastrophe can occur if repulsion between the pair of charged particles is too weak. This style solves partial charges on atoms via the matrix inversion method. A tolerance of 1.0e-6 is usually a good number.

The *qeq/shielded* style describes partial charges on atoms also as point charges, but uses a shielded Coulomb potential to describe the interaction between a pair of charged particles. Interaction through the shielded Coulomb is given by equation (13) of the ReaxFF force field paper. The shielding accounts for charge overlap between charged particles at small separation. This style is the same as fix qeq/reax, and can be used with pair_style reax/c. Only the *chi*, *eta*, and *gamma* parameters from the *qfile* file are used. This style solves partial charges on atoms via the matrix inversion method. A tolerance of 1.0e-6 is usually a good number.

The *qeq/slater* style describes partial charges on atoms as spherical charge densities centered around atoms via the Slater 1*s* orbital, so that the interaction between a pair of charged particles is the product of two Slater 1*s* orbitals. The expression for the Slater 1*s* orbital is given under equation (6) of the Streitz-Mintmire paper. Only the *chi*, *eta*, *zeta*, and *qcore* parameters from the *qfile* file are used. This style solves partial charges on atoms via the matrix inversion method. A tolerance of 1.0e-6 is usually a good number. Keyword *alpha* can be used to change the Slater type orbital exponent.

The *qeq/dynamic* style describes partial charges on atoms as point charges that interact through 1/r, but the extended Lagrangian method is used to solve partial charges on atoms. Only the *chi* and *eta* parameters from the

qfile file are used. Note that Coulomb catastrophe can occur if repulsion between the pair of charged particles is too weak. A tolerance of 1.0e-3 is usually a good number. Keyword *qdamp* can be used to change the damping factor, while keyword *qstep* can be used to change the time step size.

The *qeq/fire* style describes the same charge model and charge solver as the *qeq/dynamic* style, but employs a FIRE minimization algorithm to solve for equilibrium charges. Keyword *qdamp* can be used to change the damping factor, while keyword *qstep* can be used to change the time step size.

Note that *qeq/point*, *qeq/shielded*, and *qeq/slater* describe different charge models, whereas the matrix inversion method and the extended Lagrangian method (*qeq/dynamic* and *qeq/fire*) are different solvers.

Note that *qeq/point*, *qeq/dynamic* and *qeq/fire* styles all describe charges as point charges that interact through 1/r relationship, but solve partial charges on atoms using different solvers. These three styles should yield comparable results if the QEq parameters and *Nevery*, *cutoff*, and *tolerance* are the same. Style *qeq/point* is typically faster, *qeq/dynamic* scales better on larger sizes, and *qeq/fire* is faster than *qeq/dynamic*.

NOTE: To avoid the evaluation of the derivative of charge with respect to position, which is typically ill-defined, the system should have a zero net charge.

NOTE: Developing QEq parameters (chi, eta, gamma, zeta, and qcore) is non-trivial. Charges on atoms are not guaranteed to equilibrate with arbitrary choices of these parameters. We do not develop these QEq paramters. See the examples/qeq directory for some examples.

Restart, fix_modify, output, run start/stop, minimize info:

No information about these fixes is written to binary restart files. No global scalar or vector or per-atom quantities are stored by these fixes for access by various output commands. No parameter of these fixes can be used with the *start/stop* keywords of the run command.

Thexe fixes are invoked during energy minimization.

Restrictions:

These fixes are part of the QEQ package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix qeq/reax, fix qeq/comb

Default: none

(Rappe and Goddard) A. K. Rappe and W. A. Goddard III, J Physical Chemistry, 95, 3358-3363 (1991).

(Nakano) A. Nakano, Computer Physics Communications, 104, 59-69 (1997).

(Rick and Stuart) S. W. Rick, S. J. Stuart, B. J. Berne, J Chemical Physics 101, 16141 (1994).

(Streitz-Mintmire) F. H. Streitz, J. W. Mintmire, Physical Review B, 50, 16, 11996 (1994)

(ReaxFF) A. C. T. van Duin, S. Dasgupta, F. Lorant, W. A. Goddard III, J Physical Chemistry, 105, 9396-9049 (2001)

(QEq/Fire) T.-R. Shan, A. P. Thompson, S. J. Plimpton, in preparation

fix qeq/comb command

fix qeq/comb/omp command

Syntax:

```
fix ID group-ID qeq/comb Nevery precision keyword value ...
```

- ID, group-ID are documented in fix command
- qeq/comb = style name of this fix command
- Nevery = perform charge equilibration every this many steps
- precision = convergence criterion for charge equilibration
- zero or more keyword/value pairs may be appended
- keyword = *file*

```
  file value = filename
      filename = name of file to write QEQ equilibration info to
```

Examples:

```
fix 1 surface qeq/comb 10 0.0001
```

Description:

Perform charge equilibration (QeQ) in conjunction with the COMB (Charge-Optimized Many-Body) potential as described in (COMB_1) and (COMB_2). It performs the charge equilibration portion of the calculation using the so-called QEq method, whereby the charge on each atom is adjusted to minimize the energy of the system. This fix can only be used with the COMB potential; see the fix qeq/reax command for a QeQ calculation that can be used with any potential.

Only charges on the atoms in the specified group are equilibrated. The fix relies on the pair style (COMB in this case) to calculate the per-atom electronegativity (effective force on the charges). An electronegativity equalization calculation (or QEq) is performed in an interative fashion, which in parallel requires communication at each iteration for processors to exchange charge information about nearby atoms with each other. See Rappe_and_Goddard and Rick_and_Stuart for details.

During a run, charge equilibration is peformed every *Nevery* time steps. Charge equilibration is also always enforced on the first step of each run. The *precision* argument controls the tolerance for the difference in electronegativity for all atoms during charge equilibration. *Precision* is a trade-off between the cost of performing charge equilibration (more iterations) and accuracy.

If the *file* keyword is used, then information about each equilibration calculation is written to the specifed file.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making

LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix produces a per-atom vector which can be accessed by various output commands. The vector stores the gradient of the charge on each atom. The per-atom values be accessed on any timestep.

No parameter of this fix can be used with the *start/stop* keywords of the run command.

This fix can be invoked during energy minimization.

Restrictions:

This fix command currently only supports pair style *comb*.

Related commands:

pair_style comb

Default:

No file output is performed.

(COMB_1) J. Yu, S. B. Sinnott, S. R. Phillpot, Phys Rev B, 75, 085311 (2007),

(COMB_2) T.-R. Shan, B. D. Devine, T. W. Kemper, S. B. Sinnott, S. R. Phillpot, Phys Rev B, 81, 125328 (2010).

(Rappe_and_Goddard) A. K. Rappe, W. A. Goddard, J Phys Chem 95, 3358 (1991).

(Rick_and_Stuart) S. W. Rick, S. J. Stuart, B. J. Berne, J Chem Phys 101, 16141 (1994).

fix qeq/reax command

Syntax:

```
fix ID group-ID qeq/reax Nevery cutlo cuthi tolerance params
```

- ID, group-ID are documented in fix command
- qeq/reax = style name of this fix command
- Nevery = perform QEq every this many steps
- cutlo,cuthi = lo and hi cutoff for Taper radius
- tolerance = precision to which charges will be equilibrated
- params = reax/c or a filename

Examples:

```
fix 1 all qeq/reax 1 0.0 10.0 1.0e-6 reax/c
fix 1 all qeq/reax 1 0.0 10.0 1.0e-6 param.qeq
```

Description:

Perform the charge equilibration (QEq) method as described in (Rappe and Goddard) and formulated in (Nakano). It is typically used in conjunction with the ReaxFF force field model as implemented in the pair_style reax/c command, but it can be used with any potential in LAMMPS, so long as it defines and uses charges on each atom. The fix qeq/comb command should be used to perform charge equliibration with the COMB potential. For more technical details about the charge equilibration performed by fix qeq/reax, see the (Aktulga) paper.

The QEq method minimizes the electrostatic energy of the system by adjusting the partial charge on individual atoms based on interactions with their neighbors. It reqires some parameters for each atom type. If the *params* setting above is the word "reax/c", then these are extracted from the pair_style reax/c command and the ReaxFF force field file it reads in. If a file name is specified for *params*, then the parameters are taken from the specified file and the file must contain one line for each atom type. The latter form must be used when performing QeQ with a non-ReaxFF potential. Each line should be formatted as follows:

```
itype chi eta gamma
```

where *itype* is the atom type from 1 to Ntypes, *chi* denotes the electronegativity in eV, *eta* denotes the self-Coulomb potential in eV, and *gamma* denotes the valence orbital exponent. Note that these 3 quantities are also in the ReaxFF potential file, except that eta is defined here as twice the eta value in the ReaxFF file. Note that unlike the rest of LAMMPS, the units of this fix are hard-coded to be A, eV, and electronic charge.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. No global scalar or vector or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command.

This fix is invoked during energy minimization.

Restrictions:

This fix is part of the USER-REAXC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix does not correctly handle interactions involving multiple periodic images of the same atom. Hence, it should not be used for periodic cell dimensions less than 10 angstroms.

Related commands:

pair_style reax/c

Default: none

(Rappe) Rappe and Goddard III, Journal of Physical Chemistry, 95, 3358-3363 (1991).

(Nakano) Nakano, Computer Physics Communications, 104, 59-69 (1997).

(Aktulga) Aktulga, Fogarty, Pandit, Grama, Parallel Computing, 38, 245-259 (2012).

fix qmmm command

Syntax:

```
fix ID group-ID qmmm
```

- ID, group-ID are documented in fix command
- qmmm = style name of this fix command

Examples:

fix 1 qmol qmmm

Description:

This fix provides functionality to enable a quantum mechanics/molecular mechanice (QM/MM) coupling of LAMMPS to a quantum mechanical code. The current implementation only supports an ONIOM style mechanical coupling to the Quantum ESPRESSO plane wave DFT package. Electrostatic coupling is in preparation and the interface has been written in a manner that coupling to other QM codes should be possible without changes to LAMMPS itself.

The interface code for this is in the lib/qmmm directory of the LAMMPS distribution and is being made available at this early stage of development in order to encourage contributions for interfaces to other QM codes. This will allow the LAMMPS side of the implementation to be adapted if necessary before being finalized.

Details about how to use this fix are currently documented in the description of the QM/MM interface code itself in lib/qmmm/README.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global scalar or vector or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the USER-QMMM package. It is only enabled if LAMMPS was built with that package. It also requires building a library provided with LAMMPS. See the Making LAMMPS section for more info.

The fix is only functional when LAMMPS is built as a library and linked with a compatible QM program and a QM/MM frontend into a QM/MM executable. See the lib/qmmm/README file for details.

Related commands: none

Default: none

fix qtb command

Syntax:

```
fix ID group-ID qtb keyword value ...
```

- ID, group-ID are documented in fix command
- qtb = style name of this fix
- zero or more keyword/value pairs may be appended
- keyword = *temp* or *damp* or *seed* or *f_max* or *N_f*

```
  temp value = target quantum temperature (temperature units)
    damp value = damping parameter (time units) inverse of friction &gamma;
    seed value = random number seed (positive integer)
    f_max value = upper cutoff frequency of the vibration spectrum (1/time units)
    N_f value = number of frequency bins (positive integer)
```

Examples:

```
fix 1 all nve
fix 1 all qtb temp 110 damp 200 seed 35082 f_max 0.3 N_f 100 (liquid methane modeled with the REAX f
fix 2 all nph iso 1.01325 1.01325 1
fix 2 all qtb temp 300 damp 1 seed 47508 f_max 120.0 N_f 100 (quartz modeled with the BKS force fiel
```

Description:

This command performs the quantum thermal bath scheme proposed by (Dammak) to include self-consistent quantum nuclear effects, when used in conjunction with the fix nve or fix nph commands.

Classical molecular dynamics simulation does not include any quantum nuclear effect. Quantum treatment of the vibrational modes will introduce zero point energy into the system, alter the energy power spectrum and bias the heat capacity from the classical limit. Missing all the quantum nuclear effects, classical MD cannot model systems at temperatures lower than their classical limits. This effect is especially important for materials with a large population of hydrogen atoms and thus higher classical limits.

The equation of motion implemented by this command follows a Langevin form:

$$m_i a_i = f_i + R_i - m_i \quad v_i.$$

Here m_i, a_i, f_i , R_i, and v_i represent mass, acceleration, force exerted by all other atoms, random force, frictional coefficient (the inverse of damping parameter damp), and velocity. The random force R_i is "colored" so that any vibrational mode with frequency will have a temperature-sensitive energy (,T) which resembles the energy expectation for a quantum harmonic oscillator with the same natural frequency:

$$(\ ,T) = \quad /2 + \quad [\exp(\quad /k_B T)-1]^{-1}$$

To efficiently generate the random forces, we employ the method of (Barrat), that circumvents the need to generate all random forces for all times before the simulation. The memory requirement of this approach is less demanding and independent of the simulation duration. Since the total random force R_{tot} does not necessarily vanish for a finite number of atoms, R_i is replaced by $R_i - R_{tot}/N_{tot}$ to avoid collective motion of the system.

The *temp* parameter sets the target quantum temperature. LAMMPS will still have an output temperature in its thermo style. That is the instantaneous classical temperature T^{cl} derived from the atom velocities at thermal equilibrium. A non-zero T^{cl} will be present even when the quantum temperature approaches zero. This is associated with zero-point energy at low temperatures.

$$T^{\mathrm{cl}} = \sum m_i v_i^2 / 3Nk_{\mathrm{B}}$$

The *damp* parameter is specified in time units, and it equals the inverse of the frictional coefficient . should be as small as possible but slightly larger than the timescale of anharmonic coupling in the system which is about 10 ps to 100 ps. When is too large, it gives an energy spectrum that differs from the desired Bose-Einstein spectrum. When is too small, the quantum thermal bath coupling to the system will be less significant than anharmonic effects, reducing to a classical limit. We find that setting between 5 THz and 1 THz could be appropriate depending on the system.

The random number *seed* is a positive integer used to initiate a Marsaglia random number generator. Each processor uses the input seed to generate its own unique seed and its own stream of random numbers. Thus the dynamics of the system will not be identical on two runs on different numbers of processors.

The *f_max* parameter truncate the noise frequency domain so that vibrational modes with frequencies higher than *f_max* will not be modulated. If we denote Δt as the time interval for the MD integration, *f_max* is always reset by the code to make = (int)$(2f\_max\Delta t)^{-1}$ a positive integer and print out relative information. An appropriate value for the cutoff frequency *f_max* would be around 2~3 f_{D}, where f_{D} is the Debye frequency.

The *N_f* parameter is the frequency grid size, the number of points from 0 to *f_max* in the frequency domain that will be sampled. *3×2 N_f* per-atom random numbers are required in the random force generation and there could be as many atoms as in the whole simulation that can migrate into every individual processor. A larger *N_f* provides a more accurate sampling of the spectrum while consumes more memory. With fixed *f_max* and , *N_f* should be big enough to converge the classical temperature T^{cl} as a function of target quantum bath temperature. Memory usage per processor could be from 10 to 100 Mbytes.

NOTE: Unlike the fix nvt command which performs Nose/Hoover thermostatting AND time integration, this fix does NOT perform time integration. It only modifies forces to a colored thermostat. Thus you must use a separate time integration fix, like fix nve or fix nph to actually update the velocities and positions of atoms (as shown in the examples). Likewise, this fix should not normally be used with other fixes or commands that also specify system temperatures , e.g. fix nvt and fix temp/rescale.

Restart, fix_modify, output, run start/stop, minimizie info:

No information about this fix is written to binary restart files. Because the state of the random number generator is not saved in restart files, this means you cannot do "exact" restarts with this fix. However, in a statistical sense, a restarted simulation should produce similar behaviors of the system.

This fix is not invoked during energy minimization.

Restrictions:

This fix style is part of the USER-QTB package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix nve, fix nph, fix langevin, fix qbmsst

Default:

The keyword defaults are temp = 300, damp = 1, seed = 880302, f_max=200.0 and N_f = 100.

(Dammak) Dammak, Chalopin, Laroche, Hayoun, and Greffet, Phys Rev Lett, 103, 190601 (2009).

(Barrat) Barrat and Rodney, J. Stat. Phys, 144, 679 (2011).

fix reax/bonds command

fix reax/c/bonds command

Syntax:

```
fix ID group-ID reax/bonds Nevery filename
```

- ID, group-ID are documented in fix command
- reax/bonds = style name of this fix command
- Nevery = output interval in timesteps
- filename = name of output file

Examples:

```
fix 1 all reax/bonds 100 bonds.tatb
fix 1 all reax/c/bonds 100 bonds.reaxc
```

Description:

Write out the bond information computed by the ReaxFF potential specified by pair_style reax or pair_style reax/c in the exact same format as the original stand-alone ReaxFF code of Adri van Duin. The bond information is written to *filename* on timesteps that are multiples of *Nevery*, including timestep 0. For time-averaged chemical species analysis, please see the fix species command.

The format of the output file should be self-explantory.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

The fix reax/bonds command requires that the pair_style reax be invoked. This fix is part of the REAX package. It is only enabled if LAMMPS was built with that package, which also requires the REAX library be built and linked with LAMMPS. The fix reax/c/bonds command requires that the pair_style reax/c be invoked. This fix is part of the USER-REAXC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_style reax, pair_style reax/c, fix reax/c/species

Default: none

fix reax/c/species command

Syntax:

```
fix ID group-ID reax/c/species Nevery Nrepeat Nfreq filename keyword value ...
```

- ID, group-ID are documented in fix command
- reax/c/species = style name of this command
- Nevery = sample bond-order every this many timesteps
- Nrepeat = # of bond-order samples used for calculating averages
- Nfreq = calculate average bond-order every this many timesteps
- filename = name of output file
- zero or more keyword/value pairs may be appended
- keyword = *cutoff* or *element* or *position*

```
  cutoff value = I J Cutoff
      I, J = atom types
      Cutoff = Bond-order cutoff value for this pair of atom types
    element value = Element1, Element2, ...
    position value = posfreq filepos
      posfreq = write position files every this many timestep
      filepos = name of position output file
```

Examples:

```
fix 1 all reax/c/species 10 10 100 species.out
fix 1 all reax/c/species 1 2 20 species.out cutoff 1 1 0.40 cutoff 1 2 0.55
fix 1 all reax/c/species 1 100 100 species.out element Au O H position 1000 AuOH.pos
```

Description:

Write out the chemical species information computed by the ReaxFF potential specified by pair_style reax/c. Bond-order values (either averaged or instantaneous, depending on value of *Nrepeat*) are used to determine chemical bonds. Every *Nfreq* timesteps, chemical species information is written to *filename* as a two line output. The first line is a header containing labels. The second line consists of the following: timestep, total number of molecules, total number of distinct species, number of molecules of each species. In this context, "species" means a unique molecule. The chemical formula of each species is given in the first line.

Optional keyword *cutoff* can be assigned to change the minimum bond-order values used in identifying chemical bonds between pairs of atoms. Bond-order cutoffs should be carefully chosen, as bond-order cutoffs that are too small may include too many bonds (which will result in an error), while cutoffs that are too large will result in fragmented molecules. The default cutoff of 0.3 usually gives good results.

The optional keyword *element* can be used to specify the chemical symbol printed for each LAMMPS atom type. The number of symbols must match the number of LAMMPS atom types and each symbol must consist of 1 or 2 alphanumeric characters. Normally, these symbols should be chosen to match the chemical identity of each LAMMPS atom type, as specified using the reax/c pair_coeff command and the ReaxFF force field file.

The optional keyword *position* writes center-of-mass positions of each identified molecules to file *filepos* every *posfreq* timesteps. The first line contains information on timestep, total number of molecules, total number of distinct species, and box dimensions. The second line is a header containing labels. From the third line downward, each molecule writes a line of output containing the following information: molecule ID, number of atoms in this

molecule, chemical formula, total charge, and center-of-mass xyz positions of this molecule. The xyz positions are in fractional coordinates relative to the box dimensions.

For the keyword *position*, the *filepos* is the name of the output file. It can contain the wildcard character "*". If the "*" character appears in *filepos*, then one file per snapshot is written at *posfreq* and the "*" character is replaced with the timestep value. For example, AuO.pos.* becomes AuO.pos.0, AuO.pos.1000, etc.

The *Nevery*, *Nrepeat*, and *Nfreq* arguments specify on what timesteps the bond-order values are sampled to get the average bond order. The species analysis is performed using the average bond-order on timesteps that are a multiple of *Nfreq*. The average is over *Nrepeat* bond-order samples, computed in the preceding portion of the simulation every *Nevery* timesteps. *Nfreq* must be a multiple of *Nevery* and *Nevery* must be non-zero even if *Nrepeat* is 1. Also, the timesteps contributing to the average bond-order cannot overlap, i.e. Nrepeat*Nevery can not exceed Nfreq.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then bond-order values on timesteps 90,92,94,96,98,100 will be used to compute the average bond-order for the species analysis output on timestep 100.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes both a global vector of length 2 and a per-atom vector, either of which can be accessed by various output commands. The values in the global vector are "intensive".

The 2 values in the global vector are as follows:

- 1 = total number of molecules
- 2 = total number of distinct species

The per-atom vector stores the molecule ID for each atom as identified by the fix. If an atom is not in a molecule, its ID will be 0. For atoms in the same molecule, the molecule ID for all of them will be the same and will be equal to the smallest atom ID of any atom in the molecule.

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

The fix species currently only works with pair_style reax/c and it requires that the pair_style reax/c be invoked. This fix is part of the USER-REAXC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

It should be possible to extend it to other reactive pair_styles (such as rebo, airebo, comb, and bop), but this has not yet been done.

Related commands:

pair_style reax/c, fix reax/bonds

Default:

The default values for bond-order cutoffs are 0.3 for all I-J pairs. The default element symbols are C, H, O, N. Position files are not written by default.

fix recenter command

Syntax:

```
fix ID group-ID recenter x y z keyword value ...
```

- ID, group-ID are documented in fix command
- recenter = style name of this fix command
- x,y,z = constrain center-of-mass to these coords (distance units), any coord can also be NULL or INIT (see below)
- zero or more keyword/value pairs may be appended
- keyword = *shift* or *units*

```
shift value = group-ID
    group-ID = group of atoms whose coords are shifted
  units value = box or lattice or fraction
```

Examples:

```
fix 1 all recenter 0.0 0.5 0.0
fix 1 all recenter INIT INIT NULL
fix 1 all recenter INIT 0.0 0.0 units box
```

Description:

Constrain the center-of-mass position of a group of atoms by adjusting the coordinates of the atoms every timestep. This is simply a small shift that does not alter the dynamics of the system or change the relative coordinates of any pair of atoms in the group. This can be used to insure the entire collection of atoms (or a portion of them) do not drift during the simulation due to random perturbations (e.g. fix langevin thermostatting).

Distance units for the x,y,z values are determined by the setting of the *units* keyword, as discussed below. One or more x,y,z values can also be specified as NULL, which means exclude that dimension from this operation. Or it can be specified as INIT which means to constrain the center-of-mass to its initial value at the beginning of the run.

The center-of-mass (COM) is computed for the group specified by the fix. If the current COM is different than the specified x,y,z, then a group of atoms has their coordinates shifted by the difference. By default the shifted group is also the group specified by the fix. A different group can be shifted by using the *shift* keyword. For example, the COM could be computed on a protein to keep it in the center of the simulation box. But the entire system (protein + water) could be shifted.

If the *units* keyword is set to *box*, then the distance units of x,y,z are defined by the units command - e.g. Angstroms for *real* units. A *lattice* value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacing. A *fraction* value means a fractional distance between the lo/hi box boundaries, e.g. 0.5 = middle of the box. The default is to use lattice units.

Note that the velocity command can be used to create velocities with zero aggregate linear and/or angular momentum.

NOTE: This fix performs its operations at the same point in the timestep as other time integration fixes, such as fix nve, fix nvt, or fix npt. Thus fix recenter should normally be the last such fix specified in the input script, since

the adjustments it makes to atom coordinates should come after the changes made by time integration. LAMMPS will warn you if your fixes are not ordered this way.

NOTE: If you use this fix on a small group of atoms (e.g. a molecule in solvent) without using the *shift* keyword to adjust the positions of all atoms in the system, then the results can be unpredictable. For example, if the molecule is pushed in one direction by the solvent, its velocity will increase. But its coordinates will be recentered, meaning it is pushed back towards the force. Thus over time, the velocity and temperature of the molecule could become very large (though it won't appear to be moving due to the recentering). If you are thermostatting the entire system, then the solvent would be cooled to compensate. A better solution for this simulation scenario is to use the fix spring command to tether the molecule in place.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the distance the group is moved by fix recenter.

This fix also computes global 3-vector which can be accessed by various output commands. The 3 quantities in the vector are xyz components of displacement applied to the group of atoms by the fix.

The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix should not be used with an x,y,z setting that causes a large shift in the system on the 1st timestep, due to the requested COM being very different from the initial COM. This could cause atoms to be lost, especially in parallel. Instead, use the displace_atoms command, which can be used to move atoms a large distance.

Related commands:

fix momentum, velocity

Default:

The option defaults are shift = fix group-ID, and units = lattice.

fix restrain command

Syntax:

```
fix ID group-ID restrain keyword args ...
```

- ID, group-ID are documented in fix command
- restrain = style name of this fix command
- one or more keyword/arg pairs may be appended
- keyword = *bond* or *angle* or *dihedral*

```
  bond args = atom1 atom2 Kstart Kstop r0
      atom1,atom2 = IDs of 2 atoms in bond
      Kstart,Kstop = restraint coefficients at start/end of run (energy units)
      r0 = equilibrium bond distance (distance units)
    angle args = atom1 atom2 atom3 Kstart Kstop theta0
      atom1,atom2,atom3 = IDs of 3 atoms in angle, atom2 = middle atom
      Kstart,Kstop = restraint coefficients at start/end of run (energy units)
      theta0 = equilibrium angle theta (degrees)
    dihedral args = atom1 atom2 atom3 atom4 Kstart Kstop phi0
      atom1,atom2,atom3,atom4 = IDs of 4 atoms in dihedral in linear order
      Kstart,Kstop = restraint coefficients at start/end of run (energy units)
      phi0 = equilibrium dihedral angle phi (degrees)
```

Examples:

```
fix holdem all restrain bond 45 48 2000.0 2000.0 2.75
fix holdem all restrain dihedral 1 2 3 4 2000.0 2000.0 120.0
fix holdem all restrain bond 45 48 2000.0 2000.0 2.75 dihedral 1 2 3 4 2000.0 2000.0 120.0
fix texas_holdem all restrain dihedral 1 2 3 4 0.0 2000.0 120.0 dihedral 1 2 3 5 0.0 2000.0 -120.0 d
```

Description:

Restrain the motion of the specified sets of atoms by making them part of a bond or angle or dihedral interaction whose strength can vary over time during a simulation. This is functionally equivalent to creating a bond or angle or dihedral for the same atoms in a data file, as specified by the read_data command, albeit with a time-varying pre-factor coefficient. For the purpose of forcefield parameter-fitting or mapping a molecular potential energy surface, this fix reduces the hassle and risk associated with modifying data files. In other words, use this fix to temporarily force a molecule to adopt a particular conformation. To create a permanent bond or angle or dihedral, you should modify the data file.

The group-ID specified by this fix is ignored.

The second example above applies a restraint to hold the dihedral angle formed by atoms 1, 2, 3, and 4 near 120 degrees using a constant restraint coefficient. The fourth example applies similar restraints to multiple dihedral angles using a restraint coefficient that increases from 0.0 to 2000.0 over the course of the run.

NOTE: Adding a force to atoms implies a change in their potential energy as they move due to the applied force field. For dynamics via the run command, this energy can be added to the system's potential energy for thermodynamic output (see below). For energy minimization via the minimize command, this energy must be added to the system's potential energy to formulate a self-consistent minimization problem (see below).

In order for a restraint to be effective, the restraint force must typically be significantly larger than the forces associated with conventional forcefield terms. If the restraint is applied during a dynamics run (as opposed to during an energy minimization), a large restraint coefficient can significantly reduce the stable timestep size, especially if the atoms are initially far from the preferred conformation. You may need to experiment to determine what value of K works best for a given application.

For the case of finding a minimum energy structure for a single molecule with particular restratins (e.g. for fitting forcefield parameters or constructing a potential energy surface), commands such as the following may be useful:

```
# minimize molecule energy with restraints
velocity all create 600.0 8675309 mom yes rot yes dist gaussian
fix NVE all nve
fix TFIX all langevin 600.0 0.0 100 24601
fix REST all restrain dihedral 2 1 3 8 0.0 5000.0 ${angle1} dihedral 3 1 2 9 0.0 5000.0 ${angle2}
fix_modify REST energy yes
run 10000
fix TFIX all langevin 0.0 0.0 100 24601
fix REST all restrain dihedral 2 1 3 8 5000.0 5000.0 ${angle1} dihedral 3 1 2 9 5000.0 5000.0 ${angl
fix_modify REST energy yes
run 10000
# sanity check for convergence
minimize 1e-6 1e-9 1000 100000
# report unrestrained energies
unfix REST
run 0
```

The *bond* keyword applies a bond restraint to the specified atoms using the same functional form used by the bond_style harmonic command. The potential associated with the restraint is

$$E = K(r - r_0)^2$$

with the following coefficients:

- K (energy/distance^2)
- r0 (distance)

K and r0 are specified with the fix. Note that the usual 1/2 factor is included in K.

The *angle* keyword applies an angle restraint to the specified atoms using the same functional form used by the angle_style harmonic command. The potential associated with the restraint is

$$E = K(\theta - \theta_0)^2$$

with the following coefficients:

- K (energy/radian^2)
- theta0 (degrees)

K and theta0 are specified with the fix. Note that the usual 1/2 factor is included in K.

The *dihedral* keyword applies a dihedral restraint to the specified atoms using a simplified form of the function used by the dihedral_style charmm command. The potential associated with the restraint is

$$E = K[1 + \cos(n\phi - d)]$$

with the following coefficients:

- K (energy)
- n = 1
- d (degrees) = phi0 + 180

K and phi0 are specified with the fix. Note that the value of n is hard-wired to 1. Also note that the energy will be a minimum when the current dihedral angle phi is equal to phi0.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *energy* option is supported by this fix to add the potential energy associated with this fix to the system's potential energy as part of thermodynamic output.

NOTE: If you want the fictitious potential energy associated with the added forces to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the fix_modify *energy* option for this fix.

This fix computes a global scalar, which can be accessed by various output commands. The scalar is the potential energy for all the restraints as discussed above. The scalar value calculated by this fix is "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command.

Restrictions: none

Related commands: none

Default: none

fix rigid command

fix rigid/nve command

fix rigid/nvt command

fix rigid/npt command

fix rigid/nph command

fix rigid/small command

fix rigid/nve/small command

fix rigid/nvt/small command

fix rigid/npt/small command

fix rigid/nph/small command

Syntax:

```
fix ID group-ID style bodystyle args keyword values ...
```

- ID, group-ID are documented in fix command
- style = *rigid* or *rigid/nve* or *rigid/nvt* or *rigid/npt* or *rigid/nph* or *rigid/small* or *rigid/nve/small* or *rigid/nvt/small* or *rigid/npt/small* or *rigid/nph/small*
- bodystyle = *single* or *molecule* or *group*

```
  single args = none
    molecule args = none
    group args = N groupID1 groupID2 ...
      N = # of groups
      groupID1, groupID2, ... = list of N group IDs
```

- zero or more keyword/value pairs may be appended
- keyword = *langevin* or *temp* or *iso* or *aniso* or *x* or *y* or *z* or *couple* or *tparam* or *pchain* or *dilate* or *force* or *torque* or *infile*

```
  langevin values = Tstart Tstop Tperiod seed
      Tstart,Tstop = desired temperature at start/stop of run (temperature units)
      Tdamp = temperature damping parameter (time units)
      seed = random number seed to use for white noise (positive integer)
    temp values = Tstart Tstop Tdamp
      Tstart,Tstop = desired temperature at start/stop of run (temperature units)
      Tdamp = temperature damping parameter (time units)
    iso or aniso values = Pstart Pstop Pdamp
      Pstart,Pstop = scalar external pressure at start/end of run (pressure units)
      Pdamp = pressure damping parameter (time units)
    x or y or z values = Pstart Pstop Pdamp
      Pstart,Pstop = external stress tensor component at start/end of run (pressure units)
      Pdamp = stress damping parameter (time units)
```

```
      couple = none or xyz or xy or yz or xz
      tparam values = Tchain Titer Torder
        Tchain = length of Nose/Hoover thermostat chain
        Titer = number of thermostat iterations performed
        Torder = 3 or 5 = Yoshida-Suzuki integration parameters
      pchain values = Pchain
        Pchain = length of the Nose/Hoover thermostat chain coupled with the barostat
      dilate value = dilate-group-ID
        dilate-group-ID = only dilate atoms in this group due to barostat volume changes
      force values = M xflag yflag zflag
        M = which rigid body from 1-Nbody (see asterisk form below)
        xflag,yflag,zflag = off/on if component of center-of-mass force is active
      torque values = M xflag yflag zflag
        M = which rigid body from 1-Nbody (see asterisk form below)
        xflag,yflag,zflag = off/on if component of center-of-mass torque is active
      infile filename
        filename = file with per-body values of mass, center-of-mass, moments of inertia
      mol value = template-ID
        template-ID = ID of molecule template specified in a separate molecule command
```

Examples:

```
fix 1 clump rigid single
fix 1 clump rigid/small molecule
fix 1 clump rigid single force 1 off off on langevin 1.0 1.0 1.0 428984
fix 1 polychains rigid/nvt molecule temp 1.0 1.0 5.0
fix 1 polychains rigid molecule force 1*5 off off off force 6*10 off off on
fix 1 polychains rigid/small molecule langevin 1.0 1.0 1.0 428984
fix 2 fluid rigid group 3 clump1 clump2 clump3 torque * off off off
fix 1 rods rigid/npt molecule temp 300.0 300.0 100.0 iso 0.5 0.5 10.0
fix 1 particles rigid/npt molecule temp 1.0 1.0 5.0 x 0.5 0.5 1.0 z 0.5 0.5 1.0 couple xz
fix 1 water rigid/nph molecule iso 0.5 0.5 1.0
fix 1 particles rigid/npt/small molecule temp 1.0 1.0 1.0 iso 0.5 0.5 1.0
```

Description:

Treat one or more sets of atoms as independent rigid bodies. This means that each timestep the total force and torque on each rigid body is computed as the sum of the forces and torques on its constituent particles. The coordinates, velocities, and orientations of the atoms in each body are then updated so that the body moves and rotates as a single entity.

Examples of large rigid bodies are a colloidal particle, or portions of a biomolecule such as a protein.

Example of small rigid bodies are patchy nanoparticles, such as those modeled in this paper by Sharon Glotzer's group, clumps of granular particles, lipid molecules consiting of one or more point dipoles connected to other spheroids or ellipsoids, irregular particles built from line segments (2d) or triangles (3d), and coarse-grain models of nano or colloidal particles consisting of a small number of constituent particles. Note that the fix shake command can also be used to rigidify small molecules of 2, 3, or 4 atoms, e.g. water molecules. That fix treats the constituent atoms as point masses.

These fixes also update the positions and velocities of the atoms in each rigid body via time integration, in the NVE, NVT, NPT, or NPH ensemble, as described below.

There are two main variants of this fix, fix rigid and fix rigid/small. The NVE/NVT/NPT/NHT versions belong to one of the two variants, as their style names indicate.

NOTE: Not all of the *bodystyle* options and keyword/value options are available for both the *rigid* and *rigid/small* variants. See details below.

The *rigid* variant is typically the best choice for a system with a small number of large rigid bodies, each of which can extend across the domain of many processors. It operates by creating a single global list of rigid bodies, which all processors contribute to. MPI_Allreduce operations are performed each timestep to sum the contributions from each processor to the force and torque on all the bodies. This operation will not scale well in parallel if large numbers of rigid bodies are simulated.

The *rigid/small* variant is typically best for a system with a large number of small rigid bodies. Each body is assigned to the atom closest to the geometrical center of the body. The fix operates using local lists of rigid bodies owned by each processor and information is exchanged and summed via local communication between neighboring processors when ghost atom info is accumlated.

NOTE: To use *rigid/small* the ghost atom cutoff must be large enough to span the distance between the atom that owns the body and every other atom in the body. This distance value is printed out when the rigid bodies are defined. If the pair_style cutoff plus neighbor skin does not span this distance, then you should use the comm_modify cutoff command with a setting epsilon larger than the distance.

Which of the two variants is faster for a particular problem is hard to predict. The best way to decide is to perform a short test run. Both variants should give identical numerical answers for short runs. Long runs should give statistically similar results, but round-off differences may accumulate to produce divergent trajectories.

NOTE: You should not update the atoms in rigid bodies via other time-integration fixes (e.g. fix nve, fix nvt, fix npt), or you will be integrating their motion more than once each timestep. When performing a hybrid simulation with some atoms in rigid bodies, and some not, a separate time integration fix like fix nve or fix nvt should be used for the non-rigid particles.

NOTE: These fixes are overkill if you simply want to hold a collection of atoms stationary or have them move with a constant velocity. A simpler way to hold atoms stationary is to not include those atoms in your time integration fix. E.g. use "fix 1 mobile nve" instead of "fix 1 all nve", where "mobile" is the group of atoms that you want to move. You can move atoms with a constant velocity by assigning them an initial velocity (via the velocity command), setting the force on them to 0.0 (via the fix setforce command), and integrating them as usual (e.g. via the fix nve command).

NOTE: The aggregate properties of each rigid body are calculated one time at the start of the first simulation run after this fix is specified. The properties include the position and velocity of the center-of-mass of the body, its moments of inertia, and its angular momentum. This is done using the properties of the constituent atoms of the body at that point in time (or see the *infile* keyword option). Thereafter, changing properties of individual atoms in the body will have no effect on a rigid body's dynamics, unless they effect the pair_style interactions that individual particles are part of. For example, you might think you could displace the atoms in a body or add a large velocity to each atom in a body to make it move in a desired direction before a 2nd run is performed, using the set or displace_atoms or velocity command. But these commands will not affect the internal attributes of the body, and the position and velocity or individual atoms in the body will be reset when time integration starts.

Each rigid body must have two or more atoms. An atom can belong to at most one rigid body. Which atoms are in which bodies can be defined via several options.

NOTE: With fix rigid/small, which requires bodystyle *molecule*, you can define a system that has no rigid bodies initially. This is useful when you are using the *mol* keyword in conjunction with another fix that is adding rigid bodies on-the-fly, such as fix deposit or fix pour.

For bodystyle *single* the entire fix group of atoms is treated as one rigid body. This option is only allowed for fix rigid and its sub-styles.

For bodystyle *molecule*, each set of atoms in the fix group with a different molecule ID is treated as a rigid body. This option is allowed for fix rigid and fix rigid/small, and their sub-styles. Note that atoms with a molecule ID = 0 will be treated as a single rigid body. For a system with atomic solvent (typically this is atoms with molecule ID = 0) surrounding rigid bodies, this may not be what you want. Thus you should be careful to use a fix group that only includes atoms you want to be part of rigid bodies.

For bodystyle *group*, each of the listed groups is treated as a separate rigid body. Only atoms that are also in the fix group are included in each rigid body. This option is only allowed for fix rigid and its sub-styles.

NOTE: To compute the initial center-of-mass position and other properties of each rigid body, the image flags for each atom in the body are used to "unwrap" the atom coordinates. Thus you must insure that these image flags are consistent so that the unwrapping creates a valid rigid body (one where the atoms are close together), particularly if the atoms in a single rigid body straddle a periodic boundary. This means the input data file or restart file must define the image flags for each atom consistently or that you have used the set command to specify them correctly. If a dimension is non-periodic then the image flag of each atom must be 0 in that dimension, else an error is generated.

The *force* and *torque* keywords discussed next are only allowed for fix rigid and its sub-styles.

By default, each rigid body is acted on by other atoms which induce an external force and torque on its center of mass, causing it to translate and rotate. Components of the external center-of-mass force and torque can be turned off by the *force* and *torque* keywords. This may be useful if you wish a body to rotate but not translate, or vice versa, or if you wish it to rotate or translate continuously unaffected by interactions with other particles. Note that if you expect a rigid body not to move or rotate by using these keywords, you must insure its initial center-of-mass translational or angular velocity is 0.0. Otherwise the initial translational or angular momentum the body has will persist.

An xflag, yflag, or zflag set to *off* means turn off the component of force of torque in that dimension. A setting of *on* means turn on the component, which is the default. Which rigid body(s) the settings apply to is determined by the first argument of the *force* and *torque* keywords. It can be an integer M from 1 to Nbody, where Nbody is the number of rigid bodies defined. A wild-card asterisk can be used in place of, or in conjunction with, the M argument to set the flags for multiple rigid bodies. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of rigid bodies, then an asterisk with no numeric values means all bodies from 1 to N. A leading asterisk means all bodies from 1 to n (inclusive). A trailing asterisk means all bodies from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that you can use the *force* or *torque* keywords as many times as you like. If a particular rigid body has its component flags set multiple times, the settings from the final keyword are used.

NOTE: For computational efficiency, you may wish to turn off pairwise and bond interactions within each rigid body, as they no longer contribute to the motion. The neigh_modify exclude and delete_bonds commands are used to do this. If the rigid bodies have strongly overalapping atoms, you may need to turn off these interactions to avoid numerical problems due to large equal/opposite intra-body forces swamping the contribution of small inter-body forces.

For computational efficiency, you should typically define one fix rigid or fix rigid/small command which includes all the desired rigid bodies. LAMMPS will allow multiple rigid fixes to be defined, but it is more expensive.

The constituent particles within a rigid body can be point particles (the default in LAMMPS) or finite-size particles, such as spheres or ellipsoids or line segments or triangles. See the atom_style sphere and ellipsoid and line and tri commands for more details on these kinds of particles. Finite-size particles contribute differently to the moment of inertia of a rigid body than do point particles. Finite-size particles can also experience torque (e.g. due to frictional granular interactions) and have an orientation. These contributions are accounted for by these

fixes.

Forces between particles within a body do not contribute to the external force or torque on the body. Thus for computational efficiency, you may wish to turn off pairwise and bond interactions between particles within each rigid body. The neigh_modify exclude and delete_bonds commands are used to do this. For finite-size particles this also means the particles can be highly overlapped when creating the rigid body.

The *rigid* and *rigid/small* and *rigid/nve* styles perform constant NVE time integration. The only difference is that the *rigid* and *rigid/small* styles use an integration technique based on Richardson iterations. The *rigid/nve* style uses the methods described in the paper by Miller, which are thought to provide better energy conservation than an iterative approach.

The *rigid/nvt* and *rigid/nvt/small* styles performs constant NVT integration using a Nose/Hoover thermostat with chains as described originally in (Hoover) and (Martyna), which thermostats both the translational and rotational degrees of freedom of the rigid bodies. The rigid-body algorithm used by *rigid/nvt* is described in the paper by Kamberaj.

The *rigid/npt* and *rigid/nph* (and their /small counterparts) styles perform constant NPT or NPH integration using a Nose/Hoover barostat with chains. For the NPT case, the same Nose/Hoover thermostat is also used as with *rigid/nvt*.

The barostat parameters are specified using one or more of the *iso*, *aniso*, *x*, *y*, *z* and *couple* keywords. These keywords give you the ability to specify 3 diagonal components of the external stress tensor, and to couple these components together so that the dimensions they represent are varied together during a constant-pressure simulation. The effects of these keywords are similar to those defined in fix npt/nph

NOTE: Currently the *rigid/npt* and *rigid/nph* (and their /small counterparts) styles do not support triclinic (non-orthongonal) boxes.

The target pressures for each of the 6 components of the stress tensor can be specified independently via the *x*, *y*, *z* keywords, which correspond to the 3 simulation box dimensions. For each component, the external pressure or tensor component at each timestep is a ramped value during the run from *Pstart* to *Pstop*. If a target pressure is specified for a component, then the corresponding box dimension will change during a simulation. For example, if the *y* keyword is used, the y-box length will change. A box dimension will not change if that component is not specified, although you have the option to change that dimension via the fix deform command.

For all barostat keywords, the *Pdamp* parameter operates like the *Tdamp* parameter, determining the time scale on which pressure is relaxed. For example, a value of 10.0 means to relax the pressure in a timespan of (roughly) 10 time units (e.g. tau or fmsec or psec - see the units command).

Regardless of what atoms are in the fix group (the only atoms which are time integrated), a global pressure or stress tensor is computed for all atoms. Similarly, when the size of the simulation box is changed, all atoms are re-scaled to new positions, unless the keyword *dilate* is specified with a *dilate-group-ID* for a group that represents a subset of the atoms. This can be useful, for example, to leave the coordinates of atoms in a solid substrate unchanged and controlling the pressure of a surrounding fluid. Another example is a system consisting of rigid bodies and point particles where the barostat is only coupled with the rigid bodies. This option should be used with care, since it can be unphysical to dilate some atoms and not others, because it can introduce large, instantaneous displacements between a pair of atoms (one dilated, one not) that are far from the dilation origin.

The *couple* keyword allows two or three of the diagonal components of the pressure tensor to be "coupled" together. The value specified with the keyword determines which are coupled. For example, *xz* means the *Pxx* and *Pzz* components of the stress tensor are coupled. *Xyz* means all 3 diagonal components are coupled. Coupling

means two things: the instantaneous stress will be computed as an average of the corresponding diagonal components, and the coupled box dimensions will be changed together in lockstep, meaning coupled dimensions will be dilated or contracted by the same percentage every timestep. The *Pstart*, *Pstop*, *Pdamp* parameters for any coupled dimensions must be identical. *Couple xyz* can be used for a 2d simulation; the *z* dimension is simply ignored.

The *iso* and *aniso* keywords are simply shortcuts that are equivalent to specifying several other keywords together.

The keyword *iso* means couple all 3 diagonal components together when pressure is computed (hydrostatic pressure), and dilate/contract the dimensions together. Using "iso Pstart Pstop Pdamp" is the same as specifying these 4 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple xyz
```

The keyword *aniso* means *x*, *y*, and *z* dimensions are controlled independently using the *Pxx*, *Pyy*, and *Pzz* components of the stress tensor as the driving forces, and the specified scalar external pressure. Using "aniso Pstart Pstop Pdamp" is the same as specifying these 4 keywords:

```
x Pstart Pstop Pdamp
y Pstart Pstop Pdamp
z Pstart Pstop Pdamp
couple none
```

The keyword/value option pairs are used in the following ways.

The *langevin* and *temp* and *tparam* keywords perform thermostatting of the rigid bodies, altering both their translational and rotational degrees of freedom. What is meant by "temperature" of a collection of rigid bodies and how it can be monitored via the fix output is discussed below.

The *langevin* keyword applies a Langevin thermostat to the constant NVE time integration performed by either the *rigid* or *rigid/small* or *rigid/nve* styles. It cannot be used with the *rigid/nvt* style. The desired temperature at each timestep is a ramped value during the run from *Tstart* to *Tstop*. The *Tdamp* parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 100.0 means to relax the temperature in a timespan of (roughly) 100 time units (tau or fmsec or psec - see the units command). The random # *seed* must be a positive integer.

The way that Langevin thermostatting operates is explained on the fix langevin doc page. If you wish to simply viscously damp the rotational motion without thermostatting, you can set *Tstart* and *Tstop* to 0.0, which means only the viscous drag term in the Langevin thermostat will be applied. See the discussion on the fix viscous doc page for details.

NOTE: When the *langevin* keyword is used with fix rigid versus fix rigid/small, different dynamics will result for parallel runs. This is because of the way random numbers are used in the two cases. The dynamics for the two cases should be statistically similar, but will not be identical, even for a single timestep.

The *temp* and *tparam* keywords apply a Nose/Hoover thermostat to the NVT time integration performed by the *rigid/nvt* style. They cannot be used with the *rigid* or *rigid/small* or *rigid/nve* styles. The desired temperature at each timestep is a ramped value during the run from *Tstart* to *Tstop*. The *Tdamp* parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 100.0 means to relax the temperature in a timespan of (roughly) 100 time units (tau or fmsec or psec - see the units command).

Nose/Hoover chains are used in conjunction with this thermostat. The *tparam* keyword can optionally be used to change the chain settings used. *Tchain* is the number of thermostats in the Nose Hoover chain. This value, along with *Tdamp* can be varied to dampen undesirable oscillations in temperature that can occur in a simulation. As a rule of thumb, increasing the chain length should lead to smaller oscillations. The keyword *pchain* specifies the number of thermostats in the chain thermostatting the barostat degrees of freedom.

NOTE: There are alternate ways to thermostat a system of rigid bodies. You can use fix langevin to treat the individual particles in the rigid bodies as effectively immersed in an implicit solvent, e.g. a Brownian dynamics model. For hybrid systems with both rigid bodies and solvent particles, you can thermostat only the solvent particles that surround one or more rigid bodies by appropriate choice of groups in the compute and fix commands for temperature and thermostatting. The solvent interactions with the rigid bodies should then effectively thermostat the rigid body temperature as well without use of the Langevin or Nose/Hoover options associated with the fix rigid commands.

The *mol* keyword can only be used with fix rigid/small. It must be used when other commands, such as fix deposit or fix pour, add rigid bodies on-the-fly during a simulation. You specify a *template-ID* previously defined using the molecule command, which reads a file that defines the molecule. You must use the same *template-ID* that the other fix which is adding rigid bodies uses. The coordinates, atom types, atom diameters, center-of-mass, and moments of inertia can be specified in the molecule file. See the molecule command for details. The only settings required to be in this file are the coordinates and types of atoms in the molecule, in which case the molecule command calculates the other quantities itself.

Note that these other fixes create new rigid bodies, in addition to those defined initially by this fix via the *bodystyle* setting.

Also note that when using the *mol* keyword, extra restart information about all rigid bodies is written out whenever a restart file is written out. See the NOTE in the next section for details.

The *infile* keyword allows a file of rigid body attributes to be read in from a file, rather then having LAMMPS compute them. There are 5 such attributes: the total mass of the rigid body, its center-of-mass position, its 6 moments of inertia, its center-of-mass velocity, and the 3 image flags of the center-of-mass position. For rigid bodies consisting of point particles or non-overlapping finite-size particles, LAMMPS can compute these values accurately. However, for rigid bodies consisting of finite-size particles which overlap each other, LAMMPS will ignore the overlaps when computing these 4 attributes. The amount of error this induces depends on the amount of overlap. To avoid this issue, the values can be pre-computed (e.g. using Monte Carlo integration).

The format of the file is as follows. Note that the file does not have to list attributes for every rigid body integrated by fix rigid. Only bodies which the file specifies will have their computed attributes overridden. The file can contain initial blank lines or comment lines starting with "#" which are ignored. The first non-blank, non-comment line should list N = the number of lines to follow. The N successive lines contain the following information:

```
ID1 masstotal xcm ycm zcm ixx iyy izz ixy ixz iyz vxcm vycm vzcm lx ly lz ixcm iycm izcm
ID2 masstotal xcm ycm zcm ixx iyy izz ixy ixz iyz vxcm vycm vzcm lx ly lz ixcm iycm izcm
...
IDN masstotal xcm ycm zcm ixx iyy izz ixy ixz iyz vxcm vycm vzcm lx ly lz ixcm iycm izcm
```

The rigid body IDs are all positive integers. For the *single* bodystyle, only an ID of 1 can be used. For the *group* bodystyle, IDs from 1 to Ng can be used where Ng is the number of specified groups. For the *molecule* bodystyle, use the molecule ID for the atoms in a specific rigid body as the rigid body ID.

The masstotal and center-of-mass coordinates (xcm,ycm,zcm) are self-explanatory. The center-of-mass should be consistent with what is calculated for the position of the rigid body with all its atoms unwrapped by their

respective image flags. If this produces a center-of-mass that is outside the simulation box, LAMMPS wraps it back into the box.

The 6 moments of inertia (ixx,iyy,izz,ixy,ixz,iyz) should be the values consistent with the current orientation of the rigid body around its center of mass. The values are with respect to the simulation box XYZ axes, not with respect to the prinicpal axes of the rigid body itself. LAMMPS performs the latter calculation internally.

The (vxcm,vycm,vzcm) values are the velocity of the center of mass. The (lx,ly,lz) values are the angular momentum of the body. The (vxcm,vycm,vzcm) and (lx,ly,lz) values can simply be set to 0 if you wish the body to have no initial motion.

The (ixcm,iycm,izcm) values are the image flags of the center of mass of the body. For periodic dimensions, they specify which image of the simulation box the body is considered to be in. An image of 0 means it is inside the box as defined. A value of 2 means add 2 box lengths to get the true value. A value of -1 means subtract 1 box length to get the true value. LAMMPS updates these flags as the rigid bodies cross periodic boundaries during the simulation.

NOTE: If you use the *infile* or *mol* keywords and write restart files during a simulation, then each time a restart file is written, the fix also write an auxiliary restart file with the name rfile.rigid, where "rfile" is the name of the restart file, e.g. tmp.restart.10000 and tmp.restart.10000.rigid. This auxiliary file is in the same format described above. Thus it can be used in a new input script that restarts the run and re-specifies a rigid fix using an *infile* keyword and the appropriate filename. Note that the auxiliary file will contain one line for every rigid body, even if the original file only listed a subset of the rigid bodies.

If you use a temperature compute with a group that includes particles in rigid bodies, the degrees-of-freedom removed by each rigid body are accounted for in the temperature (and pressure) computation, but only if the temperature group includes all the particles in a particular rigid body.

A 3d rigid body has 6 degrees of freedom (3 translational, 3 rotational), except for a collection of point particles lying on a straight line, which has only 5, e.g a dimer. A 2d rigid body has 3 degrees of freedom (2 translational, 1 rotational).

NOTE: You may wish to explicitly subtract additional degrees-of-freedom if you use the *force* and *torque* keywords to eliminate certain motions of one or more rigid bodies. LAMMPS does not do this automatically.

The rigid body contribution to the pressure of the system (virial) is also accounted for by this fix.

If your simlulation is a hybrid model with a mixture of rigid bodies and non-rigid particles (e.g. solvent) there are several ways these rigid fixes can be used in tandem with fix nve, fix nvt, fix npt, and fix nph.

If you wish to perform NVE dynamics (no thermostatting or barostatting), use fix rigid or fix rigid/nve to integrate the rigid bodies, and fix nve to integrate the non-rigid particles.

If you wish to perform NVT dynamics (thermostatting, but no barostatting), you can use fix rigid/nvt for the rigid bodies, and any thermostatting fix for the non-rigid particles (fix nvt, fix langevin, fix temp/berendsen). You can also use fix rigid or fix rigid/nve for the rigid bodies and thermostat them using fix langevin on the group that contains all the particles in the rigid bodies. The net force added by fix langevin to each rigid body effectively thermostats its translational center-of-mass motion. Not sure how well it does at thermostatting its rotational motion.

If you with to perform NPT or NPH dynamics (barostatting), you cannot use both fix npt and fix rigid/npt (or the nph variants). This is because there can only be one fix which monitors the global pressure and changes the

simulation box dimensions. So you have 3 choices:

- Use fix rigid/npt for the rigid bodies. Use the *dilate* all option so that it will dilate the positions of the non-rigid particles as well. Use fix nvt (or any other thermostat) for the non-rigid particles.
- Use fix npt for the group of non-rigid particles. Use the *dilate* all option so that it will dilate the center-of-mass positions of the rigid bodies as well. Use fix rigid/nvt for the rigid bodies.
- Use fix press/berendsen to compute the pressure and change the box dimensions. Use fix rigid/nvt for the rigid bodies. Use fix nvt (or any other thermostat) for the non-rigid particles.

In all case, the rigid bodies and non-rigid particles both contribute to the global pressure and the box is scaled the same by any of the barostatting fixes.

You could even use the 2nd and 3rd options for a non-hybrid simulation consisting of only rigid bodies, assuming you give fix npt an empty group, though it's an odd thing to do. The barostatting fixes (fix npt and fix press/berensen) will monitor the pressure and change the box dimensions, but not time integrate any particles. The integration of the rigid bodies will be performed by fix rigid/nvt.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about the *rigid* and *rigid/small* and *rigid/nve* fixes are written to binary restart files. The exception is if the *infile* or *mol* keyword is used, in which case an auxiliary file is written out with rigid body information each time a restart file is written, as explained above for the *infile* keyword. For style *rigid/nvt* the state of the Nose/Hoover thermostat is written to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify *energy* option is supported by the rigid/nvt fix to add the energy change induced by the thermostatting to the system's potential energy as part of thermodynamic output.

The fix_modify *temp* and *press* options are supported by the rigid/npt and rigid/nph fixes to change the computes used to calculate the instantaneous pressure tensor. Note that the rigid/nvt fix does not use any external compute to compute instantaneous temperature.

The *rigid* and *rigid/small* and *rigid/nve* fixes compute a global scalar which can be accessed by various output commands. The scalar value calculated by these fixes is "intensive". The scalar is the current temperature of the collection of rigid bodies. This is averaged over all rigid bodies and their translational and rotational degrees of freedom. The translational energy of a rigid body is 1/2 m v^2, where m = total mass of the body and v = the

velocity of its center of mass. The rotational energy of a rigid body is 1/2 I w^2, where I = the moment of inertia tensor of the body and w = its angular velocity. Degrees of freedom constrained by the *force* and *torque* keywords are removed from this calculation, but only for the *rigid* and *rigid/nve* fixes.

The *rigid/nvt*, *rigid/npt*, and *rigid/nph* fixes compute a global scalar which can be accessed by various output commands. The scalar value calculated by these fixes is "extensive". The scalar is the cumulative energy change due to the thermostatting and barostatting the fix performs.

All of the *rigid* fixes except *rigid/small* compute a global array of values which can be accessed by various output commands. The number of rows in the array is equal to the number of rigid bodies. The number of columns is 15. Thus for each rigid body, 15 values are stored: the xyz coords of the center of mass (COM), the xyz components of the COM velocity, the xyz components of the force acting on the COM, the xyz components of the torque acting on the COM, and the xyz image flags of the COM.

The center of mass (COM) for each body is similar to unwrapped coordinates written to a dump file. It will always be inside (or slightly outside) the simulation box. The image flags have the same meaning as image flags for atom positions (see the "dump" command). This means you can calculate the unwrapped COM by applying the image flags to the COM, the same as when unwrapped coordinates are written to a dump file.

The force and torque values in the array are not affected by the *force* and *torque* keywords in the fix rigid command; they reflect values before any changes are made by those keywords.

The ordering of the rigid bodies (by row in the array) is as follows. For the *single* keyword there is just one rigid body. For the *molecule* keyword, the bodies are ordered by ascending molecule ID. For the *group* keyword, the list of group IDs determines the ordering of bodies.

The array values calculated by these fixes are "intensive", meaning they are independent of the number of atoms in the simulation.

No parameter of these fixes can be used with the *start/stop* keywords of the run command. These fixes are not invoked during energy minimization.

Restrictions:

These fixes are all part of the RIGID package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Assigning a temperature via the velocity create command to a system with rigid bodies may not have the desired outcome for two reasons. First, the velocity command can be invoked before the rigid-body fix is invoked or initialized and the number of adjusted degrees of freedom (DOFs) is known. Thus it is not possible to compute the target temperature correctly. Second, the assigned velocities may be partially canceled when constraints are first enforced, leading to a different temperature than desired. A workaround for this is to perform a run 0 command, which insures all DOFs are accounted for properly, and then rescale the temperature to the desired value before performing a simulation. For example:

```
velocity all create 300.0 12345
run 0                           # temperature may not be 300K
velocity all scale 300.0        # now it should be
```

Related commands:

delete_bonds, neigh_modify exclude, fix shake

Default:

The option defaults are force * on on on and torque * on on on, meaning all rigid bodies are acted on by center-of-mass force and torque. Also Tchain = Pchain = 10, Titer = 1, Torder = 3.

(Hoover) Hoover, Phys Rev A, 31, 1695 (1985).

(Kamberaj) Kamberaj, Low, Neal, J Chem Phys, 122, 224114 (2005).

(Martyna) Martyna, Klein, Tuckerman, J Chem Phys, 97, 2635 (1992); Martyna, Tuckerman, Tobias, Klein, Mol Phys, 87, 1117.

(Miller) Miller, Eleftheriou, Pattnaik, Ndirango, and Newns, J Chem Phys, 116, 8649 (2002).

(Zhang) Zhang, Glotzer, Nanoletters, 4, 1407-1413 (2004).

fix saed/vtk command

Syntax:

```
fix ID group-ID saed/vtk Nevery Nrepeat Nfreak c_ID attribute args ... keyword args ...
```

- ID, group-ID are documented in fix command
- saed/vtk = style name of this fix command
- Nevery = use input values every this many timesteps
- Nrepeat = # of times to use input values for calculating averages
- Nfreq = calculate averages every this many timesteps
- c_ID = saed compute ID

```
keyword = file or ave or start or file or overwrite:l
  ave args = one or running or window M
    one = output a new average value every Nfreq steps
    running = output cumulative average of all previous Nfreq steps
    window M = output average of M most recent Nfreq steps
  start args = Nstart
    Nstart = start averaging on this timestep
  file arg = filename
    filename = name of file to output time averages to
  overwrite arg = none = overwrite output file with only latest output
```

Examples:

```
compute 1 all saed 0.0251 Al O Kmax 1.70 Zone 0 0 1 dR_Ewald 0.01 c 0.5 0.5 0.5
compute 2 all saed 0.0251 Ni Kmax 1.70 Zone 0 0 0 c 0.05 0.05 0.05 manual echo

fix saed/vtk 1 1 1 c_1 file Al2O3_001.saed
fix saed/vtk 1 1 1 c_2 file Ni_000.saed
```

Description:

Time average computed intensities from compute_saed and write output to a file in the 3rd generation vtk image data format for visualization directly in parallelized visualization software packages like ParaView and VisIt. Note that if no time averaging is done, this command can be used as a convenient way to simply output diffraction intensities at a single snapshot.

To produce output in the image data vtk format ghost data is added outside the *Kmax* range assigned in the compute saed. The ghost data is assigned a value of -1 and can be removed setting a minimum isovolume of 0 within the vizualiziton software. SAED images can be created by visualizing a spherical slice of the data that is centered at R_Ewald*[h k l]/norm([h k l]), where R_Ewald=1/lambda.

The group specified within this command is ignored. However, note that specified values may represent calculations performed by saed computes which store their own "group" definitions.

Fix saed/vtk is designed to work only with compute_saed values, e.g.

```
compute 3 top saed 0.0251 Al O
fix saed/vtk 1 1 1 c_3 file Al2O3_001.saed
```

The *Nevery*, *Nrepeat*, and *Nfreq* arguments specify on what timesteps the input values will be used in order to contribute to the average. The final averaged quantities are generated on timesteps that are a multiple of *Nfreq*. The average is over *Nrepeat* quantities, computed in the preceding portion of the simulation every *Nevery* timesteps. *Nfreq* must be a multiple of *Nevery* and *Nevery* must be non-zero even if *Nrepeat* is 1. Also, the timesteps contributing to the average value cannot overlap, i.e. Nrepeat*Nevery can not exceed Nfreq.

For example, if Nevery=2, Nrepeat=6, and Nfreq=100, then values on timesteps 90,92,94,96,98,100 will be used to compute the final average on timestep 100. Similarly for timesteps 190,192,194,196,198,200 on timestep 200, etc. If Nrepeat=1 and Nfreq = 100, then no time averaging is done; values are simply generated on timesteps 100,200,etc.

The output for fix ave/time/saed is a file writen with the 3rd generation vtk image data formatting. The filename assigned by the *file* keyword is appended with _N.vtk where N is an index (0,1,2...) to account for multiple diffraction intensity outputs.

By default the header contains the following information (with example data):

```
# vtk DataFile Version 3.0 c_SAED
Image data set
ASCII
DATASET STRUCTURED_POINTS
DIMENSIONS 337 219 209
ASPECT_RATIO 0.00507953 0.00785161 0.00821458
ORIGIN -0.853361 -0.855826 -0.854316
POINT_DATA 15424827
SCALARS intensity float
LOOKUP_TABLE default
...data
```

In this example, kspace is sampled across a 337 x 219 x 209 point mesh where the mesh spacing is approximately 0.005, 0.007, and 0.008 inv(length) units in the k1, k2, and k3 directions, respectively. The data is shifted by -0.85, -0.85, -0.85 inv(length) units so that the origin will lie at 0, 0, 0. Here, 15,424,827 kspace points are sampled in total.

Additional optional keywords also affect the operation of this fix.

The *ave* keyword determines how the values produced every *Nfreq* steps are averaged with values produced on previous steps that were multiples of *Nfreq*, before they are accessed by another output command or written to a file.

If the *ave* setting is *one*, then the values produced on timesteps that are multiples of *Nfreq* are independent of each other; they are output as-is without further averaging.

If the *ave* setting is *running*, then the values produced on timesteps that are multiples of *Nfreq* are summed and averaged in a cumulative sense before being output. Each output value is thus the average of the value produced on that timestep with all preceding values. This running average begins when the fix is defined; it can only be restarted by deleting the fix via the unfix command, or by re-defining the fix by re-specifying it.

If the *ave* setting is *window*, then the values produced on timesteps that are multiples of *Nfreq* are summed and averaged within a moving "window" of time, so that the last M values are used to produce the output. E.g. if M = 3 and Nfreq = 1000, then the output on step 10000 will be the average of the individual values on steps 8000,9000,10000. Outputs on early steps will average over less than M values if they are not available.

The *start* keyword specifies what timestep averaging will begin on. The default is step 0. Often input values can be 0.0 at time 0, so setting *start* to a larger value can avoid including a 0.0 in a running or windowed average.

The *file* keyword allows a filename to be specified. Every *Nfreq* steps, the vector of saed intensity data is written to a new file using the 3rd generation vtk format. The base of each file is assigned by the *file* keyword and this string is appended with _N.vtk where N is an index (0,1,2...) to account for situations with multiple diffraction intensity outputs.

The *overwrite* keyword will continuously overwrite the output file with the latest output, so that it only contains one timestep worth of output. This option can only be used with the *ave running* setting.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

The attributes for fix_saed_vtk must match the values assigned in the associated compute_saed command.

Related commands:

compute_saed

Default:

The option defaults are ave = one, start = 0, no file output.

(Coleman) Coleman, Spearot, Capolungo, MSMSE, 21, 055020 (2013).

fix setforce command

fix setforce/cuda command

fix setforce/kk command

Syntax:

```
fix ID group-ID setforce fx fy fz keyword value ...
```

- ID, group-ID are documented in fix command
- setforce = style name of this fix command
- fx,fy,fz = force component values
- any of fx,fy,fz can be a variable (see below)
- zero or more keyword/value pairs may be appended to args
- keyword = *region*

```
region value = region-ID
    region-ID = ID of region atoms must be in to have added force
```

Examples:

```
fix freeze indenter setforce 0.0 0.0 0.0
fix 2 edge setforce NULL 0.0 0.0
fix 2 edge setforce NULL 0.0 v_oscillate
```

Description:

Set each component of force on each atom in the group to the specified values fx,fy,fz. This erases all previously computed forces on the atom, though additional fixes could add new forces. This command can be used to freeze certain atoms in the simulation by zeroing their force, either for running dynamics or performing an energy minimization. For dynamics, this assumes their initial velocity is also zero.

Any of the fx,fy,fz values can be specified as NULL which means do not alter the force component in that dimension.

Any of the 3 quantities defining the force components can be specified as an equal-style or atom-style variable, namely *fx*, *fy*, *fz*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the force component.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent force field.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent force field with optional time-dependence as well.

If the *region* keyword is used, the atom must also be in the specified geometric region in order to have force added to it.

Styles with a *cuda* or *kk* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

The region keyword is also supported by Kokkos, but a Kokkos-enabled region must be used. See the region region command for more information.

These accelerated styles are part of the USER-CUDA or Kokkos package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global 3-vector of forces, which can be accessed by various output commands. This is the total force on the group of atoms before the forces on individual atoms are changed by the fix. The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command, but you cannot set forces to any value besides zero when performing a minimization. Use the fix addforce command if you want to apply a non-zero force to atoms during a minimization.

Restrictions: none

Related commands:

fix addforce, fix aveforce

Default: none

fix shake command

fix shake/cuda command

fix rattle command

Syntax:

```
fix ID group-ID style tol iter N constraint values ... keyword value ...
```

- ID, group-ID are documented in fix command
- style = shake or rattle = style name of this fix command
- tol = accuracy tolerance of SHAKE solution
- iter = max # of iterations in each SHAKE solution
- N = print SHAKE statistics every this many timesteps (0 = never)
- one or more constraint/value pairs are appended
- constraint = *b* or *a* or *t* or *m*

```
  b values = one or more bond types
    a values = one or more angle types
    t values = one or more atom types
    m value = one or more mass values
```

- zero or more keyword/value pairs may be appended
- keyword = *mol*

```
  mol value = template-ID
      template-ID = ID of molecule template specified in a separate molecule command
```

Examples:

```
fix 1 sub shake 0.0001 20 10 b 4 19 a 3 5 2
fix 1 sub shake 0.0001 20 10 t 5 6 m 1.0 a 31
fix 1 sub shake 0.0001 20 10 t 5 6 m 1.0 a 31 mol myMol
fix 1 sub rattle 0.0001 20 10 t 5 6 m 1.0 a 31
fix 1 sub rattle 0.0001 20 10 t 5 6 m 1.0 a 31 mol myMol
```

Description:

Apply bond and angle constraints to specified bonds and angles in the simulation by either the SHAKE or RATTLE algorithms. This typically enables a longer timestep.

SHAKE vs RATTLE:

The SHAKE algorithm was invented for schemes such as standard Verlet timesteppnig, where only the coordinates are integrated and the velocities are approximated as finite differences to the trajectories (Ryckaert et al. (1977)). If the velocities are integrated explicitly, as with velocity Verlet which is what LAMMPS uses as an integration method, a second set of constraining forces is required in order to eliminate velocity components along the bonds (Andersen (1983)).

In order to formulate individual constraints for SHAKE and RATTLE, focus on a single molecule whose bonds are constrained. Let Ri and Vi be the position and velocity of atom i at time n, for i=1,...,N, where N is the number of sites of our reference molecule. The distance vector between sites i and j is given by

$$\mathbf{r}_{ij}^{n+1} = \mathbf{r}_j^n - \mathbf{r}_i^n$$

The constraints can then be formulated as

$$\mathbf{r}_{ij}^{n+1} \cdot \mathbf{r}_{ij}^{n+1} = d_{ij}^2 \quad \text{and}$$
$$\mathbf{v}_{ij}^{n+1} \cdot \mathbf{r}_{ij}^{n+1} = 0,$$

The SHAKE algorithm satisfies the first condition, i.e. the sites at time *n+1* will have the desired separations Dij immediately after the coordinates are integrated. If we also enforce the second condition, the velocity components along the bonds will vanish. RATTLE satisfies both conditions. As implemented in LAMMPS, fix rattle uses fix shake for satisfying the coordinate constraints. Therefore the settings and optional keywords are the same for both fixes, and all the information below about SHAKE is also relevant for RATTLE.

SHAKE:

Each timestep the specified bonds and angles are reset to their equilibrium lengths and angular values via the SHAKE algorithm (Ryckaert et al. (1977)). This is done by applying an additional constraint force so that the new positions preserve the desired atom separations. The equations for the additional force are solved via an iterative method that typically converges to an accurate solution in a few iterations. The desired tolerance (e.g. 1.0e-4 = 1 part in 10000) and maximum # of iterations are specified as arguments. Setting the N argument will print statistics to the screen and log file about regarding the lengths of bonds and angles that are being constrained. Small delta values mean SHAKE is doing a good job.

In LAMMPS, only small clusters of atoms can be constrained. This is so the constraint calculation for a cluster can be performed by a single processor, to enable good parallel performance. A cluster is defined as a central atom connected to others in the cluster by constrained bonds. LAMMPS allows for the following kinds of clusters to be constrained: one central atom bonded to 1 or 2 or 3 atoms, or one central atom bonded to 2 others and the angle between the 3 atoms also constrained. This means water molecules or CH2 or CH3 groups may be constrained, but not all the C-C backbone bonds of a long polymer chain.

The *b* constraint lists bond types that will be constrained. The *t* constraint lists atom types. All bonds connected to an atom of the specified type will be constrained. The *m* constraint lists atom masses. All bonds connected to atoms of the specified masses will be constrained (within a fudge factor of MASSDELTA specified in fix_shake.cpp). The *a* constraint lists angle types. If both bonds in the angle are constrained then the angle will also be constrained if its type is in the list.

For all constraints, a particular bond is only constrained if both atoms in the bond are in the group specified with the SHAKE fix.

The degrees-of-freedom removed by SHAKE bonds and angles are accounted for in temperature and pressure computations. Similarly, the SHAKE contribution to the pressure of the system (virial) is also accounted for.

NOTE: This command works by using the current forces on atoms to caculate an additional constraint force which when added will leave the atoms in positions that satisfy the SHAKE constraints (e.g. bond length) after the next time integration step. If you define fixes (e.g. fix efield) that add additional force to the atoms after fix shake operates, then this fix will not take them into account and the time integration will typically not satisfy the SHAKE constraints. The solution for this is to make sure that fix shake is defined in your input script after any other fixes which add or change forces (to atoms that fix shake operates on).

The *mol* keyword should be used when other commands, such as fix deposit or fix pour, add molecules on-the-fly during a simulation, and you wish to contrain the new molecules via SHAKE. You specify a *template-ID* previously defined using the molecule command, which reads a file that defines the molecule. You must use the same *template-ID* that the command adding molecules uses. The coordinates, atom types, special bond restrictions, and SHAKE info can be specified in the molecule file. See the molecule command for details. The only settings required to be in this file (by this command) are the SHAKE info of atoms in the molecule.

Styles with a *cuda* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

RATTLE:

The velocity constraints lead to a linear system of equations which can be solved analytically. The implementation of the algorithm in LAMMPS closely follows (Andersen (1983)).

NOTE: The fix rattle command modifies forces and velocities and thus should be defined after all other integration fixes in your input script. If you define other fixes that modify velocities or forces after fix rattle operates, then fix rattle will not take them into account and the overall time integration will typically not satisfy the RATTLE constraints. You can check whether the constraints work correctly by setting the value of RATTLE_DEBUG in src/fix_rattle.cpp to 1 and recompiling LAMMPS.

Restart, fix_modify, output, run start/stop, minimize info:

No information about these fixes is written to binary restart files. None of the fix_modify options are relevant to these fixes. No global or per-atom quantities are stored by these fixes for access by various output commands. No parameter of these fixes can be used with the *start/stop* keywords of the run command. These fixes are not invoked during energy minimization.

Restrictions:

These fixes are part of the RIGID package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

For computational efficiency, there can only be one shake or rattle fix defined in a simulation.

If you use a tolerance that is too large or a max-iteration count that is too small, the constraints will not be enforced very strongly, which can lead to poor energy conservation. You can test for this in your system by running a constant NVE simulation with a particular set of SHAKE parameters and monitoring the energy versus time.

SHAKE or RATTLE should not be used to contrain an angle at 180 degrees (e.g. linear CO2 molecule). This causes numeric difficulties.

Related commands: none

Default: none

(Ryckaert) J.-P. Ryckaert, G. Ciccotti and H. J. C. Berendsen, J of Comp Phys, 23, 327-341 (1977).

(Andersen) H. Andersen, J of Comp Phys, 52, 24-34 (1983).

fix shardlow command

Syntax:

```
fix ID group-ID shardlow
```

- ID, group-ID are documented in fix command
- shardlow = style name of this fix command

Examples:

```
fix 1 all shardlow
```

Description:

Specifies that the Shardlow splitting algorithm (SSA) is to be used to integrate the DPD equations of motion. The SSA splits the integration into a stochastic and deterministic integration step. The fix *shardlow* performs the stochastic integration step and must be used in conjunction with a deterministic integrator (e.g. fix nve or fix nph). The stochastic integration of the dissipative and random forces is performed prior to the deterministic integration of the conservative force. Further details regarding the method are provided in (Lisal) and (Larentzos).

The fix *shardlow* must be used with the pair_style dpd/fdt or pair_style dpd/fdt/energy command to properly initialize the fluctuation-dissipation theorem parameter(s) sigma (and kappa, if necessary).

Note that numerous variants of DPD can be specified by choosing an appropriate combination of the integrator and pair_style dpd/fdt command. DPD under isothermal conditions can be specified by using fix *shardlow*, fix *nve* and pair_style *dpd/fdt*. DPD under isoenergetic conditions can be specified by using fix *shardlow*, fix *nve* and pair_style *dpd/fdt/energy*. DPD under isobaric conditions can be specified by using fix shardlow, fix *nph* and pair_style *dpd/fdt*. DPD under isoenthalpic conditions can be specified by using fix shardlow, fix *nph* and pair_style *dpd/fdt/energy*. Examples of each DPD variant are provided in the examples/USER/dpd directory.

Restrictions:

This fix is only available if LAMMPS is built with the USER-DPD package. See the Making LAMMPS section for more info.

This fix is currently limited to orthogonal simulation cell geometries.

This fix must be used with an additional fix that specifies time integration, e.g. fix nve or fix nph.

The Shardlow splitting algorithm requires the sizes of the sub-domain lengths to be larger than twice the cutoff+skin. Generally, the domain decomposition is dependant on the number of processors requested.

Related commands:

pair_style dpd/fdt, fix eos/cv

Default: none

(Lisal) M. Lisal, J.K. Brennan, J. Bonet Avalos, "Dissipative particle dynamics as isothermal, isobaric, isoenergetic, and isoenthalpic conditions using Shardlow-like splitting algorithms.", J. Chem. Phys., 135, 204105 (2011).

(Larentzos) J.P. Larentzos, J.K. Brennan, J.D. Moore, M. Lisal and W.D. Mattson, "Parallel Implementation of Isothermal and Isoenergetic Dissipative Particle Dynamics Using Shardlow-Like Splitting Algorithms", Comput. Phys. Commun., 185, 1987-1998 (2014).

(Larentzos) J.P. Larentzos, J.K. Brennan, J.D. Moore, and W.D. Mattson, "LAMMPS Implementation of Constant Energy Dissipative Particle Dynamics (DPD-E)", ARL-TR-6863, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD (2014).

fix smd command

Syntax:

```
fix ID group-ID smd type values keyword values
```

- ID, group-ID are documented in fix command
- smd = style name of this fix command
- mode = *cvel* or *cfor* to select constant velocity or constant force SMD

```
  cvel values = K vel
      K = spring constant (force/distance units)
      vel = velocity of pulling (distance/time units)
    cfor values = force
      force = pulling force (force units)
```

- keyword = *tether* or *couple*

```
  tether values = x y z R0
      x,y,z = point to which spring is tethered
      R0 = distance of end of spring from tether point (distance units)
    couple values = group-ID2 x y z R0
      group-ID2 = 2nd group to couple to fix group with a spring
      x,y,z = direction of spring, automatically computed with 'auto'
      R0 = distance of end of spring (distance units)
```

Examples:

```
fix  pull    cterm smd cvel 20.0 -0.00005 tether NULL NULL 100.0 0.0
fix  pull    cterm smd cvel 20.0 -0.0001 tether 25.0 25 25.0 0.0
fix  stretch cterm smd cvel 20.0  0.0001 couple nterm auto auto auto 0.0
fix  pull    cterm smd cfor  5.0 tether 25.0 25.0 25.0 0.0
```

Description:

This fix implements several options of steered MD (SMD) as reviewed in (Izrailev), which allows to induce conformational changes in systems and to compute the potential of mean force (PMF) along the assumed reaction coordinate (Park) based on Jarzynski's equality (Jarzynski). This fix borrows a lot from fix spring and fix setforce.

You can apply a moving spring force to a group of atoms (*tether* style) or between two groups of atoms (*couple* style). The spring can then be used in either constant velocity (*cvel*) mode or in constant force (*cfor*) mode to induce transitions in your systems. When running in *tether* style, you may need some way to fix some other part of the system (e.g. via fix spring/self)

The *tether* style attaches a spring between a point at a distance of R0 away from a fixed point *x,y,z* and the center of mass of the fix group of atoms. A restoring force of magnitude K (R - R0) Mi / M is applied to each atom in the group where *K* is the spring constant, Mi is the mass of the atom, and M is the total mass of all atoms in the group. Note that *K* thus represents the total force on the group of atoms, not a per-atom force.

In *cvel* mode the distance R is incremented or decremented monotonously according to the pulling (or pushing) velocity. In *cfor* mode a constant force is added and the actual distance in direction of the spring is recorded.

The *couple* style links two groups of atoms together. The first group is the fix group; the second is specified by group-ID2. The groups are coupled together by a spring that is at equilibrium when the two groups are displaced

by a vector in direction *x,y,z* with respect to each other and at a distance R0 from that displacement. Note that *x,y,z* only provides a direction and will be internally normalized. But since it represents the *absolute* displacement of group-ID2 relative to the fix group, (1,1,0) is a different spring than (-1,-1,0). For each vector component, the displacement can be described with the *auto* parameter. In this case the direction is recomputed in every step, which can be useful for steering a local process where the whole object undergoes some other change. When the relative positions and distance between the two groups are not in equilibrium, the same spring force described above is applied to atoms in each of the two groups.

For both the *tether* and *couple* styles, any of the x,y,z values can be specified as NULL which means do not include that dimension in the distance calculation or force application.

For constant velocity pulling (*cvel* mode), the running integral over the pulling force in direction of the spring is recorded and can then later be used to compute the potential of mean force (PMF) by averaging over multiple independent trajectories along the same pulling path.

Restart, fix_modify, output, run start/stop, minimize info:

The fix stores the direction of the spring, current pulling target distance and the running PMF to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

None of the fix_modify options are relevant to this fix.

This fix computes a vector list of 7 quantities, which can be accessed by various output commands. The quantities in the vector are in this order: the x-, y-, and z-component of the pulling force, the total force in direction of the pull, the equilibrium distance of the spring, the distance between the two reference points, and finally the accumulated PMF (the sum of pulling forces times displacement).

The force is the total force on the group of atoms by the spring. In the case of the *couple* style, it is the force on the fix group (group-ID) or the negative of the force on the 2nd group (group-ID2). The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix drag, fix spring, fix spring/self, fix spring/rg

Default: none

(Izrailev) Izrailev, Stepaniants, Isralewitz, Kosztin, Lu, Molnar, Wriggers, Schulten. Computational Molecular Dynamics: Challenges, Methods, Ideas, volume 4 of Lecture Notes in Computational Science and Engineering, pp. 39-65. Springer-Verlag, Berlin, 1998.

(Park) Park, Schulten, J. Chem. Phys. 120 (13), 5946 (2004)

(Jarzynski) Jarzynski, Phys. Rev. Lett. 78, 2690 (1997)

fix smd/adjust_dt command

Syntax:

```
fix ID group-ID smd/adjust_dt arg
```

- ID, group-ID are documented in fix command
- smd/adjust_dt = style name of this fix command
- arg = *s_fact*

  s_fact = safety factor

Examples:

```
fix 1 all smd/adjust_dt 0.1
```

Description:

The fix calculates a new stable time increment for use with the SMD time integrators.

The stable time increment is based on multiple conditions. For the SPH pair styles, a CFL criterion (Courant, Friedrichs & Lewy, 1928) is evaluated, which determines the the speed of sound cannot propagate further than a typical spacing between particles within a single time step to ensure no information is lost. For the contact pair styles, a linear analysis of the pair potential determines a stable maximum time step.

This fix inquires the minimum stable time increment across all particles contained in the group for which this fix is defined. An additional safety factor *s_fact* is applied to the time increment.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Restart, fix_modify, output, run start/stop, minimize info:

Currently, no part of USER-SMD supports restarting nor minimization.

Restrictions:

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

smd/tlsph_dt

Default: none

fix smd/integrate_tlsph command

Syntax:

```
fix ID group-ID smd/integrate_tlsph keyword values
```

- ID, group-ID are documented in fix command
- smd/integrate_tlsph = style name of this fix command
- zero or more keyword/value pairs may be appended

- keyword = *limit_velocity*

```
limit_velocity value = max_vel
    max_vel = maximum allowed velocity
```

Examples:

```
fix 1 all smd/integrate_tlsph
fix 1 all smd/integrate_tlsph limit_velocity 1000
```

Description:

The fix performs explicit time integration for particles which interact according with the Total-Lagrangian SPH pair style.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

The *limit_velocity* keyword will control the velocity, scaling the norm of the velocity vector to max_vel in case it exceeds this velocity limit.

Restart, fix_modify, output, run start/stop, minimize info:

Currently, no part of USER-SMD supports restarting nor minimization. This fix has no outputs.

Restrictions:

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

smd/integrate_ulsph

Default: none

fix smd/integrate_ulsph command

Syntax:

```
fix ID group-ID smd/integrate_ulsph keyword
```

- ID, group-ID are documented in fix command
- smd/integrate_ulsph = style name of this fix command
- zero or more keyword/value pairs may be appended

keyword = adjust_radius or limit_velocity

adjust_radius values = adjust_radius_factor min_nn max_nn adjust_radius_factor = factor which scale the smooth/kernel radius min_nn = minimum number of neighbors max_nn = maximum number of neighbors limit_velocity values = max_velocity max_velocity = maximum allowed velocity.

Examples:

```
fix 1 all smd/integrate_ulsph adjust_radius 1.02 25 50

fix 1 all smd/integrate_ulsph limit_velocity 1000
```

Description:

The fix performs explicit time integration for particles which interact with the updated Lagrangian SPH pair style. See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

The *adjust_radius* keyword activates dynamic adjustment of the per-particle SPH smoothing kernel radius such that the number of neighbors per particles remains within the interval *min_nn* to *max_nn*. The parameter *adjust_radius_factor* determines the amount of adjustment per timestep. Typical values are *adjust_radius_factor*=1.02, *min_nn*=15, and *max_nn*=20.

The *limit_velocity* keyword will control the velocity, scaling the norm of the velocity vector to max_vel in case it exceeds this velocity limit.

Restart, fix_modify, output, run start/stop, minimize info:

Currently, no part of USER-SMD supports restarting nor minimization. This fix has no outputs.

Restrictions:

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

Default: none

fix smd/move_tri_surf command

Syntax:

```
fix ID group-ID smd/move_tri_surf keyword
```

- ID, group-ID are documented in fix command
- smd/move_tri_surf keyword = style name of this fix command
- keyword = **LINEAR* or **WIGGLE* or **ROTATE*

```
  *LINEAR args = Vx Vy Vz
        Vx,Vy,Vz = components of velocity vector (velocity units), any component can be specifie
     *WIGGLE args = Vx Vy Vz max_travel
        vx,vy,vz = components of velocity vector (velocity units), any component can be specifie
        max_travel = wiggle amplitude
     *ROTATE args = Px Py Pz Rx Ry Rz period
        Px,Py,Pz = origin point of axis of rotation (distance units)
        Rx,Ry,Rz = axis of rotation vector
        period = period of rotation (time units)
```

Examples:

```
fix 1 tool smd/move_tri_surf *LINEAR 20 20 10
fix 2 tool smd/move_tri_surf *WIGGLE 20 20 10
fix 2 tool smd/move_tri_surf *ROTATE 0 0 0 5 2 1
```

Description:

This fix applies only to rigid surfaces read from .STL files via fix smd/wall_surface . It updates position and velocity for the particles in the group each timestep without regard to forces on the particles. The rigid surfaces can thus be moved along simple trajectories during the simulation.

The **LINEAR* style moves particles with the specified constant velocity vector V = (Vx,Vy,Vz). This style also sets the velocity of each particle to V = (Vx,Vy,Vz).

The **WIGGLE* style moves particles in an oscillatory fashion. Particles are moved along (vx, vy, vz) with constant velocity until a displacement of max_travel is reached. Then, the velocity vector is reversed. This process is repeated.

The **ROTATE* style rotates particles around a rotation axis R = (Rx,Ry,Rz) that goes through a point P = (Px,Py,Pz). The period of the rotation is also specified. This style also sets the velocity of each particle to (omega cross Rperp) where omega is its angular velocity around the rotation axis and Rperp is a perpendicular vector from the rotation axis to the particle.

See this PDF guide to using Smooth Mach Dynamics in LAMMPS.

Restart, fix_modify, output, run start/stop, minimize info:

Currently, no part of USER-SMD supports restarting nor minimization. This fix has no outputs.

Restrictions:

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

smd/triangle_mesh_vertices, smd/wall_surface

Default: none

fix smd/setvel command

Syntax:

```
fix ID group-ID smd/setvel vx vy vz keyword value ...
```

- ID, group-ID are documented in fix command
- smd/setvel = style name of this fix command
- vx,vy,vz = velocity component values
- any of vx,vy,vz can be a variable (see below)
- zero or more keyword/value pairs may be appended to args
- keyword = *region*

```
region value = region-ID
    region-ID = ID of region particles must be in to have their velocities set
```

Examples:

```
fix top_velocity top_group setvel 1.0 0.0 0.0
```

Description:

Set each component of velocity on each particle in the group to the specified values vx,vy,vz, regardless of the forces acting on the particle. This command can be used to impose velocity boundary conditions.

Any of the vx,vy,vz values can be specified as NULL which means do not alter the velocity component in that dimension.

This fix is indented to be used together with a time integration fix.

Any of the 3 quantities defining the velocity components can be specified as an equal-style or atom-style variable, namely *vx*, *vy*, *vz*. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the force component.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent velocity field.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent velocity field with optional time-dependence as well.

If the *region* keyword is used, the particle must also be in the specified geometric region in order to have its velocity set by this command.

Restart, fix_modify, output, run start/stop, minimize info:

Currently, no part of USER-SMD supports restarting nor minimization None of the fix_modify options are relevant to this fix.

This fix computes a global 3-vector of forces, which can be accessed by various output commands. This is the total force on the group of atoms. The vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command.

Restrictions:

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands: none

Default: none

fix smd/wall_surface command

Syntax:

```
fix ID group-ID smd/wall_surface arg type mol-ID
```

- ID, group-ID are documented in fix command
- smd/wall_surface = style name of this fix command
- arg = *file*

  file = file name of a triangular mesh in stl format
- type = particle type to be given to the new particles created by this fix
- mol-ID = molecule-ID to be given to the new particles created by this fix (must be >= 65535)

Examples:

```
fix stl_surf all smd/wall_surface tool.stl 2 65535
```

Description:

This fix creates reads a traingulated surface from a file in .STL format. For each triangle, a new particle is created which stores the barycenter of the triangle and the vertex positions. The radius of the new particle is that of the minimum circle which encompasses the triangle vertices.

The triangulated surface can be used as a complex rigid wall via the smd/tri_surface pair style. It is possible to move the triangulated surface via the smd/move_tri_surf fix style.

Immediately after a .STL file has been read, the simulation needs to be run for 0 timesteps in order to properly register the new particles in the system. See the "funnel_flow" example in the USER-SMD examples directory.

See this PDF guide to use Smooth Mach Dynamics in LAMMPS.

Restart, fix_modify, output, run start/stop, minimize info:

Currently, no part of USER-SMD supports restarting nor minimization. This fix has no outputs.

Restrictions:

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info. The molecule ID given to the particles created by this fix have to be equal to or larger than 65535.

Within each .STL file, only a single triangulated object must be present, even though the STL format allows for the possibility of multiple objects in one file.

Related commands:

smd/triangle_mesh_vertices, smd/move_tri_surf, smd/tri_surface

Default: none

fix spring command

Syntax:

```
fix ID group-ID spring keyword values
```

- ID, group-ID are documented in fix command
- spring = style name of this fix command
- keyword = *tether* or *couple*

```
  tether values = K x y z R0
      K = spring constant (force/distance units)
      x,y,z = point to which spring is tethered
      R0 = equilibrium distance from tether point (distance units)
    couple values = group-ID2 K x y z R0
      group-ID2 = 2nd group to couple to fix group with a spring
      K = spring constant (force/distance units)
      x,y,z = direction of spring
      R0 = equilibrium distance of spring (distance units)
```

Examples:

```
fix pull ligand spring tether 50.0 0.0 0.0 0.0 0.0
fix pull ligand spring tether 50.0 0.0 0.0 0.0 5.0
fix pull ligand spring tether 50.0 NULL NULL 2.0 3.0
fix 5 bilayer1 spring couple bilayer2 100.0 NULL NULL 10.0 0.0
fix longitudinal pore spring couple ion 100.0 NULL NULL -20.0 0.0
fix radial pore spring couple ion 100.0 0.0 0.0 NULL 5.0
```

Description:

Apply a spring force to a group of atoms or between two groups of atoms. This is useful for applying an umbrella force to a small molecule or lightly tethering a large group of atoms (e.g. all the solvent or a large molecule) to the center of the simulation box so that it doesn't wander away over the course of a long simulation. It can also be used to hold the centers of mass of two groups of atoms at a given distance or orientation with respect to each other.

The *tether* style attaches a spring between a fixed point *x,y,z* and the center of mass of the fix group of atoms. The equilibrium position of the spring is R0. At each timestep the distance R from the center of mass of the group of atoms to the tethering point is computed, taking account of wrap-around in a periodic simulation box. A restoring force of magnitude K (R - R0) Mi / M is applied to each atom in the group where *K* is the spring constant, Mi is the mass of the atom, and M is the total mass of all atoms in the group. Note that *K* thus represents the total force on the group of atoms, not a per-atom force.

The *couple* style links two groups of atoms together. The first group is the fix group; the second is specified by group-ID2. The groups are coupled together by a spring that is at equilibrium when the two groups are displaced by a vector *x,y,z* with respect to each other and at a distance R0 from that displacement. Note that *x,y,z* is the equilibrium displacement of group-ID2 relative to the fix group. Thus (1,1,0) is a different spring than (-1,-1,0). When the relative positions and distance between the two groups are not in equilibrium, the same spring force described above is applied to atoms in each of the two groups.

For both the *tether* and *couple* styles, any of the x,y,z values can be specified as NULL which means do not include that dimension in the distance calculation or force application.

The first example above pulls the ligand towards the point (0,0,0). The second example holds the ligand near the surface of a sphere of radius 5 around the point (0,0,0). The third example holds the ligand a distance 3 away from the z=2 plane (on either side).

The fourth example holds 2 bilayers a distance 10 apart in z. For the last two examples, imagine a pore (a slab of atoms with a cylindrical hole cut out) oriented with the pore axis along z, and an ion moving within the pore. The fifth example holds the ion a distance of -20 below the z = 0 center plane of the pore (umbrella sampling). The last example holds the ion a distance 5 away from the pore axis (assuming the center-of-mass of the pore in x,y is the pore axis).

NOTE: The center of mass of a group of atoms is calculated in "unwrapped" coordinates using atom image flags, which means that the group can straddle a periodic boundary. See the dump doc page for a discussion of unwrapped coordinates. It also means that a spring connecting two groups or a group and the tether point can cross a periodic boundary and its length be calculated correctly. One exception is for rigid bodies, which should not be used with the fix spring command, if the rigid body will cross a periodic boundary. This is because image flags for rigid bodies are used in a different way, as explained on the fix rigid doc page.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *energy* option is supported by this fix to add the energy stored in the spring to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the spring energy = 0.5 * K * r^2.

This fix also computes global 4-vector which can be accessed by various output commands. The first 3 quantities in the vector are xyz components of the total force added to the group of atoms by the spring. In the case of the *couple* style, it is the force on the fix group (group-ID) or the negative of the force on the 2nd group (group-ID2). The 4th quantity in the vector is the magnitude of the force added by the spring, as a positive value if (r-R0) > 0 and a negative value if (r-R0) < 0. This sign convention can be useful when using the spring force to compute a potential of mean force (PMF).

The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command.

NOTE: If you want the spring energy to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the fix_modify *energy* option for this fix.

Restrictions: none

Related commands:

fix drag, fix spring/self, fix spring/rg, fix smd

Default: none

fix spring/rg command

Syntax:

```
fix ID group-ID spring/rg K RG0
```

- ID, group-ID are documented in fix command
- spring/rg = style name of this fix command
- K = harmonic force constant (force/distance units)
- RG0 = target radius of gyration to constrain to (distance units)

```
  if RG0 = NULL, use the current RG as the target value
```

Examples:

```
fix 1 protein spring/rg 5.0 10.0
fix 2 micelle spring/rg 5.0 NULL
```

Description:

Apply a harmonic restraining force to atoms in the group to affect their central moment about the center of mass (radius of gyration). This fix is useful to encourage a protein or polymer to fold/unfold and also when sampling along the radius of gyration as a reaction coordinate (i.e. for protein folding).

The radius of gyration is defined as RG in the first formula. The energy of the constraint and associated force on each atom is given by the second and third formulas, when the group is at a different RG than the target value RG0.

$$R_G{}^2 = \frac{1}{M} \sum_i^N m_i \left(x_i - \frac{1}{M} \sum_j^N m_j x_j \right)^2$$

$$E = K \left(R_G - R_{G0} \right)^2$$

$$F_i = 2K \frac{m_i}{M} \left(1 - \frac{R_{G0}}{R_G} \right) \left(x_i - \frac{1}{M} \sum_j^N m_j x_j \right)$$

The (xi - center-of-mass) term is computed taking into account periodic boundary conditions, m_i is the mass of the atom, and M is the mass of the entire group. Note that K is thus a force constant for the aggregate force on the group of atoms, not a per-atom force.

If RG0 is specified as NULL, then the RG of the group is computed at the time the fix is specified, and that value is used as the target.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

fix spring, fix spring/self fix drag, fix smd

Default: none

fix spring/self command

Syntax:

```
fix ID group-ID spring/self K dir
```

- ID, group-ID are documented in fix command
- spring/self = style name of this fix command
- K = spring constant (force/distance units)
- dir = xyz, xy, xz, yz, x, y, or z (optional, default: xyz)

Examples:

```
fix tether boundary-atoms spring/self 10.0
fix zrest  move spring/self 10.0 z
```

Description:

Apply a spring force independently to each atom in the group to tether it to its initial position. The initial position for each atom is its location at the time the fix command was issued. At each timestep, the magnitude of the force on each atom is -Kr, where r is the displacement of the atom from its current position to its initial position. The distance r correctly takes into account any crossings of periodic boundary by the atom since it was in its intitial position.

With the (optional) dir flag, one can select in which direction the spring force is applied. By default, the restraint is applied in all directions, but it can be limited to the xy-, xz-, yz-plane and the x-, y-, or z-direction, thus restraining the atoms to a line or a plane, respectively.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the original coordinates of tethered atoms to binary restart files, so that the spring effect will be the same in a restarted simulation. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix_modify *energy* option is supported by this fix to add the energy stored in the per-atom springs to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar which can be accessed by various output commands. The scalar is an energy which is the sum of the spring energy for each atom, where the per-atom energy is 0.5 * K * r^2. The scalar value calculated by this fix is "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command.

NOTE: If you want the per-atom spring energy to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the fix_modify *energy* option for this fix.

Restrictions: none

Related commands:

fix drag, fix spring, fix smd, fix spring/rg

Default: none

fix srd command

Syntax:

```
fix ID group-ID srd N groupbig-ID Tsrd hgrid seed keyword value ...
```

- ID, group-ID are documented in fix command
- srd = style name of this fix command
- N = reset SRD particle velocities every this many timesteps
- groupbig-ID = ID of group of large particles that SRDs interact with
- Tsrd = temperature of SRD particles (temperature units)
- hgrid = grid spacing for SRD grouping (distance units)
- seed = random # seed (positive integer)

- zero or more keyword/value pairs may be appended
- keyword = *lamda* or *collision* or *overlap* or *inside* or *exact* or *radius* or *bounce* or *search* or *cubic* or *shift* or *tstat* or *rescale*

```
lamda value = mean free path of SRD particles (distance units)
  collision value = noslip or slip = collision model
  overlap value = yes or no = whether big particles may overlap
  inside value = error or warn or ignore = how SRD particles which end up inside a big particl
  exact value = yes or no
  radius value = rfactor = scale collision radius by this factor
  bounce value = Nbounce = max # of collisions an SRD particle can undergo in one timestep
  search value = sgrid = grid spacing for collision partner searching (distance units)
  cubic values = style tolerance
    style = error or warn
    tolerance = fractional difference allowed (0 <= tol <= 1)
  shift values = flag shiftseed
    flag = yes or no or possible = SRD bin shifting for better statistics
      yes = perform bin shifting each time SRD velocities are rescaled
      no = no shifting
      possible = shift depending on mean free path and bin size
    shiftseed = random # seed (positive integer)
  tstat value = yes or no = thermostat SRD particles or not
  rescale value = yes or no or rotate or collide = rescaling of SRD velocities
    yes = rescale during velocity rotation and collisions
    no = no rescaling
    rotate = rescale during velocity rotation, but not collisions
    collide = rescale during collisions, but not velocity rotation
```

Examples:

```
fix 1 srd srd 10 big 1.0 0.25 482984
fix 1 srd srd 10 big 0.5 0.25 482984 collision slip search 0.5
```

Description:

Treat a group of partilces as stochastic rotation dynamics (SRD) particles that serve as a background solvent when interacting with big (colloidal) particles in groupbig-ID. The SRD formalism is described in (Hecht). The key idea behind using SRD particles as a cheap coarse-grained solvent is that SRD particles do not interact with each other, but only with the solute particles, which in LAMMPS can be spheroids, ellipsoids, or line segments, or triangles, or rigid bodies containing multiple spherioids or ellipsoids or line segments or triangles. The collision and rotation properties of the model imbue the SRD particles with fluid-like properties, including an effective viscosity. Thus

simulations with large solute particles can be run more quickly, to measure solute propoerties like diffusivity and viscosity in a background fluid. The usual LAMMPS fixes for such simulations, such as fix deform, fix viscosity, and fix nvt/sllod, can be used in conjunction with the SRD model.

For more details on how the SRD model is implemented in LAMMPS, this paper describes the implementation and usage of pure SRD fluids. This paper, which is nearly complete, describes the implementation and usage of mixture systems (solute particles in an SRD fluid). See the examples/srd directory for sample input scripts using SRD particles in both settings.

This fix does 2 things:

(1) It advects the SRD particles, performing collisions between SRD and big particles or walls every timestep, imparting force and torque to the big particles. Collisions also change the position and velocity of SRD particles.

(2) It resets the velocity distribution of SRD particles via random rotations every N timesteps.

SRD particles have a mass, temperature, characteristic timestep dt_SRD, and mean free path between collisions (lamda). The fundamental equation relating these 4 quantities is

```
lamda = dt_SRD * sqrt(Kboltz * Tsrd / mass)
```

The mass of SRD particles is set by the mass command elsewhere in the input script. The SRD timestep dt_SRD is N times the step dt defined by the timestep command. Big particles move in the normal way via a time integration fix with a short timestep dt. SRD particles advect with a large timestep dt_SRD >= dt.

If the *lamda* keyword is not specified, the the SRD temperature *Tsrd* is used in the above formula to compute lamda. If the *lamda* keyword is specified, then the *Tsrd* setting is ignored and the above equation is used to compute the SRD temperature.

The characteristic length scale for the SRD fluid is set by *hgrid* which is used to bin SRD particles for purposes of resetting their velocities. Normally hgrid is set to be 1/4 of the big particle diameter or smaller, to adequately resolve fluid properties around the big particles.

Lamda cannot be smaller than 0.6 * hgrid, else an error is generated (unless the *shift* keyword is used, see below). The velocities of SRD particles are bounded by Vmax, which is set so that an SRD particle will not advect further than Dmax = 4*lamda in dt_SRD. This means that roughly speaking, Dmax should not be larger than a big particle diameter, else SRDs may pass thru big particles without colliding. A warning is generated if this is the case.

Collisions between SRD particles and big particles or walls are modeled as a lightweight SRD point particle hitting a heavy big particle of given diameter or a wall at a point on its surface and bouncing off with a new velocity. The collision changes the momentum of the SRD particle. It imparts a force and torque to the big particle. It imparts a force to a wall. Static or moving SRD walls are setup via the fix wall/srd command. For the remainder of this doc page, a collision of an SRD particle with a wall can be viewed as a collision with a big particle of infinite radius and mass.

The *collision* keyword sets the style of collisions. The *slip* style means that the tangential component of the SRD particle momentum is preserved. Thus a force is imparted to a big particle, but no torque. The normal component of the new SRD velocity is sampled from a Gaussian distribution at temperature *Tsrd*.

For the *noslip* style, both the normal and tangential components of the new SRD velocity are sampled from a Gaussian distribution at temperature *Tsrd*. Additionally, a new tangential direction for the SRD velocity is chosen randomly. This collision style imparts torque to a big particle. Thus a time integrator fix that rotates the big

particles appropriately should be used.

The *overlap* keyword should be set to *yes* if two (or more) big particles can ever overlap. This depends on the pair potential interaction used for big-big interactions, or could be the case if multiple big particles are held together as rigid bodies via the fix rigid command. If the *overlap* keyword is *no* and big particles do in fact overlap, then SRD/big collisions can generate an error if an SRD ends up inside two (or more) big particles at once. How this error is treated is determined by the *inside* keyword. Running with *overlap* set to *no* allows for faster collision checking, so it should only be set to *yes* if needed.

The *inside* keyword determines how a collision is treated if the computation determines that the timestep started with the SRD particle already inside a big particle. If the setting is *error* then this generates an error message and LAMMPS stops. If the setting is *warn* then this generates a warning message and the code continues. If the setting is *ignore* then no message is generated. One of the output quantities logged by the fix (see below) tallies the number of such events, so it can be monitored. Note that once an SRD particle is inside a big particle, it may remain there for several steps until it drifts outside the big particle.

The *exact* keyword determines how accurately collisions are computed. A setting of *yes* computes the time and position of each collision as SRD and big particles move together. A setting of *no* estimates the position of each collision based on the end-of-timestep positions of the SRD and big particle. If *overlap* is set to yes, the setting of the *exact* keyword is ignored since time-accurate collisions are needed.

The *radius* keyword scales the effective size of big particles. If big particles will overlap as they undergo dynamics, then this keyword can be used to scale down their effective collision radius by an amount *rfactor*, so that SRD particle will only collide with one big particle at a time. For example, in a Lennard-Jones system at a temperature of 1.0 (in reduced LJ units), the minimum separation bewteen two big particles is as small as about 0.88 sigma. Thus an *rfactor* value of 0.85 should prevent dual collisions.

The *bounce* keyword can be used to limit the maximum number of collisions an SRD particle undergoes in a single timestep as it bounces between nearby big particles. Note that if the limit is reached, the SRD can be left inside a big particle. A setting of 0 is the same as no limit.

There are 2 kinds of bins created and maintained when running an SRD simulation. The first are "SRD bins" which are used to bin SRD particles and reset their velocities, as discussed above. The second are "search bins" which are used to identify SRD/big particle collisions.

The *search* keyword can be used to choose a search bin size for identifying SRD/big particle collisions. The default is to use the *hgrid* parameter for SRD bins as the search bin size. Choosing a smaller or large value may be more efficient, depending on the problem. But, in a statistical sense, it should not change the simulation results.

The *cubic* keyword can be used to generate an error or warning when the bin size chosen by LAMMPS creates SRD bins that are non-cubic or different than the requested value of *hgrid* by a specified *tolerance*. Note that using non-cubic SRD bins can lead to undetermined behavior when rotating the velocities of SRD particles, hence LAMMPS tries to protect you from this problem.

LAMMPS attempts to set the SRD bin size to exactly *hgrid*. However, there must be an integer number of bins in each dimension of the simulation box. Thus the actual bin size will depend on the size and shape of the overall simulation box. The actual bin size is printed as part of the SRD output when a simulation begins.

If the actual bin size in non-cubic by an amount exceeding the tolerance, an error or warning is printed, depending on the style of the *cubic* keyword. Likewise, if the actual bin size differs from the requested *hgrid* value by an amount exceeding the tolerance, then an error or warning is printed. The *tolerance* is a fractional difference. E.g. a tolerance setting of 0.01 on the shape means that if the ratio of any 2 bin dimensions exceeds (1 +/- tolerance)

then an error or warning is generated. Similarly, if the ratio of any bin dimension with *hgrid* exceeds (1 +/- tolerance), then an error or warning is generated.

NOTE: The fix srd command can be used with simluations the size and/or shape of the simulation box changes. This can be due to non-periodic boundary conditions or the use of fixes such as the fix deform or fix wall/srd commands to impose a shear on an SRD fluid or an interaction with an external wall. If the box size changes then the size of SRD bins must be recalculated every reneighboring. This is not necessary if only the box shape changes. This re-binning is always done so as to fit an integer number of bins in the current box dimension, whether it be a fixed, shrink-wrapped, or periodic boundary, as set by the boundary command. If the box size or shape changes, then the size of the search bins must be recalculated avery reneighboring. Note that changing the SRD bin size may alter the properties of the SRD fluid, such as its viscosity.

The *shift* keyword determines whether the coordinates of SRD particles are randomly shifted when binned for purposes of rotating their velocities. When no shifting is performed, SRD particles are binned and the velocity distribution of the set of SRD particles in each bin is adjusted via a rotation operator. This is a statistically valid operation if SRD particles move sufficiently far between successive rotations. This is determined by their mean-free path lamda. If lamda is less than 0.6 of the SRD bin size, then shifting is required. A shift means that all of the SRD particles are shifted by a vector whose coordinates are chosen randomly in the range [-1/2 bin size, 1/2 bin size]. Note that all particles are shifted by the same vector. The specified random number *shiftseed* is used to generate these vectors. This operation sufficiently randomizes which SRD particles are in the same bin, even if lamda is small.

If the *shift* flag is set to *no*, then no shifting is performed, but bin data will be communicated if bins overlap processor boundaries. An error will be generated if lamda < 0.6 of the SRD bin size. If the *shift* flag is set to *possible*, then shifting is performed only if lamda < 0.6 of the SRD bin size. A warning is generated to let you know this is occurring. If the *shift* flag is set to *yes* then shifting is performed regardless of the magnitude of lamda. Note that the *shiftseed* is not used if the *shift* flag is set to *no*, but must still be specified.

Note that shifting of SRD coordinates requires extra communication, hence it should not normally be enabled unless required.

The *tstat* keyword will thermostat the SRD particles to the specified *Tsrd*. This is done every N timesteps, during the velocity rotation operation, by rescaling the thermal velocity of particles in each SRD bin to the desired temperature. If there is a streaming velocity associated with the system, e.g. due to use of the fix deform command to perform a simulation undergoing shear, then that is also accounted for. The mean velocity of each bin of SRD particles is set to the position-dependent streaming velocity, based on the coordinates of the center of the SRD bin. Note that collisions of SRD particles with big particles or walls has a thermostatting effect on the colliding particles, so it may not be necessary to thermostat the SRD particles on a bin by bin basis in that case. Also note that for streaming simulations, if no thermostatting is performed (the default), then it may take a long time for the SRD fluid to come to equilibrium with a velocity profile that matches the simulation box deformation.

The *rescale* keyword enables rescaling of an SRD particle's velocity if it would travel more than 4 mean-free paths in an SRD timestep. If an SRD particle exceeds this velocity it is possible it will be lost when migrating to other processors or that collisions with big particles will be missed, either of which will generate errors. Thus the safest mode is to run with rescaling enabled. However rescaling removes kinetic energy from the system (the particle's velocity is reduced). The latter will not typically be a problem if thermostatting is enabled via the *tstat* keyword or if SRD collisions with big particles or walls effectively thermostat the system. If you wish to turn off rescaling (on is the default), e.g. for a pure SRD system with no thermostatting so that the temperature does not decline over time, the *rescale* keyword can be used. The *no* value turns rescaling off during collisions and the per-bin velocity rotation operation. The *collide* and *rotate* values turn it on for one of the operations and off for the other.

NOTE: This fix is normally used for simulations with a huge number of SRD particles relative to the number of big particles, e.g. 100 to 1. In this scenario, computations that involve only big particles (neighbor list creation, communication, time integration) can slow down dramatically due to the large number of background SRD particles.

Three other input script commands will largely overcome this effect, speeding up an SRD simulation by a significant amount. These are the atom_modify first, neigh_modify include, and comm_modify group commands. Each takes a group-ID as an argument, which in this case should be the group-ID of the big solute particles.

Additionally, when a pair_style for big/big particle interactions is specified, the pair_coeff command should be used to turn off big/SRD interactions, e.g. by setting their epsilon or cutoff length to 0.0.

The "delete_atoms overlap" command may be useful in setting up an SRD simulation to insure there are no initial overlaps between big and SRD particles.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix tabulates several SRD statistics which are stored in a vector of length 12, which can be accessed by various output commands. The vector values calculated by this fix are "intensive", meaning they do not scale with the size of the simulation. Technically, the first 8 do scale with the size of the simulation, but treating them as intensive means they are not scaled when printed as part of thermodyanmic output.

These are the 12 quantities. All are values for the current timestep, except for quantity 5 and the last three, each of which are cummulative quantities since the beginning of the run.

- (1) # of SRD/big collision checks performed
- (2) # of SRDs which had a collision
- (3) # of SRD/big colllisions (including multiple bounces)
- (4) # of SRD particles inside a big particle
- (5) # of SRD particles whose velocity was rescaled to be < Vmax
- (6) # of bins for collision searching
- (7) # of bins for SRD velocity rotation
- (8) # of bins in which SRD temperature was computed
- (9) SRD temperature
- (10) # of SRD particles which have undergone max # of bounces
- (11) max # of bounces any SRD particle has had in a single step
- (12) # of reneighborings due to SRD particles moving too far

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This command can only be used if LAMMPS was built with the SRD package. See the Making LAMMPS section for more info on packages.

Related commands:

Default:

The option defaults are lamda inferred from Tsrd, collision = noslip, overlap = no, inside = error, exact = yes, radius = 1.0, bounce = 0, search = hgrid, cubic = error 0.01, shift = no, tstat = no, and rescale = yes.

(Hecht) Hecht, Harting, Ihle, Herrmann, Phys Rev E, 72, 011408 (2005).

(Petersen) Petersen, Lechman, Plimpton, Grest, in' t Veld, Schunk, J Chem Phys, 132, 174106 (2010).

(Lechman) Lechman, et al, in preparation (2010).

fix store/force command

Syntax:

```
fix ID group-ID store/force
```

- ID, group-ID are documented in fix command
- store/force = style name of this fix command

Examples:

```
fix 1 all store/force
```

Description:

Store the forces on atoms in the group at the point during each timestep when the fix is invoked, as described below. This is useful for storing forces before constraints or other boundary conditions are computed which modify the forces, so that unmodified forces can be written to a dump file or accessed by other output commands that use per-atom quantities.

This fix is invoked at the point in the velocity-Verlet timestepping immediately after pair, bond, angle, dihedral, improper, and long-range forces have been calculated. It is the point in the timestep when various fixes that compute constraint forces are calculated and potentially modify the force on each atom. Examples of such fixes are fix shake, fix wall, and fix indent.

NOTE: The order in which various fixes are applied which operate at the same point during the timestep, is the same as the order they are specified in the input script. Thus normally, if you want to store per-atom forces due to force field interactions, before constraints are applied, you should list this fix first within that set of fixes, i.e. before other fixes that apply constraints. However, if you wish to include certain constraints (e.g. fix shake) in the stored force, then it could be specified after some fixes and before others.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix produces a per-atom array which can be accessed by various output commands. The number of columns for each atom is 3, and the columns store the x,y,z forces on each atom. The per-atom values be accessed on any timestep.

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

fix store_state

Default: none

fix store/state command

Syntax:

```
fix ID group-ID store/state N input1 input2 ... keyword value ...
```

- ID, group-ID are documented in fix command
- store/state = style name of this fix command
- N = store atom attributes every N steps, N = 0 for initial store only
- input = one or more atom attributes

```
possible attributes = id, mol, type, mass,
                      x, y, z, xs, ys, zs, xu, yu, zu, xsu, ysu, zsu, ix, iy, iz,
                      vx, vy, vz, fx, fy, fz,
                      q, mux, muy, muz, mu,
                      radius, diameter, omegax, omegay, omegaz,
                      angmomx, angmomy, angmomz, tqx, tqy, tqz,
                      c_ID, c_ID[N], f_ID, f_ID[N], v_name,
                      d_name, i_name
```

```
id = atom ID
mol = molecule ID
type = atom type
mass = atom mass
x,y,z = unscaled atom coordinates
xs,ys,zs = scaled atom coordinates
xu,yu,zu = unwrapped atom coordinates
xsu,ysu,zsu = scaled unwrapped atom coordinates
ix,iy,iz = box image that the atom is in
vx,vy,vz = atom velocities
fx,fy,fz = forces on atoms
q = atom charge
mux,muy,muz = orientation of dipolar atom
mu = magnitued of dipole moment of atom
radius,diameter = radius.diameter of spherical particle
omegax,omegay,omegaz = angular velocity of spherical particle
angmomx,angmomy,angmomz = angular momentum of aspherical particle
tqx,tqy,tqz = torque on finite-size particles
c_ID = per-atom vector calculated by a compute with ID
c_ID[I] = Ith column of per-atom array calculated by a compute with ID
f_ID = per-atom vector calculated by a fix with ID
f_ID[I] = Ith column of per-atom array calculated by a fix with ID
v_name = per-atom vector calculated by an atom-style variable with name
d_name = per-atom floating point vector name, managed by fix property/atom
i_name = per-atom integer vector name, managed by fix property/atom
```

- zero or more keyword/value pairs may be appended
- keyword = *com*

```
com value = yes or no
```

Examples:

```
fix 1 all store/state 0 x y z
fix 1 all store/state 0 xu yu zu com yes
fix 2 all store/state 1000 vx vy vz
```

Description:

Define a fix that stores attributes for each atom in the group at the time the fix is defined. If *N* is 0, then the values are never updated, so this is a way of archiving an atom attribute at a given time for future use in a calculation or output. See the discussion of output commands that take fixes as inputs.

If *N* is not zero, then the attributes will be updated every *N* steps.

NOTE: Actually, only atom attributes specified by keywords like *xu* or *vy* or *radius* are initially stored immediately at the point in your input script when the fix is defined. Attributes specified by a compute, fix, or variable are not initially stored until the first run following the fix definition begins. This is because calculating those attributes may require quantities that are not defined in between runs.

The list of possible attributes is the same as that used by the dump custom command, which describes their meaning.

If the *com* keyword is set to *yes* then the *xu*, *yu*, and *zu* inputs store the position of each atom relative to the center-of-mass of the group of atoms, instead of storing the absolute position.

The requested values are stored in a per-atom vector or array as discussed below. Zeroes are stored for atoms not in the specified group.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the per-atom values it stores to binary restart files, so that the values can be restored when a simulation is restarted. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

None of the fix_modify options are relevant to this fix.

If a single input is specified, this fix produces a per-atom vector. If multiple inputs are specified, a per-atom array is produced where the number of columns for each atom is the number of inputs. These can be accessed by various output commands. The per-atom values be accessed on any timestep.

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

dump custom, compute property/atom, fix property/atom, variable

Default:

The option default is com = no.

fix temp/berendsen command

fix temp/berendsen/cuda command

Syntax:

```
fix ID group-ID temp/berendsen Tstart Tstop Tdamp
```

- ID, group-ID are documented in fix command
- temp/berendsen = style name of this fix command
- Tstart,Tstop = desired temperature at start/end of run

```
   Tstart can be a variable (see below)
```

- Tdamp = temperature damping parameter (time units)

Examples:

```
fix 1 all temp/berendsen 300.0 300.0 100.0
```

Description:

Reset the temperature of a group of atoms by using a Berendsen thermostat (Berendsen), which rescales their velocities every timestep.

The thermostat is applied to only the translational degrees of freedom for the particles, which is an important consideration for finite-size particles which have rotational degrees of freedom are being thermostatted with this fix. The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

The desired temperature at each timestep is a ramped value during the run from *Tstart* to *Tstop*. The *Tdamp* parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 100.0 means to relax the temperature in a timespan of (roughly) 100 time units (tau or fmsec or psec - see the units command).

Tstart can be specified as an equal-style variable. In this case, the *Tstop* setting is ignored. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the target temperature.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent temperature.

NOTE: Unlike the fix nvt command which performs Nose/Hoover thermostatting AND time integration, this fix does NOT perform time integration. It only modifies velocities to effect thermostatting. Thus you must use a separate time integration fix, like fix nve to actually update the positions of atoms using the modified velocities. Likewise, this fix should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by fix nvt or fix langevin commands.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp", as if this command had been issued:

```
compute fix-ID_temp group-ID temp
```

See the compute temp command for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp*. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the compute_modify command or print this temperature during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with compute commands that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute commands to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a *cuda* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *temp* option is supported by this fix. You can use it to assign a temperature compute you have defined to this fix which will be used in its thermostatting procedure, as described above. For consistency, the group used by this fix and by the compute should be the same.

The fix_modify *energy* option is supported by this fix to add the energy change implied by a velocity rescaling to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the cummulative energy change due to this fix. The scalar value calculated by this fix is "extensive".

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

This fix can be used with dynamic groups as defined by the group command. Likewise it can be used with groups to which atoms are added or deleted over time, e.g. a deposition simulation. However, the conservation properties of the thermostat and barostat are defined for systems with a static set of atoms. You may observe odd behavior if the atoms in a group vary dramatically over time or the atom count becomes very small.

Related commands:

fix nve, fix nvt, fix temp/rescale, fix langevin, fix_modify, compute temp, fix press/berendsen

Default: none

(Berendsen) Berendsen, Postma, van Gunsteren, DiNola, Haak, J Chem Phys, 81, 3684 (1984).

fix temp/csvr command

fix temp/csld command

Syntax:

```
fix ID group-ID temp/csvr Tstart Tstop Tdamp seed

fix ID group-ID temp/csld Tstart Tstop Tdamp seed
```

- ID, group-ID are documented in fix command
- temp/csvr or temp/csld = style name of this fix command
- Tstart,Tstop = desired temperature at start/end of run

```
  Tstart can be a variable (see below)
```

- Tdamp = temperature damping parameter (time units)
- seed = random number seed to use for white noise (positive integer)

Examples:

```
fix 1 all temp/csvr 300.0 300.0 100.0 54324

fix 1 all temp/csld 100.0 300.0 10.0 123321
```

Description:

Adjust the temperature with a canonical sampling thermostat that uses global velocity rescaling with Hamiltonian dynamics (*temp/csvr*) (Bussi1), or Langevin dynamics (*temp/csld*) (Bussi2). In the case of *temp/csvr* the thermostat is similar to the empirical Berendsen thermostat in temp/berendsen, but chooses the actual scaling factor from a suitably chosen (gaussian) distribution rather than having it determined from the time constant directly. In the case of *temp/csld* the velocities are updated to a linear combination of the current velocities with a gaussian distribution of velocities at the desired temperature. Both termostats are applied every timestep.

The thermostat is applied to only the translational degrees of freedom for the particles, which is an important consideration for finite-size particles which have rotational degrees of freedom are being thermostatted with these fixes. The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

The desired temperature at each timestep is a ramped value during the run from *Tstart* to *Tstop*. The *Tdamp* parameter is specified in time units and determines how rapidly the temperature is relaxed. For example, a value of 100.0 means to relax the temperature in a timespan of (roughly) 100 time units (tau or fmsec or psec - see the units command).

Tstart can be specified as an equal-style variable. In this case, the *Tstop* setting is ignored. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the target temperature.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent temperature.

NOTE: Unlike the fix nvt command which performs Nose/Hoover thermostatting AND time integration, these fixes do NOT perform time integration. They only modify velocities to effect thermostatting. Thus you must use a separate time integration fix, like fix nve to actually update the positions of atoms using the modified velocities. Likewise, these fixes should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by fix nvt or fix langevin commands.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

These fixes compute a temperature each timestep. To do this, the fix creates its own compute of style "temp", as if this command had been issued:

```
compute fix-ID_temp group-ID temp
```

See the compute temp command for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp*. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the compute_modify command or print this temperature during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* will have no effect on this fix.

Like other fixes that perform thermostatting, these fixes can be used with compute commands that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute commands to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Restart, fix_modify, output, run start/stop, minimize info:

No information about these fixes are written to binary restart files.

The fix_modify *temp* option is supported by these fixes. You can use it to assign a temperature compute you have defined to these fixes which will be used in its thermostatting procedure, as described above. For consistency, the group used by these fixes and by the compute should be the same.

These fixes can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

These fixes are not invoked during energy minimization.

These fixes compute a global scalar which can be accessed by various output commands. The scalar is the cummulative energy change due to the fix. The scalar value calculated by this fix is "extensive".

Restrictions:

These fixes are not compatible with fix shake.

The fix can be used with dynamic groups as defined by the group command. Likewise it can be used with groups to which atoms are added or deleted over time, e.g. a deposition simulation. However, the conservation properties of the thermostat and barostat are defined for systems with a static set of atoms. You may observe odd behavior if the atoms in a group vary dramatically over time or the atom count becomes very small.

Related commands:

fix nve, fix nvt, fix temp/rescale, fix langevin, fix_modify, compute temp, fix temp/berendsen

Default: none

(Bussi1) Bussi, Donadio and Parrinello, J. Chem. Phys. 126, 014101(2007)

(Bussi2) Bussi and Parrinello, Phys. Rev. E 75, 056707 (2007)

fix temp/rescale command

fix temp/rescale/cuda command

fix temp/rescale/limit/cuda command

Syntax:

```
fix ID group-ID temp/rescale N Tstart Tstop window fraction
```

- ID, group-ID are documented in fix command
- temp/rescale = style name of this fix command
- N = perform rescaling every N steps
- Tstart,Tstop = desired temperature at start/end of run (temperature units)

  ```
  Tstart can be a variable (see below)
  ```
- window = only rescale if temperature is outside this window (temperature units)
- fraction = rescale to target temperature by this fraction

Examples:

```
fix 3 flow temp/rescale 100 1.0 1.1 0.02 0.5
fix 3 boundary temp/rescale 1 1.0 1.5 0.05 1.0
fix 3 boundary temp/rescale 1 1.0 1.5 0.05 1.0
```

Description:

Reset the temperature of a group of atoms by explicitly rescaling their velocities.

The rescaling is applied to only the translational degrees of freedom for the particles, which is an important consideration if finite-size particles which have rotational degrees of freedom are being thermostatted with this fix. The translational degrees of freedom can also have a bias velocity removed from them before thermostatting takes place; see the description below.

Rescaling is performed every N timesteps. The target temperature is a ramped value between the *Tstart* and *Tstop* temperatures at the beginning and end of the run.

Tstart can be specified as an equal-style variable. In this case, the *Tstop* setting is ignored. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the target temperature.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent temperature.

Rescaling is only performed if the difference between the current and desired temperatures is greater than the *window* value. The amount of rescaling that is applied is a *fraction* (from 0.0 to 1.0) of the difference between the actual and desired temperature. E.g. if *fraction* = 1.0, the temperature is reset to exactly the desired value.

NOTE: Unlike the fix nvt command which performs Nose/Hoover thermostatting AND time integration, this fix does NOT perform time integration. It only modifies velocities to effect thermostatting. Thus you must use a separate time integration fix, like fix nve to actually update the positions of atoms using the modified velocities. Likewise, this fix should not normally be used on atoms that also have their temperature controlled by another fix - e.g. by fix nvt or fix langevin commands.

See this howto section of the manual for a discussion of different ways to compute temperature and perform thermostatting.

This fix computes a temperature each timestep. To do this, the fix creates its own compute of style "temp", as if one of this command had been issued:

```
compute fix-ID_temp group-ID temp
```

See the compute temp for details. Note that the ID of the new compute is the fix-ID + underscore + "temp", and the group for the new compute is the same as the fix group.

Note that this is NOT the compute used by thermodynamic output (see the thermo_style command) with ID = *thermo_temp*. This means you can change the attributes of this fix's temperature (e.g. its degrees-of-freedom) via the compute_modify command or print this temperature during thermodynamic output via the thermo_style custom command using the appropriate compute-ID. It also means that changing attributes of *thermo_temp* will have no effect on this fix.

Like other fixes that perform thermostatting, this fix can be used with compute commands that calculate a temperature after removing a "bias" from the atom velocities. E.g. removing the center-of-mass velocity from a group of atoms or only calculating temperature on the x-component of velocity or only calculating temperature for atoms in a geometric region. This is not done by default, but only if the fix_modify command is used to assign a temperature compute to this fix that includes such a bias term. See the doc pages for individual compute commands to determine which ones include a bias. In this case, the thermostat works in the following manner: the current temperature is calculated taking the bias into account, bias is removed from each atom, thermostatting is performed on the remaining thermal degrees of freedom, and the bias is added back in.

Styles with a *cuda* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *temp* option is supported by this fix. You can use it to assign a temperature compute you have defined to this fix which will be used in its thermostatting procedure, as described above. For consistency, the

group used by this fix and by the compute should be the same.

The fix_modify *energy* option is supported by this fix to add the energy change implied by a velocity rescaling to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the cummulative energy change due to this fix. The scalar value calculated by this fix is "extensive".

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

fix langevin, fix nvt, fix_modify

Default: none

fix temp/rescale/eff command

Syntax:

```
fix ID group-ID temp/rescale/eff N Tstart Tstop window fraction
```

- ID, group-ID are documented in fix command
- temp/rescale/eff = style name of this fix command
- N = perform rescaling every N steps
- Tstart,Tstop = desired temperature at start/end of run (temperature units)
- window = only rescale if temperature is outside this window (temperature units)
- fraction = rescale to target temperature by this fraction

Examples:

```
fix 3 flow temp/rescale/eff 10 1.0 100.0 0.02 1.0
```

Description:

Reset the temperature of a group of nuclei and electrons in the electron force field model by explicitly rescaling their velocities.

The operation of this fix is exactly like that described by the fix temp/rescale command, except that the rescaling is also applied to the radial electron velocity for electron particles.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *temp* option is supported by this fix. You can use it to assign a temperature compute you have defined to this fix which will be used in its thermostatting procedure, as described above. For consistency, the group used by this fix and by the compute should be the same.

The fix_modify *energy* option is supported by this fix to add the energy change implied by a velocity rescaling to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the cummulative energy change due to this fix. The scalar value calculated by this fix is "extensive".

This fix can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the USER-EFF package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

fix langevin/eff, fix nvt/eff, fix_modify, fix_temp_rescale,

Default: none

fix tfmc command

Syntax:

```
fix ID group-ID tfmc Delta Temp seed keyword value
```

- ID, group-ID are documented in fix command
- tfmc = style name of this fix command
- Delta = maximal displacement length (distance units)
- Temp = imposed temperature of the system
- seed = random number seed (positive integer)
- zero or more keyword/arg pairs may be appended
- keyword = *com* or *rot*

```
com args = xflag yflag zflag
    xflag,yflag,zflag = 0/1 to exclude/include each dimension
  rot args = none
```

Examples:

```
fix 1 all tfmc 0.1 1000.0 159345
fix 1 all tfmc 0.05 600.0 658943 com 1 1 0
fix 1 all tfmc 0.1 750.0 387068 com 1 1 1 rot
```

Description:

Perform uniform-acceptance force-bias Monte Carlo (fbMC) simulations, using the time-stamped force-bias Monte Carlo (tfMC) algorithm described in (Mees) and (Bal).

One successful use case of force-bias Monte Carlo methods is that they can be used to extend the time scale of atomistic simulations, in particular when long time scale relaxation effects must be considered; some interesting examples are given in the review by (Neyts). An example of a typical use case would be the modelling of chemical vapour deposition (CVD) processes on a surface, in which impacts by gas-phase species can be performed using MD, but subsequent relaxation of the surface is too slow to be done using MD only. Using tfMC can allow for a much faster relaxation of the surface, so that higher fluxes can be used, effectively extending the time scale of the simulation. (Such an alternating simulation approach could be set up using a loop.)

The initial version of tfMC algorithm in (Mees) contained an estimation of the effective time scale of such a simulation, but it was later shown that the speed-up one can gain from a tfMC simulation is system- and process-dependent, ranging from none to several orders of magnitude. In general, solid-state processes such as (re)crystallisation or growth can be accelerated by up to two or three orders of magnitude, whereas diffusion in the liquid phase is not accelerated at all. The observed pseudodynamics when using the tfMC method is not the actual dynamics one would obtain using MD, but the relative importance of processes can match the actual relative dynamics of the system quite well, provided *Delta* is chosen with care. Thus, the system's equilibrium is reached faster than in MD, along a path that is generally roughly similar to a typical MD simulation (but not necessarily so). See (Bal) for details.

Each step, all atoms in the selected group are displaced using the stochastic tfMC algorithm, which is designed to sample the canonical (NVT) ensemble at the temperature *Temp*. Although tfMC is a Monte Carlo algorithm and thus strictly speaking does not perform time integration, it is similar in the sense that it uses the forces on all atoms in order to update their positions. Therefore, it is implemented as a time integration fix, and no other fixes

of this type (such as fix nve) should be used at the same time. Because velocities do not play a role in this kind of Monte Carlo simulations, instantaneous temperatures as calculated by temperature computes or thermodynamic output have no meaning: the only relevant temperature is the sampling temperature *Temp*. Similarly, performing tfMC simulations does not require setting a timestep and the simulated time as calculated by LAMMPS is meaningless.

The critical parameter determining the success of a tfMC simulation is *Delta*, the maximal displacement length of the lightest element in the system: the larger it is, the longer the effective time scale of the simulation will be (there is an approximately quadratic dependence). However, *Delta* must also be chosen sufficiently small in order to comply with detailed balance; in general values between 5 and 10 % of the nearest neighbor distance are found to be a good choice. For a more extensive discussion with specific examples, please refer to (Bal), which also describes how the code calculates element-specific maximal displacements from *Delta*, based on the fourth root of their mass.

Because of the uncorrelated movements of the atoms, the center-of-mass of the fix group will not necessarily be stationary, just like its orientation. When the *com* keyword is used, all atom positions will be shifted (after every tfMC iteration) in order to fix the position of the center-of-mass along the included directions, by setting the corresponding flag to 1. The *rot* keyword does the same for the rotational component of the tfMC displacements after every iteration.

NOTE: the *com* and *rot* keywords should not be used if an external force is acting on the specified fix group, along the included directions. This can be either a true external force (e.g. through fix wall) or forces due to the interaction with atoms not included in the fix group. This is because in such cases, translations or rotations of the fix group could be induced by these external forces, and removing them will lead to a violation of detailed balance.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

None of the fix_modify options are relevant to this fix.

This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the MC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This fix is not compatible with fix shake.

Related commands:

fix gcmc, fix nvt

Default:

The option default is com = 0 0 0

(Bal) K. M Bal and E. C. Neyts, J. Chem. Phys. 141, 204104 (2014).

(Mees) M. J. Mees, G. Pourtois, E. C. Neyts, B. J. Thijsse, and A. Stesmans, Phys. Rev. B 85, 134301 (2012).

(Neyts) E. C. Neyts and A. Bogaerts, Theor. Chem. Acc. 132, 1320 (2013).

fix thermal/conductivity command

Syntax:

```
fix ID group-ID thermal/conductivity N edim Nbin keyword value ...
```

- ID, group-ID are documented in fix command
- thermal/conductivity = style name of this fix command
- N = perform kinetic energy exchange every N steps
- edim = *x* or *y* or *z* = direction of kinetic energy transfer
- Nbin = # of layers in edim direction (must be even number)
- zero or more keyword/value pairs may be appended
- keyword = *swap*

```
  swap value = Nswap = number of swaps to perform every N steps
```

Examples:

```
fix 1 all thermal/conductivity 100 z 20
fix 1 all thermal/conductivity 50 z 20 swap 2
```

Description:

Use the Muller-Plathe algorithm described in this paper to exchange kinetic energy between two particles in different regions of the simulation box every N steps. This induces a temperature gradient in the system. As described below this enables the thermal conductivity of a material to be calculated. This algorithm is sometimes called a reverse non-equilibrium MD (reverse NEMD) approach to computing thermal conductivity. This is because the usual NEMD approach is to impose a temperature gradient on the system and measure the response as the resulting heat flux. In the Muller-Plathe method, the heat flux is imposed, and the temperature gradient is the system's response.

See the compute heat/flux command for details on how to compute thermal conductivity in an alternate way, via the Green-Kubo formalism.

The simulation box is divided into *Nbin* layers in the *edim* direction, where the layer 1 is at the low end of that dimension and the layer *Nbin* is at the high end. Every N steps, Nswap pairs of atoms are chosen in the following manner. Only atoms in the fix group are considered. The hottest Nswap atoms in layer 1 are selected. Similarly, the coldest Nswap atoms in the "middle" layer (see below) are selected. The two sets of Nswap atoms are paired up and their velocities are exchanged. This effectively swaps their kinetic energies, assuming their masses are the same. If the masses are different, an exchange of velocities relative to center of mass motion of the 2 atoms is performed, to conserve kinetic energy. Over time, this induces a temperature gradient in the system which can be measured using commands such as the following, which writes the temperature profile (assuming z = edim) to the file tmp.profile:

```
compute   ke all ke/atom
variable  temp atom c_ke/1.5
fix       3 all ave/spatial 10 100 1000 z lower 0.05 v_temp &
            file tmp.profile units reduced
```

Note that by default, Nswap = 1, though this can be changed by the optional *swap* keyword. Setting this parameter appropriately, in conjunction with the swap rate N, allows the heat flux to be adjusted across a wide range of

values, and the kinetic energy to be exchanged in large chunks or more smoothly.

The "middle" layer for velocity swapping is defined as the *Nbin*/2 + 1 layer. Thus if *Nbin* = 20, the two swapping layers are 1 and 11. This should lead to a symmetric temperature profile since the two layers are separated by the same distance in both directions in a periodic sense. This is why *Nbin* is restricted to being an even number.

As described below, the total kinetic energy transferred by these swaps is computed by the fix and can be output. Dividing this quantity by time and the cross-sectional area of the simulation box yields a heat flux. The ratio of heat flux to the slope of the temperature profile is proportional to the thermal conductivity of the fluid, in appropriate units. See the Muller-Plathe paper for details.

NOTE: If your system is periodic in the direction of the heat flux, then the flux is going in 2 directions. This means the effective heat flux in one direction is reduced by a factor of 2. You will see this in the equations for thermal conductivity (kappa) in the Muller-Plathe paper. LAMMPS is simply tallying kinetic energy which does not account for whether or not your system is periodic; you must use the value appropriately to yield a kappa for your system.

NOTE: After equilibration, if the temperature gradient you observe is not linear, then you are likely swapping energy too frequently and are not in a regime of linear response. In this case you cannot accurately infer a thermal conductivity and should try increasing the Nevery parameter.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the cummulative kinetic energy transferred between the bottom and middle of the simulation box (in the *edim* direction) is stored as a scalar quantity by this fix. This quantity is zeroed when the fix is defined and accumlates thereafter, once every N steps. The units of the quantity are energy; see the units command for details. The scalar value calculated by this fix is "intensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Swaps conserve both momentum and kinetic energy, even if the masses of the swapped atoms are not equal. Thus you should not need to thermostat the system. If you do use a thermostat, you may want to apply it only to the non-swapped dimensions (other than *vdim*).

LAMMPS does not check, but you should not use this fix to swap the kinetic energy of atoms that are in constrained molecules, e.g. via fix shake or fix rigid. This is because application of the constraints will alter the amount of transferred momentum. You should, however, be able to use flexible molecules. See the Zhang paper for a discussion and results of this idea.

When running a simulation with large, massive particles or molecules in a background solvent, you may want to only exchange kinetic energy bewteen solvent particles.

Related commands:

fix ave/spatial, fix viscosity, compute heat/flux

Default:

The option defaults are swap = 1.

(Muller-Plathe) Muller-Plathe, J Chem Phys, 106, 6082 (1997).

(Zhang) Zhang, Lussetti, de Souza, Muller-Plathe, J Phys Chem B, 109, 15060-15067 (2005).

fix ti/rs command

Syntax:

```
fix ID group-ID ti/rs lambda_initial lambda_final t_switch t_equil keyword value ...
```

- ID, group-ID are documented in fix command
- ti/rs = style name of this fix command
- lambda_initial/lambda_final = initial/final values of the coupling parameter
- t_switch/t_equil = number of steps of the switching/equilibration procedure
- keyword = *function*

```
function value = function-ID
    function-ID = ID of the switching function (1, 2 or 3)
```

Example:

```
fix ref all ti/rs 50.0 2000 1000
fix vf vacancy ti/rs 10.0 70000 50000 function 2
```

Description:

This fix allows you to compute the free energy temperature dependence by performing a thermodynamic integration procedure known as Reversible Scaling (de Koning99, de Koning00a). The thermodynamic integration is performed using the nonequilibrium method of Adiabatic Switching (Watanabe, de Koning96).

The forces on the atoms are dynamically scaled during the simulation, the rescaling is done in the following manner:

$$F_{\mathrm{total}} = \lambda F_{\mathrm{int}}$$

where F_int is the total force on the atoms due to the interatomic potential and lambda is the coupling parameter of the thermodynamic integration.

The fix acts as follows: during the first *t_equil* steps after the fix is defined the value of lambda is *lambda_initial* , this is the period to equilibrate the system in the lambda = *lambda_initial* state. After this the value of lambda changes continuously from *lambda_initial* to *lambda_final* according to the function defined using the keyword *function* (described below), this is done in *t_switch* steps. Then comes the second equilibration period of *t_equil* to equilibrate the system in the lambda = *lambda_final* state. After that the switching back to the lambda = *lambda_initial* state is done using *t_switch* timesteps and following the same switching function. After this period the value of lambda is kept equal to *lambda_initial* indefinitely or until a unfix erase the fix.

The description of thermodynamic integration in both directions is done in de Koning00b, the main reason is to try to eliminate the dissipated heat due to the nonequilibrium process.

The *function* keyword allows the use of three different switching rates. The option *1* results in a constant rescaling where the lambda parameter changes at a constant rate during the switching time according to the switching function

$$\lambda(\tau) = \lambda_i + \tau\left(\lambda_f - \lambda_i\right)$$

where tau is the scaled time variable t/t_switch. This switching function has the characteristic that the temperature scaling is faster at temperatures closer to the final temperature of the procedure. The option number *2* performs the switching at a rate defined by the following switching function

$$\lambda(\tau) = \frac{\lambda_i}{1 + \tau\left(\frac{\lambda_i}{\lambda_f} - 1\right)}$$

This switching function has the characteristic that the temperature scaling occurs at a constant rate during all the procedure. The option number *3* performs the switching at a rate defined by the following switching function

$$\lambda(\tau) = \frac{\lambda_i}{1 + \log_2(1+\tau)\left(\frac{\lambda_i}{\lambda_f} - 1\right)}$$

This switching function has the characteristic that the temperature scaling is faster at temperatures closer to the initial temperature of the procedure.

An example script using this command is provided in the examples/USER/misc/ti directory.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

This fix computes a global vector quantitie which can be accessed by various output commands. The vector has 2 positions, the first one is the coupling parameter lambda and the second one is the time derivative of lambda. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command.

Related commands:

fix ti/spring

Restrictions:

This command is part of the USER-MISC package. It is only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

Default:

The keyword default is function = 1.

(de Koning 99) M. de Koning, A. Antonelli and S. Yip, Phys Rev Lett, 83, 3973 (1999).

(Watanabe) M. Watanabe and W. P. Reinhardt, Phys Rev Lett, 65, 3301 (1990).

(de Koning 96) M. de Koning and A. Antonelli, Phys Rev E, 53, 465 (1996).

(de Koning 00a) M. de Koning, A. Antonelli and S. Yip, J Chem Phys, 115, 11025 (2000).

(de Koning 00b) M. de Koning et al., Computing in Science & Engineering, 2, 88 (2000).

fix ti/spring command

Syntax:

```
fix ID group-ID ti/spring K t_switch t_equil keyword value ...
```

- ID, group-ID are documented in fix command
- ti/spring = style name of this fix command
- K = spring constant (force/distance units)
- t_switch/t_equil = number of steps of the switching/equilibration procedure
- zero or more keyword/value pairs may be appended to args
- keyword = *function*

```
function value = function-ID
    function-ID = ID of the switching function (1 or 2)
```

Example:

```
fix ref all ti/spring 50.0 2000 1000 function 2
```

Description:

This fix allows you to compute the free energy of solids by performing a thermodynamic integration between the solid of interest and an Einstein crystal (Frenkel). The thermodynamic integration is performed using the nonequilibrium method of Adiabatic Switching (Watanabe, de Koning96).

A spring force is applied independently to each atom in the group to tether it to its initial position. The initial position for each atom is its location at the time the fix command was issued. More details about the springs are available in fix spring/self. The forces on the atoms are dynamically scaled during the simulation, the rescaling is done in the following manner:

$$F_{\mathrm{total}} = (1 - \lambda) F_{\mathrm{solid}} + \lambda F_{\mathrm{harm}}$$

where F_harm is the force due to the springs, F_solid is the total force on the atoms due to the interatomic potential and lambda is the coupling parameter of the thermodynamic integration.

The fix acts as follows: during the first *t_equil* steps after the fix is defined the value of lambda is zero, this is the period to equilibrate the system in the lambda = 0 state. After this the value of lambda changes continuously from 0 to 1 according to the function defined using the keyword *function* (described below), this is done in *t_switch* steps. Then comes the second equilibration period of *t_equil* to equilibrate the system in the lambda = 1 state. After that the switching back to the lambda = 0 state is made using *t_switch* timesteps and following the same switching function. After this period the value of lambda is kept equal to zero and the fix has no action in the dynamics of the system anymore.

The description of thermodynamic integration in both directions is done in de Koning97, the main reason is to try to eliminate the dissipated heat due to the nonequilibrium process.

The *function* keyword allows the use of two different switching rates, the option *1* results in a constant rescaling where the lambda parameter changes at a constant rate during the switching time according to the switching function

$$\lambda(\tau) = \tau$$

where tau is the scaled time variable t/t_switch. The option number *2* performs the switching at a rate defined by the following switching function

$$\lambda(\tau) = \tau^5 \left(70\tau^4 - 315\tau^3 + 540\tau^2 - 420\tau + 126\right)$$

This function has zero slope as lambda approaches its extreme values (0 and 1), according to (de Koning96) this results in smaller fluctuations on the integral to be computed on the thermodynamic integration.

NOTE: It is importante to keep the center of mass fixed during the thermodynamic integration, a non-zero total velocity will result in divergencies during the integration due to the fact that the atoms are 'attatched' to its equilibrium positions by the Einstein crystal. Check the option *zero* of fix langevin and velocity. The use of the Nose-Hoover thermostat (fix nvt) is NOT recommended due to its well documented issues with the canonical sampling of harmonic degrees of freedom (notice that the *chain* option will NOT solve this problem). The Langevin thermostat (fix langevin) works fine.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the original coordinates of tethered atoms to binary restart files, so that the spring effect will be the same in a restarted simulation. See the read restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

The fix modify *energy* option is supported by this fix to add the energy stored in the per-atom springs to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar and a global vector quantities which can be accessed by various output commands. The scalar is an energy which is the sum of the spring energy for each atom, where the per-atom energy is 0.5 * K * r^2. The vector has 2 positions, the first one is the coupling parameter lambda and the second one is the time derivative of lambda. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command.

NOTE: If you want the per-atom spring energy to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the fix modify *energy* option for this fix.

An example script using this command is provided in the examples/USER/misc/ti directory.

Related commands:

fix spring, fix ti/rs

Restrictions:

This command is part of the USER-MISC package. It is only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

Default:

The keyword default is function = 1.

(Frenkel) Daan Frenkel and Anthony J. C. Ladd, J. Chem. Phys. 81, 3188 (1984).

(Watanabe) M. Watanabe and W. P. Reinhardt, Phys Rev Lett, 65, 3301 (1990).

(de Koning 96) M. de Koning and A. Antonelli, Phys Rev E, 53, 465 (1996).

(de Koning 97) M. de Koning and A. Antonelli, Phys Rev B, 55, 735 (1997).

fix tmd command

Syntax:

```
fix ID group-ID tmd rho_final file1 N file2
```

- ID, group-ID are documented in fix command
- tmd = style name of this fix command
- rho_final = desired value of rho at the end of the run (distance units)
- file1 = filename to read target structure from
- N = dump TMD statistics every this many timesteps, 0 = no dump
- file2 = filename to write TMD statistics to (only needed if N > 0)

Examples:

```
fix 1 all nve
fix 2 tmdatoms tmd 1.0 target_file 100 tmd_dump_file
```

Description:

Perform targeted molecular dynamics (TMD) on a group of atoms. A holonomic constraint is used to force the atoms to move towards (or away from) the target configuration. The parameter "rho" is monotonically decreased (or increased) from its initial value to rho_final at the end of the run.

Rho has distance units and is a measure of the root-mean-squared distance (RMSD) between the current configuration of the atoms in the group and the target coordinates listed in file1. Thus a value of rho_final = 0.0 means move the atoms all the way to the final structure during the course of the run.

The target file1 can be ASCII text or a gzipped text file (detected by a .gz suffix). The format of the target file1 is as follows:

```
0.0 25.0 xlo xhi
0.0 25.0 ylo yhi
0.0 25.0 zlo zhi
125     24.97311    1.69005     23.46956 0 0 -1
126     1.94691     2.79640     1.92799  1 0 0
127     0.15906     3.46099     0.79121  1 0 0
...
```

The first 3 lines may or may not be needed, depending on the format of the atoms to follow. If image flags are included with the atoms, the 1st 3 lo/hi lines must appear in the file. If image flags are not included, the 1st 3 lines should not appear. The 3 lines contain the simulation box dimensions for the atom coordinates, in the same format as in a LAMMPS data file (see the read_data command).

The remaining lines each contain an atom ID and its target x,y,z coordinates. The atom lines (all or none of them) can optionally be followed by 3 integer values: nx,ny,nz. For periodic dimensions, they specify which image of the box the atom is considered to be in, i.e. a value of N (positive or negative) means add N times the box length to the coordinate to get the true value.

The atom lines can be listed in any order, but every atom in the group must be listed in the file. Atoms not in the fix group may also be listed; they will be ignored.

TMD statistics are written to file2 every N timesteps, unless N is specified as 0, which means no statistics.

The atoms in the fix tmd group should be integrated (via a fix nve, nvt, npt) along with other atoms in the system.

Restarts can be used with a fix tmd command. For example, imagine a 10000 timestep run with a rho_initial = 11 and a rho_final = 1. If a restart file was written after 2000 time steps, then the configuration in the file would have a rho value of 9. A new 8000 time step run could be performed with the same rho_final = 1 to complete the conformational change at the same transition rate. Note that for restarted runs, the name of the TMD statistics file should be changed to prevent it being overwritten.

For more information about TMD, see (Schlitter1) and (Schlitter2).

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands.

This fix can ramp its rho parameter over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

This fix is not invoked during energy minimization.

Restrictions:

All TMD fixes must be listed in the input script after all integrator fixes (nve, nvt, npt) are applied. This ensures that atoms are moved before their positions are corrected to comply with the constraint.

Atoms that have a TMD fix applied should not be part of a group to which a SHAKE fix is applied. This is because LAMMPS assumes there are not multiple competing holonomic constraints applied to the same atoms.

To read gzipped target files, you must compile LAMMPS with the -DLAMMPS_GZIP option - see the Making LAMMPS section of the documentation.

Related commands: none

Default: none

(Schlitter1) Schlitter, Swegat, Mulders, "Distance-type reaction coordinates for modelling activated processes", J Molecular Modeling, 7, 171-177 (2001).

(Schlitter2) Schlitter and Klahn, "The free energy of a reaction coordinate at multiple constraints: a concise formulation", Molecular Physics, 101, 3439-3443 (2003).

fix ttm command

fix ttm/mod command

Syntax:

```
fix ID group-ID ttm seed C_e rho_e kappa_e gamma_p gamma_s v_0 Nx Ny Nz T_infile N T_outfile
fix ID group-ID ttm/mod seed init_file Nx Ny Nz T_infile N T_outfile
```

- ID, group-ID are documented in fix command
- style = *ttm* or *ttm_mod*
- seed = random number seed to use for white noise (positive integer)
- remaining arguments for fix ttm:

```
C_e  = electronic specific heat (energy/(electron*temperature) units)
rho_e = electronic density (electrons/volume units)
kappa_e = electronic thermal conductivity (energy/(time*distance*temperature) units)
gamma_p = friction coefficient due to electron-ion interactions (mass/time units)
gamma_s = friction coefficient due to electronic stopping (mass/time units)
v_0 = electronic stopping critical velocity (velocity units)
Nx = number of thermal solve grid points in the x-direction (positive integer)
Ny = number of thermal solve grid points in the y-direction (positive integer)
Nz = number of thermal solve grid points in the z-direction (positive integer)
T_infile = filename to read initial electronic temperature from
N = dump TTM temperatures every this many timesteps, 0 = no dump
T_outfile = filename to write TTM temperatures to (only needed if N > 0)
```

- remaining arguments for fix ttm/mod:

```
init_file = file with the parameters to TTM
Nx = number of thermal solve grid points in the x-direction (positive integer)
Ny = number of thermal solve grid points in the y-direction (positive integer)
Nz = number of thermal solve grid points in the z-direction (positive integer)
T_infile = filename to read initial electronic temperature from
N = dump TTM temperatures every this many timesteps, 0 = no dump
T_outfile = filename to write TTM temperatures to (only needed if N > 0)
```

Examples:

```
fix 2 all ttm 699489 1.0 1.0 10 0.1 0.0 2.0 1 12 1 initialTs 1000 T.out
fix 2 all ttm 123456 1.0 1.0 1.0 1.0 1.0 5.0 5 5 5 Te.in 1 Te.out
fix 2 all ttm/mod 34277 parameters.txt 5 5 5 T_init 10 T_out
```

Description:

Use a two-temperature model (TTM) to represent heat transfer through and between electronic and atomic subsystems. LAMMPS models the atomic subsystem as usual with a molecular dynamics model and the classical force field specified by the user, but the electronic subsystem is modeled as a continuum, or a background "gas", on a regular grid. Energy can be transferred spatially within the grid representing the electrons. Energy can also be transferred between the electronic and the atomic subsystems. The algorithm underlying this fix was derived by D. M. Duffy and A. M. Rutherford and is discussed in two J Physics: Condensed Matter papers: (Duffy) and (Rutherford). They used this algorithm in cascade simulations where a primary knock-on atom (PKA) was initialized with a high velocity to simulate a radiation event.

The description in this sub-section applies to both fix ttm and fix ttm/mod. Fix ttm/mod adds options to account for external heat sources (e.g. at a surface) and for specifying parameters that allow the electronic heat capacity to depend strongly on electronic temperature. It is more expensive computationally than fix ttm because it treats the thermal diffusion equation as non-linear. More details on fix ttm/mod are given below.

Heat transfer between the electronic and atomic subsystems is carried out via an inhomogeneous Langevin thermostat. This thermostat differs from the regular Langevin thermostat (fix langevin) in three important ways. First, the Langevin thermostat is applied uniformly to all atoms in the user-specified group for a single target temperature, whereas the TTM fix applies Langevin thermostatting locally to atoms within the volumes represented by the user-specified grid points with a target temperature specific to that grid point. Second, the Langevin thermostat couples the temperature of the atoms to an infinite heat reservoir, whereas the heat reservoir for fix TTM is finite and represents the local electrons. Third, the TTM fix allows users to specify not just one friction coefficient, but rather two independent friction coefficients: one for the electron-ion interactions (*gamma_p*), and one for electron stopping (*gamma_s*).

When the friction coefficient due to electron stopping, *gamma_s*, is non-zero, electron stopping effects are included for atoms moving faster than the electron stopping critical velocity, *v_0*. For further details about this algorithm, see (Duffy) and (Rutherford).

Energy transport within the electronic subsystem is solved according to the heat diffusion equation with added source terms for heat transfer between the subsystems:

$$C_e \rho_e \frac{\partial T_e}{\partial t} = \bigtriangledown (\kappa_e \bigtriangledown T_e) - g_p (T_e - T_a) + g_s T'_a$$

where C_e is the specific heat, rho_e is the density, kappa_e is the thermal conductivity, T is temperature, the "e" and "a" subscripts represent electronic and atomic subsystems respectively, g_p is the coupling constant for the electron-ion interaction, and g_s is the electron stopping coupling parameter. C_e, rho_e, and kappa_e are specified as parameters to the fix. The other quantities are derived. The form of the heat diffusion equation used here is almost the same as that in equation 6 of (Duffy), with the exception that the electronic density is explicitly reprensented, rather than being part of the the specific heat parameter.

Currently, fix ttm assumes that none of the user-supplied parameters will vary with temperature. Note that (Duffy) used a tanh() functional form for the temperature dependence of the electronic specific heat, but ignored temperature dependencies of any of the other parameters. See more discussion below for fix ttm/mod.

These fixes require use of periodic boundary conditions and a 3D simulation. Periodic boundary conditions are also used in the heat equation solve for the electronic subsystem. This varies from the approach of (Rutherford) where the atomic subsystem was embedded within a larger continuum representation of the electronic subsystem.

The initial electronic temperature input file, *T_infile*, is a text file LAMMPS reads in with no header and with four numeric columns (ix,iy,iz,Temp) and with a number of rows equal to the number of user-specified grid points (Nx by Ny by Nz). The ix,iy,iz are node indices from 0 to nxnodes-1, etc. For example, the initial electronic temperatures on a 1 by 2 by 3 grid could be specified in a *T_infile* as follows:

```
0 0 0 1.0
0 0 1 1.0
0 0 2 1.0
0 1 0 2.0
0 1 1 2.0
```

```
0 1 2 2.0
```

where the electronic temperatures along the y=0 plane have been set to 1.0, and the electronic temperatures along the y=1 plane have been set to 2.0. The order of lines in this file is no important. If all the nodal values are not specified, LAMMPS will generate an error.

The temperature output file, *T_oufile*, is created and written by this fix. Temperatures for both the electronic and atomic subsystems at every node and every N timesteps are output. If N is specified as zero, no output is generated, and no output filename is needed. The format of the output is as follows. One long line is written every output timestep. The timestep itself is given in the first column. The next Nx*Ny*Nz columns contain the temperatures for the atomic subsystem, and the final Nx*Ny*Nz columns contain the temperatures for the electronic subsystem. The ordering of the Nx*Ny*Nz columns is with the z index varing fastest, y the next fastest, and x the slowest.

These fixes do not change the coordinates of their atoms; they only scales their velocities. Thus a time integration fix (e.g. fix nve) should still be used to time integrate the affected atoms. The fixes should not normally be used on atoms that have their temperature controlled by another fix - e.g. fix nvt or fix langevin.

NOTE: The current implementations of these fixes create a copy of the electron grid that overlays the entire simulation domain, for each processor. Values on the grid are summed across all processors. Thus you should insure that this grid is not too large, else your simulation could incur high memory and communication costs.

Additional details for fix ttm/mod

Fix ttm/mod uses the heat diffusion equation with possible external heat sources (e.g. laser heating in ablation simulations):

$$C_e\rho_e\frac{\partial T_e}{\partial t} = \bigtriangledown(\kappa_e \bigtriangledown T_e) - g_p(T_e - T_a) + g_s T'_a + \theta(x - x_{surface})I_0 \exp(-x/l_{ski}$$

where theta is the Heaviside step function, I_0 is the (absorbed) laser pulse intensity for ablation simulations, l_skin is the depth of skin-layer, and all other designations have the same meaning as in the former equation. The duration of the pulse is set by the parameter *tau* in the *init_file*.

Fix ttm/mod also allows users to specify the dependencies of C_e and kappa_e on the electronic temperature. The specific heat is expressed as

$$C_e = C_0 + (a_0 + a_1 X + a_2 X^2 + a_3 X^3 + a_4 X^4)\exp(-(AX)^2)$$

where X = T_e/1000, and the thermal conductivity is defined as kappa_e = D_e*rho_e*C_e, where D_e is the thermal diffusion coefficient.

Electronic pressure effects are included in the TTM model to account for the blast force acting on ions because of electronic pressure gradient (see (Chen), (Norman)). The total force acting on an ion is:

$$\vec{F}_i = -\partial U/\partial \vec{r}_i + \vec{F}_{langevin} - \nabla P_e/n_{ion}$$

where F_langevin is a force from Langevin thermostat simulating electron-phonon coupling, and nabla P_e/n_ion is the electron blast force.

The electronic pressure is taken to be P_e = B*rho_e*C_e*T_e

The current fix ttm/mod implementation allows TTM simulations with a vacuum. The vacuum region is defined as the grid cells with zero electronic temperature. The numerical scheme does not allow energy exchange with such cells. Since the material can expand to previously unoccupied region in some simulations, the vacuum border can be allowed to move. It is controlled by the *surface_movement* parameter in the *init_file*. If it is set to 1, then "vacuum" cells can be changed to "electron-filled" cells with the temperature *T_e_min* if atoms move into them (currently only implemented for the case of 1-dimensional motion of flat surface normal to the X axis). The initial borders of vacuum can be set in the *init_file* via *lsurface* and *rsurface* parameters. In this case, electronic pressure gradient is calculated as

$$\nabla_x P_e = \left[\frac{C_e T_e(x) \lambda}{(x+\lambda)^2} + \frac{x}{x+\lambda} \frac{(C_e T_e)_{x+\Delta x} - (C_e T_e)_x}{\Delta x} \right]$$

where lambda is the electron mean free path (see (Norman), (Pisarev))

The fix ttm/mod parameter file *init_file* has the following syntax/ Every line with the odd number is considered as a comment and ignored. The lines with the even numbers are treated as follows:

```
a_0, energy/(temperature*electron) units
a_1, energy/(temperature^2*electron) units
a_2, energy/(temperature^3*electron) units
a_3, energy/(temperature^4*electron) units
a_4, energy/(temperature^5*electron) units
C_0, energy/(temperature*electron) units
A, 1/temperature units
rho_e, electrons/volume units
D_e, length^2/time units
gamma_p, mass/time units
gamma_s, mass/time units
v_0, length/time units
I_0, energy/(time*length^2) units
lsurface, electron grid units (positive integer)
rsurface, electron grid units (positive integer)
l_skin, length units
tau, time units
B, dimensionless
lambda, length units
n_ion, ions/volume units
surface_movement: 0 to disable tracking of surface motion, 1 to enable
T_e_min, temperature units
```

Restart, fix_modify, output, run start/stop, minimize info:

These fixes write the state of the electronic subsystem and the energy exchange between the subsystems to binary restart files. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

Because the state of the random number generator is not saved in the restart files, this means you cannot do "exact" restarts with this fix, where the simulation continues on the same as if no restart had taken place. However, in a statistical sense, a restarted simulation should produce the same behavior.

None of the fix_modify options are relevant to these fixes.

Both fixes compute 2 output quantities stored in a vector of length 2, which can be accessed by various output commands. The first quantity is the total energy of the electronic subsystem. The second quantity is the energy transferred from the electronic to the atomic subsystem on that timestep. Note that the velocity verlet integrator applies the fix ttm forces to the atomic subsystem as two half-step velocity updates: one on the current timestep and one on the subsequent timestep. Consequently, the change in the atomic subsystem energy is lagged by half a timestep relative to the change in the electronic subsystem energy. As a result of this, users may notice slight fluctuations in the sum of the atomic and electronic subsystem energies reported at the end of the timestep.

The vector values calculated are "extensive".

No parameter of the fixes can be used with the *start/stop* keywords of the run command. The fixes are not invoked during energy minimization.

Restrictions:

Fix *ttm* is part of the MISC package. It is only enabled if LAMMPS was built with that package. Fix *ttm/mod* is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

These fixes can only be used for 3d simulations and orthogonal simlulation boxes. You must also use periodic boundary conditions.

Related commands:

fix langevin, fix dt/reset

Default: none

(Duffy) D M Duffy and A M Rutherford, J. Phys.: Condens. Matter, 19, 016207-016218 (2007).

(Rutherford) A M Rutherford and D M Duffy, J. Phys.: Condens. Matter, 19, 496201-496210 (2007).

(Chen) J Chen, D Tzou and J Beraun, Int. J. Heat Mass Transfer, 49, 307-316 (2006).

(Norman) G E Norman, S V Starikov, V V Stegailov et al., Contrib. Plasma Phys., 53, 129-139 (2013).

(Pisarev) V V Pisarev and S V Starikov, J. Phys.: Condens. Matter, 26, 475401 (2014).

fix tune/kspace command

Syntax:

```
fix ID group-ID tune/kspace N
```

- ID, group-ID are documented in fix command
- tune/kspace = style name of this fix command
- N = invoke this fix every N steps

Examples:

```
fix 2 all tune/kspace 100
```

Description:

This fix tests each kspace style (Ewald, PPPM, and MSM), and automatically selects the fastest style to use for the remainder of the run. If the fastest style is Ewald or PPPM, the fix also adjusts the coulomb cutoff towards optimal speed. Future versions of this fix will automatically select other kspace parameters to use for maximum simulation speed. The kspace parameters may include the style, cutoff, grid points in each direction, order, Ewald parameter, MSM parallelization cut-point, MPI tasks to use, etc.

The rationale for this fix is to provide the user with as-fast-as-possible simulations that include long-range electrostatics (kspace) while meeting the user-prescribed accuracy requirement. A simple heuristic could never capture the optimal combination of parameters for every possible run-time scenario. But by performing short tests of various kspace parameter sets, this fix allows parameters to be tailored specifically to the user's machine, MPI ranks, use of threading or accelerators, the simulated system, and the simulation details. In addition, it is possible that parameters could be evolved with the simulation on-the-fly, which is useful for systems that are dynamically evolving (e.g. changes in box size/shape or number of particles).

When this fix is invoked, LAMMPS will perform short timed tests of various parameter sets to determine the optimal parameters. Tests are performed on-the-fly, with a new test initialized every N steps. N should be chosen large enough so that adequate CPU time lapses between tests, thereby providing statistically significant timings. But N should not be chosen to be so large that an unfortunate parameter set test takes an inordinate amount of wall time to complete. An N of 100 for most problems seems reasonable. Once an optimal parameter set is found, that set is used for the remainder of the run.

This fix uses heristics to guide it's selection of parameter sets to test, but the actual timed results will be used to decide which set to use in the simulation.

It is not necessary to discard trajectories produced using sub-optimal parameter sets, or a mix of various parameter sets, since the user-prescribed accuracy will have been maintained throughout. However, some users may prefer to use this fix only to discover the optimal parameter set for a given setup that can then be used on subsequent production runs.

This fix starts with kspace parameters that are set by the user with the kspace_style and kspace_modify commands. The prescribed accuracy will be maintained by this fix throughout the simulation.

None of the fix_modify options are relevant to this fix.

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the KSPACE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Do not set "neigh_modify once yes" or else this fix will never be called. Reneighboring is required.

Related commands:

kspace_style, boundary kspace_modify, pair_style lj/cut/coul/long, pair_style lj/charmm/coul/long, pair_style lj/long, pair_style lj/long/coul/long, pair_style buck/coul/long

Default:

---

fix vector command

Syntax:

```
fix ID group-ID vector Nevery value1 value2 ...
```

- ID, group-ID are documented in fix command
- vector = style name of this fix command
- Nevery = use input values every this many timesteps
- one or more input values can be listed
- value = c_ID, c_ID[N], f_ID, f_ID[N], v_name

```
c_ID = global scalar calculated by a compute with ID
c_ID[I] = Ith component of global vector calculated by a compute with ID
f_ID = global scalar calculated by a fix with ID
f_ID[I] = Ith component of global vector calculated by a fix with ID
v_name = global value calculated by an equal-style variable with name
```

Examples:

```
fix 1 all vector 100 c_myTemp
fix 1 all vector 5 c_myTemp v_integral
```

Description:

Use one or more global values as inputs every few timesteps, and simply store them. For a single specified value, the values are stored as a global vector of growing length. For multiple specified values, they are stored as rows in a global array, whose number of rows is growing. The resulting vector or array can be used by other output commands.

One way to to use this command is to accumulate a vector that is time-integrated using the variable trap() function. For example the velocity auto-correlation function (VACF) can be time-integrated, to yield a diffusion coefficient, as follows:

```
compute         2 all vacf
fix             5 all vector 1 c_2[4]
variable        diff equal dt*trap(f_5)
thermo_style    custom step v_diff
```

The group specified with this command is ignored. However, note that specified values may represent calculations performed by computes and fixes which store their own "group" definitions.

Each listed value can be the result of a compute or fix or the evaluation of an equal-style variable. In each case, the compute, fix, or variable must produce a global quantity, not a per-atom or local quantity. And the global quantity must be a scalar, not a vector or array.

Computes that produce global quantities are those which do not have the word *atom* in their style name. Only a few fixes produce global quantities. See the doc pages for individual fixes for info on which ones produce such values. Variables of style *equal* are the only ones that can be used with this fix. Variables of style *atom* cannot be used, since they produce per-atom values.

The *Nevery* argument specifies on what timesteps the input values will be used in order to be stored. Only timesteps that are a multiple of *Nevery*, including timestep 0, will contribute values.

Note that if you perform multiple runs, using the "pre no" option of the run command to avoid initialization on subsequent runs, then you need to use the *stop* keyword with the first run command with a timestep value that encompasses all the runs. This is so that the vector or array stored by this fix can be allocated to a sufficient size.

If a value begins with "c_", a compute ID must follow which has been previously defined in the input script. If no bracketed term is appended, the global scalar calculated by the compute is used. If a bracketed term is appended, the Ith element of the global vector calculated by the compute is used.

Note that there is a compute reduce command which can sum per-atom quantities into a global scalar or vector which can thus be accessed by fix vector. Or it can be a compute defined not in your input script, but by thermodynamic output or other fixes such as fix nvt or fix temp/rescale. See the doc pages for these commands which give the IDs of these computes. Users can also write code for their own compute styles and add them to LAMMPS.

If a value begins with "f_", a fix ID must follow which has been previously defined in the input script. If no bracketed term is appended, the global scalar calculated by the fix is used. If a bracketed term is appended, the Ith element of the global vector calculated by the fix is used.

Note that some fixes only produce their values on certain timesteps, which must be compatible with *Nevery*, else an error will result. Users can also write code for their own fix styles and add them to LAMMPS.

If a value begins with "v_", a variable name must follow which has been previously defined in the input script. Only equal-style variables can be referenced. See the variable command for details. Note that variables of style *equal* define a formula which can reference individual atom properties or thermodynamic keywords, or they can invoke other computes, fixes, or variables when they are evaluated, so this is a very general means of specifying quantities to be stored by fix vector.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix produces a global vector or global array which can be accessed by various output commands. The values can only be accessed on timesteps that are multiples of *Nevery*.

A vector is produced if only a single input value is specified. An array is produced if multiple input values are specified. The length of the vector or the number of rows in the array grows by 1 every *Nevery* timesteps.

If the fix prouduces a vector, then the entire vector will be either "intensive" or "extensive", depending on whether the values stored in the vector are "intensive" or "extensive". If the fix produces an array, then all elements in the array must be the same, either "intensive" or "extensive". If a compute or fix provides the value stored, then the compute or fix determines whether the value is intensive or extensive; see the doc page for that compute or fix for further info. Values produced by a variable are treated as intensive.

This fix can allocate storage for stored values accumulated over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this. If using the run pre no command option, this is required to allow the fix to allocate sufficient storage for stored values.

This fix is not invoked during energy minimization.

Restrictions: none

Related commands:

compute, variable

Default: none

fix viscosity command

Syntax:

```
fix ID group-ID viscosity N vdim pdim Nbin keyword value ...
```

- ID, group-ID are documented in fix command
- viscosity = style name of this fix command
- N = perform momentum exchange every N steps
- vdim = *x* or *y* or *z* = which momentum component to exchange
- pdim = *x* or *y* or *z* = direction of momentum transfer
- Nbin = # of layers in pdim direction (must be even number)
- zero or more keyword/value pairs may be appended
- keyword = *swap* or *target*

```
  swap value = Nswap = number of swaps to perform every N steps
    vtarget value = V or INF = target velocity of swap partners (velocity units)
```

Examples:

```
fix 1 all viscosity 100 x z 20
fix 1 all viscosity 50 x z 20 swap 2 vtarget 1.5
```

Description:

Use the Muller-Plathe algorithm described in this paper to exchange momenta between two particles in different regions of the simulation box every N steps. This induces a shear velocity profile in the system. As described below this enables a viscosity of the fluid to be calculated. This algorithm is sometimes called a reverse non-equilibrium MD (reverse NEMD) approach to computing viscosity. This is because the usual NEMD approach is to impose a shear velocity profile on the system and measure the response via an off-diagonal component of the stress tensor, which is proportional to the momentum flux. In the Muller-Plathe method, the momentum flux is imposed, and the shear velocity profile is the system's response.

The simulation box is divided into *Nbin* layers in the *pdim* direction, where the layer 1 is at the low end of that dimension and the layer *Nbin* is at the high end. Every N steps, Nswap pairs of atoms are chosen in the following manner. Only atoms in the fix group are considered. Nswap atoms in layer 1 with positive velocity components in the *vdim* direction closest to the target value *V* are selected. Similarly, Nswap atoms in the "middle" layer (see below) with negative velocity components in the *vdim* direction closest to the negative of the target value *V* are selected. The two sets of Nswap atoms are paired up and their *vdim* momenta components are swapped within each pair. This resets their velocities, typically in opposite directions. Over time, this induces a shear velocity profile in the system which can be measured using commands such as the following, which writes the profile to the file tmp.profile:

```
fix f1 all ave/spatial 100 10 1000 z lower 0.05 vx &
    file tmp.profile units reduced
```

Note that by default, Nswap = 1 and vtarget = INF, though this can be changed by the optional *swap* and *vtarget* keywords. When vtarget = INF, one or more atoms with the most positive and negative velocity components are selected. Setting these parameters appropriately, in conjunction with the swap rate N, allows the momentum flux rate to be adjusted across a wide range of values, and the momenta to be exchanged in large chunks or more smoothly.

The "middle" layer for momenta swapping is defined as the *Nbin*/2 + 1 layer. Thus if *Nbin* = 20, the two swapping layers are 1 and 11. This should lead to a symmetric velocity profile since the two layers are separated by the same distance in both directions in a periodic sense. This is why *Nbin* is restricted to being an even number.

As described below, the total momentum transferred by these velocity swaps is computed by the fix and can be output. Dividing this quantity by time and the cross-sectional area of the simulation box yields a momentum flux. The ratio of momentum flux to the slope of the shear velocity profile is proportional to the viscosity of the fluid, in appropriate units. See the Muller-Plathe paper for details.

NOTE: If your system is periodic in the direction of the momentum flux, then the flux is going in 2 directions. This means the effective momentum flux in one direction is reduced by a factor of 2. You will see this in the equations for viscosity in the Muller-Plathe paper. LAMMPS is simply tallying momentum which does not account for whether or not your system is periodic; you must use the value appropriately to yield a viscosity for your system.

NOTE: After equilibration, if the velocity profile you observe is not linear, then you are likely swapping momentum too frequently and are not in a regime of linear response. In this case you cannot accurately infer a viscosity and should try increasing the Nevery parameter.

An alternative method for calculating a viscosity is to run a NEMD simulation, as described in Section_howto 13 of the manual. NEMD simulations deform the simmulation box via the fix deform command. Thus they cannot be run on a charged system using a PPPM solver since PPPM does not currently support non-orthogonal boxes. Using fix viscosity keeps the box orthogonal; thus it does not suffer from this limitation.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global scalar which can be accessed by various output commands. The scalar is the cummulative momentum transferred between the bottom and middle of the simulation box (in the *pdim* direction) is stored as a scalar quantity by this fix. This quantity is zeroed when the fix is defined and accumlates thereafter, once every N steps. The units of the quantity are momentum = mass*velocity. The scalar value calculated by this fix is "intensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Swaps conserve both momentum and kinetic energy, even if the masses of the swapped atoms are not equal. Thus you should not need to thermostat the system. If you do use a thermostat, you may want to apply it only to the non-swapped dimensions (other than *vdim*).

LAMMPS does not check, but you should not use this fix to swap velocities of atoms that are in constrained molecules, e.g. via fix shake or fix rigid. This is because application of the constraints will alter the amount of transferred momentum. You should, however, be able to use flexible molecules. See the Maginn paper for an example of using this algorithm in a computation of alcohol molecule properties.

When running a simulation with large, massive particles or molecules in a background solvent, you may want to only exchange momenta bewteen solvent particles.

Related commands:

fix ave/spatial, fix thermal/conductivity

Default:

The option defaults are swap = 1 and vtarget = INF.

(Muller-Plathe) Muller-Plathe, Phys Rev E, 59, 4894-4898 (1999).

(Maginn) Kelkar, Rafferty, Maginn, Siepmann, Fluid Phase Equilibria, 260, 218-231 (2007).

fix viscous command

fix viscous/cuda command

Syntax:

```
fix ID group-ID viscous gamma keyword values ...
```

- ID, group-ID are documented in fix command
- viscous = style name of this fix command
- gamma = damping coefficient (force/velocity units)
- zero or more keyword/value pairs may be appended

```
keyword = scale
  scale values = type ratio
    type = atom type (1-N)
    ratio = factor to scale the damping coefficient by
```

Examples:

```
fix 1 flow viscous 0.1
fix 1 damp viscous 0.5 scale 3 2.5
```

Description:

Add a viscous damping force to atoms in the group that is proportional to the velocity of the atom. The added force can be thought of as a frictional interaction with implicit solvent, i.e. the no-slip Stokes drag on a spherical particle. In granular simulations this can be useful for draining the kinetic energy from the system in a controlled fashion. If used without additional thermostatting (to add kinetic energy to the system), it has the effect of slowly (or rapidly) freezing the system; hence it can also be used as a simple energy minimization technique.

The damping force F is given by F = - gamma * velocity. The larger the coefficient, the faster the kinetic energy is reduced. If the optional keyword *scale* is used, gamma can scaled up or down by the specified factor for atoms of that type. It can be used multiple times to adjust gamma for several atom types.

NOTE: You should specify gamma in force/velocity units. This is not the same as mass/time units, at least for some of the LAMMPS units options like "real" or "metal" that are not self-consistent.

In a Brownian dynamics context, gamma = Kb T / D, where Kb = Boltzmann's constant, T = temperature, and D = particle diffusion coefficient. D can be written as Kb T / (3 pi eta d), where eta = dynamic viscosity of the frictional fluid and d = diameter of particle. This means gamma = 3 pi eta d, and thus is proportional to the viscosity of the fluid and the particle diameter.

In the current implementation, rather than have the user specify a viscosity, gamma is specified directly in force/velocity units. If needed, gamma can be adjusted for atoms of different sizes (i.e. sigma) by using the *scale* keyword.

Note that Brownian dynamics models also typically include a randomized force term to thermostat the system at a chosen temperature. The fix langevin command does this. It has the same viscous damping term as fix viscous and adds a random force to each atom. The random force term is proportional to the sqrt of the chosen thermostatting temperature. Thus if you use fix langevin with a target T = 0, its random force term is zero, and

you are essentially performing the same operation as fix viscous. Also note that the gamma of fix viscous is related to the damping parameter of fix langevin, however the former is specified in units of force/velocity and the latter in units of time, so that it can more easily be used as a thermostat.

Styles with a *cuda* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command. This fix should only be used with damped dynamics minimizers that allow for non-conservative forces. See the min_style command for details.

Restrictions: none

Related commands:

fix langevin

Default: none

fix wall/lj93 command

fix wall/lj126 command

fix wall/lj1043 command

fix wall/colloid command

fix wall/harmonic command

Syntax:

```
fix ID group-ID style face args ... keyword value ...
```

- ID, group-ID are documented in fix command
- style = *wall/lj93* or *wall/lj126* or *wall/lj1043* or *wall/colloid* or *wall/harmonic*
- one or more face/arg pairs may be appended
- face = *xlo* or *xhi* or *ylo* or *yhi* or *zlo* or *zhi*

```
  args = coord epsilon sigma cutoff
    coord = position of wall = EDGE or constant or variable
      EDGE = current lo or hi edge of simulation box
      constant = number like 0.0 or -30.0 (distance units)
      variable = equal-style variable like v_x or v_wiggle
    epsilon = strength factor for wall-particle interaction (energy or energy/distance^2 units
      epsilon can be a variable (see below)
    sigma = size factor for wall-particle interaction (distance units)
      sigma can be a variable (see below)
    cutoff = distance from wall at which wall-particle interaction is cut off (distance units)
```

- zero or more keyword/value pairs may be appended
- keyword = *units* or *fld*

```
  units value = lattice or box
      lattice = the wall position is defined in lattice units
      box = the wall position is defined in simulation box units
    fld value = yes or no
      yes = invoke the wall constraint to be compatible with implicit FLD
      no = invoke the wall constraint in the normal way
    pbc value = yes or no
      yes = allow periodic boundary in a wall dimension
      no = require non-perioidic boundaries in any wall dimension
```

Examples:

```
fix wallhi all wall/lj93 xlo -1.0 1.0 1.0 2.5 units box
fix wallhi all wall/lj93 xhi EDGE 1.0 1.0 2.5
fix wallhi all wall/lj126 v_wiggle 23.2 1.0 1.0 2.5
fix zwalls all wall/colloid zlo 0.0 1.0 1.0 0.858 zhi 40.0 1.0 1.0 0.858
```

Description:

Bound the simulation domain on one or more of its faces with a flat wall that interacts with the atoms in the group by generating a force on the atom in a direction perpendicular to the wall. The energy of wall-particle interactions

depends on the style.

For style *wall/lj93*, the energy E is given by the 9/3 potential:

$$E = \epsilon \left[\frac{2}{15} \left(\frac{\sigma}{r} \right)^9 - \left(\frac{\sigma}{r} \right)^3 \right] \qquad r < r_c$$

For style *wall/lj126*, the energy E is given by the 12/6 potential:

$$E = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \qquad r < r_c$$

For style *wall/lj1043*, the energy E is given by the 10/4/3 potential:

$$E = 2\pi\epsilon \left[\frac{2}{5} \left(\frac{\sigma}{r} \right)^{10} - \left(\frac{\sigma}{r} \right)^4 - \frac{\sqrt{(2)}\sigma^3}{3\left(r + \left(0.61/\sqrt{(2)}\right)\sigma\right)^3} \right] \qquad r < r_c$$

For style *wall/colloid*, the energy E is given by an integrated form of the pair_style colloid potential:

$$E = \epsilon \left[\frac{\sigma^6}{7560} \left(\frac{6R - D}{D^7} + \frac{D + 8R}{(D + 2R)^7} \right) - \frac{1}{6} \left(\frac{2R(D + R) + D(D + 2R)\left[\ln D - \ln(D + 2R)\right]}{D(D + 2R)} \right) \right] \qquad r <$$

For style *wall/harmonic*, the energy E is given by a harmonic spring potential:

$$E = \epsilon \left(r - r_c\right)^2 \qquad r < r_c$$

In all cases, *r* is the distance from the particle to the wall at position *coord*, and Rc is the *cutoff* distance at which the particle and wall no longer interact. The energy of the wall potential is shifted so that the wall-particle interaction energy is 0.0 at the cutoff distance.

Up to 6 walls or faces can be specified in a single command: *xlo*, *xhi*, *ylo*, *yhi*, *zlo*, *zhi*. A *lo* face interacts with particles near the lower side of the simulation box in that dimension. A *hi* face interacts with particles near the upper side of the simulation box in that dimension.

The position of each wall can be specified in one of 3 ways: as the EDGE of the simulation box, as a constant value, or as a variable. If EDGE is used, then the corresponding boundary of the current simulation box is used. If a numeric constant is specified then the wall is placed at that position in the appropriate dimension (x, y, or z). In both the EDGE and constant cases, the wall will never move. If the wall position is a variable, it should be specified as v_name, where name is an equal-style variable name. In this case the variable is evaluated each timestep and the result becomes the current position of the reflecting wall. Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent wall position. See examples below.

For the *wall/lj93* and *wall/lj126* and *wall/lj1043* styles, *epsilon* and *sigma* are the usual Lennard-Jones parameters, which determine the strength and size of the particle as it interacts with the wall. Epsilon has energy units. Note that this *epsilon* and *sigma* may be different than any *epsilon* or *sigma* values defined for a pair style that computes particle-particle interactions.

The *wall/lj93* interaction is derived by integrating over a 3d half-lattice of Lennard-Jones 12/6 particles. The *wall/lj126* interaction is effectively a harder, more repulsive wall interaction. The *wall/lj1043* interaction is yet a different form of wall interaction, described in Magda et al in (Magda).

For the *wall/colloid* style, *R* is the radius of the colloid particle, *D* is the distance from the surface of the colloid particle to the wall (r-R), and *sigma* is the size of a constituent LJ particle inside the colloid particle and wall. Note that the cutoff distance Rc in this case is the distance from the colloid particle center to the wall. The prefactor *epsilon* can be thought of as an effective Hamaker constant with energy units for the strength of the colloid-wall interaction. More specifically, the *epsilon* pre-factor = 4 * pi^2 * rho_wall * rho_colloid * epsilon * sigma^6, where epsilon and sigma are the LJ parameters for the constituent LJ particles. Rho_wall and rho_colloid are the number density of the constituent particles, in the wall and colloid respectively, in units of 1/volume.

The *wall/colloid* interaction is derived by integrating over constituent LJ particles of size *sigma* within the colloid particle and a 3d half-lattice of Lennard-Jones 12/6 particles of size *sigma* in the wall. As mentioned in the preceeding paragraph, the density of particles in the wall and colloid can be different, as specified by the *epsilon* pre-factor.

For the *wall/harmonic* style, *epsilon* is effectively the spring constant K, and has units (energy/distance^2). The input parameter *sigma* is ignored. The minimum energy position of the harmonic spring is at the *cutoff*. This is a repulsive-only spring since the interaction is truncated at the *cutoff*

For any wall, the *epsilon* and/or *sigma* parameter can be specified as an equal-style variable, in which case it should be specified as v_name, where name is the variable name. As with a variable wall position, the variable is evaluated each timestep and the result becomes the current epsilon or sigma of the wall. Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent wall interaction.

NOTE: For all of the styles, you must insure that r is always > 0 for all particles in the group, or LAMMPS will generate an error. This means you cannot start your simulation with particles at the wall position *coord* (r = 0) or with particles on the wrong side of the wall (r < 0). For the *wall/lj93* and *wall/lj126* styles, the energy of the wall/particle interaction (and hence the force on the particle) blows up as r -> 0. The *wall/colloid* style is even

more restrictive, since the energy blows up as D = r-R -> 0. This means the finite-size particles of radius R must be a distance larger than R from the wall position *coord*. The *harmonic* style is a softer potential and does not blow up as r -> 0, but you must use a large enough *epsilon* that particles always reamin on the correct side of the wall (r > 0).

The *units* keyword determines the meaning of the distance units used to define a wall position, but only when a numeric constant or variable is used. It is not relevant when EDGE is used to specify a face position. In the variable case, the variable is assumed to produce a value compatible with the *units* setting you specify.

A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacings.

The *fld* keyword can be used with a *yes* setting to invoke the wall constraint before pairwise interactions are computed. This allows an implicit FLD model using pair_style lubricateU to include the wall force in its calculations. If the setting is *no*, wall forces are imposed after pairwise interactions, in the usual manner.

The *pbc* keyword can be used with a *yes* setting to allow walls to be specified in a periodic dimension. See the boundary command for options on simulation box boundaries. The default for *pbc* is *no*, which means the system must be non-periodic when using a wall. But you may wish to use a periodic box. E.g. to allow some particles to interact with the wall via the fix group-ID, and others to pass through it and wrap around a periodic box. In this case you should insure that the wall if sufficiently far enough away from the box boundary. If you do not, then particles may interact with both the wall and with periodic images on the other side of the box, which is probably not what you want.

Here are examples of variable definitions that move the wall position in a time-dependent fashion using equal-style variables. The wall interaction parameters (epsilon, sigma) could be varied with additional variable definitions.

```
variable ramp equal ramp(0,10)
fix 1 all wall xlo v_ramp 1.0 1.0 2.5

variable linear equal vdisplace(0,20)
fix 1 all wall xlo v_linear 1.0 1.0 2.5

variable wiggle equal swiggle(0.0,5.0,3.0)
fix 1 all wall xlo v_wiggle 1.0 1.0 2.5

variable wiggle equal cwiggle(0.0,5.0,3.0)
fix 1 all wall xlo v_wiggle 1.0 1.0 2.5
```

The ramp(lo,hi) function adjusts the wall position linearly from lo to hi over the course of a run. The vdisplace(c0,velocity) function does something similar using the equation position = c0 + velocity*delta, where delta is the elapsed time.

The swiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, where omega = 2 PI / period:

```
position = c0 + A sin(omega*delta)
```

The cwiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, which will have an initial wall velocity of 0.0, and thus may impose a gentler perturbation on the particles:

```
position = c0 + A (1 - cos(omega*delta))
```

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *energy* option is supported by this fix to add the energy of interaction between atoms and each wall to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar energy and a global vector of forces, which can be accessed by various output commands. Note that the scalar energy is the sum of interactions with all defined walls. If you want the energy on a per-wall basis, you need to use multiple fix wall commands. The length of the vector is equal to the number of walls defined by the fix. Each vector value is the normal force on a specific wall. Note that an outward force on a wall will be a negative value for *lo* walls and a positive value for *hi* walls. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command.

NOTE: If you want the atom/wall interaction energy to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the fix_modify *energy* option for this fix.

Restrictions: none

Related commands:

fix wall/reflect, fix wall/gran, fix wall/region

Default:

The option defaults units = lattice, fld = no, and pbc = no.

(Magda) Magda, Tirrell, Davis, J Chem Phys, 83, 1888-1901 (1985); erratum in JCP 84, 2901 (1986).

fix wall/gran command

Syntax:

```
fix ID group-ID wall/gran Kn Kt gamma_n gamma_t xmu dampflag wallstyle args keyword values ...
```

- ID, group-ID are documented in fix command
- wall/gran = style name of this fix command
- Kn = elastic constant for normal particle repulsion (force/distance units or pressure units - see discussion below)
- Kt = elastic constant for tangential contact (force/distance units or pressure units - see discussion below)
- gamma_n = damping coefficient for collisions in normal direction (1/time units or 1/time-distance units - see discussion below)
- gamma_t = damping coefficient for collisions in tangential direction (1/time units or 1/time-distance units - see discussion below)
- xmu = static yield criterion (unitless value between 0.0 and 1.0e4)
- dampflag = 0 or 1 if tangential damping force is excluded or included
- wallstyle = *xplane* or *yplane* or *zplane* or *zcylinder*
- args = list of arguments for a particular style

```
  xplane or yplane or zplane args = lo hi
      lo,hi = position of lower and upper plane (distance units), either can be NULL)
    zcylinder args = radius
      radius = cylinder radius (distance units)
```

- zero or more keyword/value pairs may be appended to args
- keyword = *wiggle* or *shear*

```
  wiggle values = dim amplitude period
      dim = x or y or z
      amplitude = size of oscillation (distance units)
      period = time of oscillation (time units)
    shear values = dim vshear
      dim = x or y or z
      vshear = magnitude of shear velocity (velocity units)
```

Examples:

```
fix 1 all wall/gran 200000.0 NULL 50.0 NULL 0.5 0 xplane -10.0 10.0
fix 1 all wall/gran 200000.0 NULL 50.0 NULL 0.5 0 zplane 0.0 NULL
fix 2 all wall/gran 100000.0 20000.0 50.0 30.0 0.5 1 zcylinder 15.0 wiggle z 3.0 2.0
```

Description:

Bound the simulation domain of a granular system with a frictional wall. All particles in the group interact with the wall when they are close enough to touch it.

The first set of parameters (Kn, Kt, gamma_n, gamma_t, xmu, and dampflag) have the same meaning as those specified with the pair_style granular force fields. This means a NULL can be used for either Kt or gamma_t as described on that page. If a NULL is used for Kt, then a default value is used where Kt = 2/7 Kn. If a NULL is used for gamma_t, then a default value is used where gamma_t = 1/2 gamma_n.

The nature of the wall/particle interactions are determined by which pair_style is used in your input script: *hooke*, *hooke/history*, or *hertz/history*. The equation for the force between the wall and particles touching it is the same as

the corresponding equation on the pair_style granular doc page, in the limit of one of the two particles going to infinite radius and mass (flat wall). I.e. delta = radius - r = overlap of particle with wall, m_eff = mass of particle, and sqrt(RiRj/Ri+Rj) becomes sqrt(radius of particle). The units for Kn, Kt, gamma_n, and gamma_t are as described on that doc page. The meaning of xmu and dampflag are also as described on that page. Note that you can choose different values for these 6 wall/particle coefficients than for particle/particle interactions, if you wish your wall to interact differently with the particles, e.g. if the wall is a different material.

NOTE: As discussed on the doc page for pair_style granular, versions of LAMMPS before 9Jan09 used a different equation for Hertzian interactions. This means Hertizian wall/particle interactions have also changed. They now include a sqrt(radius) term which was not present before. Also the previous versions used Kn and Kt from the pairwise interaction and hardwired dampflag to 1, rather than letting them be specified directly. This means you can set the values of the wall/particle coefficients appropriately in the current code to reproduce the results of a prevoius Hertzian monodisperse calculation. For example, for the common case of a monodisperse system with particles of diameter 1, Kn, Kt, gamma_n, and gamma_s should be set sqrt(2.0) larger than they were previously.

The *wallstyle* can be planar or cylindrical. The 3 planar options specify a pair of walls in a dimension. Wall positions are given by *lo* and *hi*. Either of the values can be specified as NULL if a single wall is desired. For a *zcylinder* wallstyle, the cylinder's axis is at x = y = 0.0, and the radius of the cylinder is specified.

Optionally, the wall can be moving, if the *wiggle* or *shear* keywords are appended. Both keywords cannot be used together.

For the *wiggle* keyword, the wall oscillates sinusoidally, similar to the oscillations of particles which can be specified by the fix_move command. This is useful in packing simulations of granular particles. The arguments to the *wiggle* keyword specify a dimension for the motion, as well as it's *amplitude* and *period*. Note that if the dimension is in the plane of the wall, this is effectively a shearing motion. If the dimension is perpendicular to the wall, it is more of a shaking motion. A *zcylinder* wall can only be wiggled in the z dimension.

Each timestep, the position of a wiggled wall in the appropriate *dim* is set according to this equation:

```
position = coord + A - A cos (omega * delta)
```

where *coord* is the specified initial position of the wall, *A* is the *amplitude*, *omega* is 2 PI / *period*, and *delta* is the time elapsed since the fix was specified. The velocity of the wall is set to the derivative of this expression.

For the *shear* keyword, the wall moves continuously in the specified dimension with velocity *vshear*. The dimension must be tangential to walls with a planar *wallstyle*, e.g. in the *y* or *z* directions for an *xplane* wall. For *zcylinder* walls, a dimension of *z* means the cylinder is moving in the z-direction along it's axis. A dimension of *x* or *y* means the cylinder is spinning around the z-axis, either in the clockwise direction for *vshear* > 0 or counter-clockwise for *vshear* < 0. In this case, *vshear* is the tangential velocity of the wall at whatever *radius* has been defined.

Restart, fix_modify, output, run start/stop, minimize info:

This fix writes the shear friction state of atoms interacting with the wall to binary restart files, so that a simulation can continue correctly if granular potentials with shear "history" effects are being used. See the read_restart command for info on how to re-specify a fix in an input script that reads a restart file, so that the operation of the fix continues in an uninterrupted fashion.

None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix is part of the GRANULAR package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Any dimension (xyz) that has a granular wall must be non-periodic.

Related commands:

fix_move, pair_style granular

Default: none

fix wall/piston command

Syntax:

```
fix ID group-ID wall/piston face ... keyword value ...
```

- ID, group-ID are documented in fix command
- wall/piston = style name of this fix command
- face = *zlo*
- zero or more keyword/value pairs may be appended
- keyword = *pos* or *vel* or *ramp* or *units*

```
  pos args = z
      z = z coordinate at which the piston begins (distance units)
    vel args = vz
      vz = final velocity of the piston (velocity units)
    ramp = use a linear velocity ramp from 0 to vz
    temp args = target damp seed extent
      target = target velocity for region immediately ahead of the piston
      damp = damping paramter (time units)
      seed = random number seed for langevin kicks
      extent = extent of thermostated region (distance units)
    units value = lattice or box
      lattice = the wall position is defined in lattice units
      box = the wall position is defined in simulation box units
```

Examples:

```
fix xwalls all wall/piston zlo
fix walls all wall/piston zlo pos 1.0 vel 10.0 units box
fix top all wall/piston zlo vel 10.0 ramp
```

Description:

Bound the simulation with a moving wall which reflect particles in the specified group and drive the system with an effective infinite-mass piston capable of driving shock waves.

A momentum mirror technique is used, which means that if an atom (or the wall) moves such that an atom is outside the wall on a timestep by a distance delta (e.g. due to fix nve), then it is put back inside the face by the same delta, and the velocity relative to the moving wall is flipped in z. For instance, a stationary particle hit with a piston wall with velocity vz, will end the timestep with a velocity of 2*vz.

Currently the *face* keyword can only be *zlo*. This creates a piston moving in the positive z direction. Particles with z coordinate less than the wall position are reflected to a z coordinate greater than the wall position. If the piston velocity is vpz and the particle velocity before reflection is vzi, the particle velocity after reflection is -vzi + 2*vpz.

The initial position of the wall can be specified by the *pos* keyword.

The final velocity of the wall can be specified by the *vel* keyword

The *ramp* keyword will cause the wall/piston to adjust the velocity linearly from zero velocity to *vel* over the course of the run. If the *ramp* keyword is omitted then the wall/piston moves at a constant velocity defined by *vel*.

The *temp* keyword will cause the region immediately in front of the wall/piston to be thermostated with a Langevin thermostat. This region moves with the piston. The damping and kicking are measured in the reference frame of the piston. So, a temperature of zero would mean all particles were moving at exactly the speed of the wall/piston.

The *units* keyword determines the meaning of the distance units used to define a wall position, but only when a numeric constant is used.

A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacings.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

This fix style is part of the SHOCK package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The face that has the wall/piston must be boundary type 's' (shrink-wrapped). The opposing face can be any boundary type other than periodic.

A wall/piston should not be used with rigid bodies such as those defined by a "fix rigid" command. This is because the wall/piston displaces atoms directly rather than exerting a force on them.

Related commands:

fix wall/reflect command, fix append/atoms command

Default:

The keyword defaults are pos = 0, vel = 0, units = lattice.

fix wall/reflect command

fix wall/reflect/kk command

Syntax:

```
fix ID group-ID wall/reflect face arg ... keyword value ...
```

- ID, group-ID are documented in fix command
- wall/reflect = style name of this fix command
- one or more face/arg pairs may be appended
- face = *xlo* or *xhi* or *ylo* or *yhi* or *zlo* or *zhi*

```
xlo,ylo,zlo arg = EDGE or constant or variable
    EDGE = current lo edge of simulation box
    constant = number like 0.0 or -30.0 (distance units)
    variable = equal-style variable like v_x or v_wiggle
  xhi,yhi,zhi arg = EDGE or constant or variable
    EDGE = current hi edge of simulation box
    constant = number like 50.0 or 100.3 (distance units)
    variable = equal-style variable like v_x or v_wiggle
```

- zero or more keyword/value pairs may be appended
- keyword = *units*

```
units value = lattice or box
    lattice = the wall position is defined in lattice units
    box = the wall position is defined in simulation box units
```

Examples:

```
fix xwalls all wall/reflect xlo EDGE xhi EDGE
fix walls all wall/reflect xlo 0.0 ylo 10.0 units box
fix top all wall/reflect zhi v_pressdown
```

Description:

Bound the simulation with one or more walls which reflect particles in the specified group when they attempt to move thru them.

Reflection means that if an atom moves outside the wall on a timestep by a distance delta (e.g. due to fix nve), then it is put back inside the face by the same delta, and the sign of the corresponding component of its velocity is flipped.

When used in conjunction with fix nve and run_style verlet, the resultant time-integration algorithm is equivalent to the primitive splitting algorithm (PSA) described by Bond. Because each reflection event divides the corresponding timestep asymmetrically, energy conservation is only satisfied to O(dt), rather than to O(dt^2) as it would be for velocity-Verlet integration without reflective walls.

Up to 6 walls or faces can be specified in a single command: *xlo*, *xhi*, *ylo*, *yhi*, *zlo*, *zhi*. A *lo* face reflects particles that move to a coordinate less than the wall position, back in the *hi* direction. A *hi* face reflects particles that move to a coordinate higher than the wall position, back in the *lo* direction.

The position of each wall can be specified in one of 3 ways: as the EDGE of the simulation box, as a constant value, or as a variable. If EDGE is used, then the corresponding boundary of the current simulation box is used. If a numeric constant is specified then the wall is placed at that position in the appropriate dimension (x, y, or z). In both the EDGE and constant cases, the wall will never move. If the wall position is a variable, it should be specified as v_name, where name is an equal-style variable name. In this case the variable is evaluated each timestep and the result becomes the current position of the reflecting wall. Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent wall position.

The *units* keyword determines the meaning of the distance units used to define a wall position, but only when a numeric constant or variable is used. It is not relevant when EDGE is used to specify a face position. In the variable case, the variable is assumed to produce a value compatible with the *units* setting you specify.

A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacings.

Here are examples of variable definitions that move the wall position in a time-dependent fashion using equal-style variables.

```
variable ramp equal ramp(0,10)
fix 1 all wall/reflect xlo v_ramp

variable linear equal vdisplace(0,20)
fix 1 all wall/reflect xlo v_linear

variable wiggle equal swiggle(0.0,5.0,3.0)
fix 1 all wall/reflect xlo v_wiggle

variable wiggle equal cwiggle(0.0,5.0,3.0)
fix 1 all wall/reflect xlo v_wiggle
```

The ramp(lo,hi) function adjusts the wall position linearly from lo to hi over the course of a run. The vdisplace(c0,velocity) function does something similar using the equation position = c0 + velocity*delta, where delta is the elapsed time.

The swiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, where omega = 2 PI / period:

```
position = c0 + A sin(omega*delta)
```

The cwiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, which will have an initial wall velocity of 0.0, and thus may impose a gentler perturbation on the particles:

```
position = c0 + A (1 - cos(omega*delta))
```

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix. No global or per-atom quantities are stored by this fix for access by various output commands. No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

Any dimension (xyz) that has a reflecting wall must be non-periodic.

A reflecting wall should not be used with rigid bodies such as those defined by a "fix rigid" command. This is because the wall/reflect displaces atoms directly rather than exerts a force on them. For rigid bodies, use a soft wall instead, such as fix wall/lj93. LAMMPS will flag the use of a rigid fix with fix wall/reflect with a warning, but will not generate an error.

Related commands:

fix wall/lj93, fix oneway

Default: none

(Bond) Bond and Leimkuhler, SIAM J Sci Comput, 30, p 134 (2007).

fix wall/region command

Syntax:

```
fix ID group-ID wall/region region-ID style epsilon sigma cutoff
```

- ID, group-ID are documented in fix command
- wall/region = style name of this fix command
- region-ID = region whose boundary will act as wall
- style = *lj93* or *lj126* or *colloid* or *harmonic*
- epsilon = strength factor for wall-particle interaction (energy or energy/distance^2 units)
- sigma = size factor for wall-particle interaction (distance units)
- cutoff = distance from wall at which wall-particle interaction is cut off (distance units)

Examples:

```
fix wall all wall/region mySphere lj93 1.0 1.0 2.5
```

Description:

Treat the surface of the geometric region defined by the *region-ID* as a bounding wall which interacts with nearby particles according to the specified style. The distance between a particle and the surface is the distance to the nearest point on the surface and the force the wall exerts on the particle is along the direction between that point and the particle, which is the direction normal to the surface at that point. Note that if the region surface is comprised of multiple "faces", then each face can exert a force on the particle if it is close enough. E.g. for region_style block, a particle in the interior, near a corner of the block, could feel wall forces from 1, 2, or 3 faces of the block.

Regions are defined using the region command. Note that the region volume can be interior or exterior to the bounding surface, which will determine in which direction the surface interacts with particles, i.e. the direction of the surface normal. The surface of the region only exerts forces on particles "inside" the region; if a particle is "outside" the region it will generate an error, because it has moved through the wall.

Regions can either be primitive shapes (block, sphere, cylinder, etc) or combinations of primitive shapes specified via the *union* or *intersect* region styles. These latter styles can be used to construct particle containers with complex shapes. Regions can also change over time via the region command keywords (move) and *rotate*. If such a region is used with this fix, then the of region surface will move over time in the corresponding manner.

NOTE: As discussed on the region command doc page, regions in LAMMPS do not get wrapped across periodic boundaries. It is up to you to insure that periodic or non-periodic boundaries are specified appropriately via the boundary command when using a region as a wall that bounds particle motion. This also means that if you embed a region in your simulation box and want it to repulse particles from its surface (using the "side out" option in the region command), that its repulsive force will not be felt across a periodic boundary.

NOTE: For primitive regions with sharp corners and/or edges (e.g. a block or cylinder), wall/particle forces are computed accurately for both interior and exterior regions. For *union* and *intersect* regions, additional sharp corners and edges may be present due to the intersection of the surfaces of 2 or more primitive volumes. These corners and edges can be of two types: concave or convex. Concave points/edges are like the corners of a cube as seen by particles in the interior of a cube. Wall/particle forces around these features are computed correctly. Convex points/edges are like the corners of a cube as seen by particles exterior to the cube, i.e. the points jut into

the volume where particles are present. LAMMPS does NOT compute the location of these convex points directly, and hence wall/particle forces in the cutoff volume around these points suffer from inaccuracies. The basic problem is that the outward normal of the surface is not continuous at these points. This can cause particles to feel no force (they don't "see" the wall) when in one location, then move a distance epsilon, and suddenly feel a large force because they now "see" the wall. In a worst-case scenario, this can blow particles out of the simulation box. Thus, as a general rule you should not use the fix wall/region command with *union* or *interesect* regions that have convex points or edges.

NOTE: Similarly, you should not define *union* or *intersert* regions for use with this command that share a common face, even if the face is smooth. E.g. two regions of style block in a *union* region, where the two blocks have the same face. This is because LAMMPS discards points that are part of multiple sub-regions when calculating wall/particle interactions, to avoid double-counting the interaction. Having two coincident faces could cause the face to become invisible to the particles. The solution is to make the two faces differ by epsilon in their position.

The energy of wall-particle interactions depends on the specified style.

For style *lj93*, the energy E is given by the 9/3 potential:

$$E = \epsilon \left[\frac{2}{15} \left(\frac{\sigma}{r} \right)^9 - \left(\frac{\sigma}{r} \right)^3 \right] \qquad r < r_c$$

For style *lj126*, the energy E is given by the 12/6 potential:

$$E = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \qquad r < r_c$$

For style *colloid*, the energy E is given by an integrated form of the pair_style colloid potential:

$$E = \epsilon \left[\frac{\sigma^6}{7560} \left(\frac{6R - D}{D^7} + \frac{D + 8R}{(D + 2R)^7} \right) - \frac{1}{6} \left(\frac{2R(D + R) + D(D + 2R) \left[\ln D - \ln(D + 2R) \right]}{D(D + 2R)} \right) \right] \qquad r <$$

For style *wall/harmonic*, the energy E is given by a harmonic spring potential:

$$E = \epsilon \left(r - r_c\right)^2 \qquad r < r_c$$

In all cases, *r* is the distance from the particle to the region surface, and Rc is the *cutoff* distance at which the particle and surface no longer interact. The energy of the wall potential is shifted so that the wall-particle interaction energy is 0.0 at the cutoff distance.

For the *lj93* and *lj126* styles, *epsilon* and *sigma* are the usual Lennard-Jones parameters, which determine the strength and size of the particle as it interacts with the wall. Epsilon has energy units. Note that this *epsilon* and *sigma* may be different than any *epsilon* or *sigma* values defined for a pair style that computes particle-particle interactions.

The *lj93* interaction is derived by integrating over a 3d half-lattice of Lennard-Jones 12/6 particles. The *lj126* interaction is effectively a harder, more repulsive wall interaction.

For the *colloid* style, *epsilon* is effectively a Hamaker constant with energy units for the colloid-wall interaction, *R* is the radius of the colloid particle, *D* is the distance from the surface of the colloid particle to the wall (r-R), and *sigma* is the size of a constituent LJ particle inside the colloid particle. Note that the cutoff distance Rc in this case is the distance from the colloid particle center to the wall.

The *colloid* interaction is derived by integrating over constituent LJ particles of size *sigma* within the colloid particle and a 3d half-lattice of Lennard-Jones 12/6 particles of size *sigma* in the wall.

For the *wall/harmonic* style, *epsilon* is effectively the spring constant K, and has units (energy/distance^2). The input parameter *sigma* is ignored. The minimum energy position of the harmonic spring is at the *cutoff*. This is a repulsive-only spring since the interaction is truncated at the *cutoff*

NOTE: For all of the styles, you must insure that r is always > 0 for all particles in the group, or LAMMPS will generate an error. This means you cannot start your simulation with particles on the region surface (r = 0) or with particles on the wrong side of the region surface (r < 0). For the *wall/lj93* and *wall/lj126* styles, the energy of the wall/particle interaction (and hence the force on the particle) blows up as r -> 0. The *wall/colloid* style is even more restrictive, since the energy blows up as D = r-R -> 0. This means the finite-size particles of radius R must be a distance larger than R from the region surface. The *harmonic* style is a softer potential and does not blow up as r -> 0, but you must use a large enough *epsilon* that particles always reamin on the correct side of the region surface (r > 0).

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files.

The fix_modify *energy* option is supported by this fix to add the energy of interaction between atoms and the wall to the system's potential energy as part of thermodynamic output.

This fix computes a global scalar energy and a global 3-length vector of forces, which can be accessed by various output commands. The scalar energy is the sum of energy interactions for all particles interacting with the wall represented by the region surface. The 3 vector quantities are the x,y,z components of the total force acting on the wall due to the particles. The scalar and vector values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command.

The forces due to this fix are imposed during an energy minimization, invoked by the minimize command.

NOTE: If you want the atom/wall interaction energy to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the fix_modify *energy* option for this fix.

Restrictions: none

Related commands:

fix wall/lj93, fix wall/lj126, fix wall/colloid, fix wall/gran

Default: none

fix wall/srd command

Syntax:

```
fix ID group-ID wall/srd face arg ... keyword value ...
```

- ID, group-ID are documented in fix command
- wall/srd = style name of this fix command
- one or more face/arg pairs may be appended
- face = *xlo* or *xhi* or *ylo* or *yhi* or *zlo* or *zhi*

```
xlo,ylo,zlo arg = EDGE or constant or variable
    EDGE = current lo edge of simulation box
    constant = number like 0.0 or -30.0 (distance units)
    variable = equal-style variable like v_x or v_wiggle
  xhi,yhi,zhi arg = EDGE or constant or variable
    EDGE = current hi edge of simulation box
    constant = number like 50.0 or 100.3 (distance units)
    variable = equal-style variable like v_x or v_wiggle
```

- zero or more keyword/value pairs may be appended
- keyword = *units*

```
units value = lattice or box
    lattice = the wall position is defined in lattice units
    box = the wall position is defined in simulation box units
```

Examples:

```
fix xwalls all wall/srd xlo EDGE xhi EDGE
fix walls all wall/srd xlo 0.0 ylo 10.0 units box
fix top all wall/srd zhi v_pressdown
```

Description:

Bound the simulation with one or more walls which interact with stochastic reaction dynamics (SRD) particles as slip (smooth) or no-slip (rough) flat surfaces. The wall interaction is actually invoked via the fix srd command, only on the group of SRD particles it defines, so the group setting for the fix wall/srd command is ignored.

A particle/wall collision occurs if an SRD particle moves outside the wall on a timestep. This alters the position and velocity of the SRD particle and imparts a force to the wall.

The *collision* and *Tsrd* settings specified via the fix srd command affect the SRD/wall collisions. A *slip* setting for the *collision* keyword means that the tangential component of the SRD particle momentum is preserved. Thus only a normal force is imparted to the wall. The normal component of the new SRD velocity is sampled from a Gaussian distribution at temperature *Tsrd*.

For a *noslip* setting of the *collision* keyword, both the normal and tangential components of the new SRD velocity are sampled from a Gaussian distribution at temperature *Tsrd*. Additionally, a new tangential direction for the SRD velocity is chosen randomly. This collision style imparts both a normal and tangential force to the wall.

Up to 6 walls or faces can be specified in a single command: *xlo*, *xhi*, *ylo*, *yhi*, *zlo*, *zhi*. A *lo* face reflects particles that move to a coordinate less than the wall position, back in the *hi* direction. A *hi* face reflects particles that move to a coordinate higher than the wall position, back in the *lo* direction.

The position of each wall can be specified in one of 3 ways: as the EDGE of the simulation box, as a constant value, or as a variable. If EDGE is used, then the corresponding boundary of the current simulation box is used. If a numeric constant is specified then the wall is placed at that position in the appropriate dimension (x, y, or z). In both the EDGE and constant cases, the wall will never move. If the wall position is a variable, it should be specified as v_name, where name is an equal-style variable name. In this case the variable is evaluated each timestep and the result becomes the current position of the reflecting wall. Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent wall position.

NOTE: Because the trajectory of the SRD particle is tracked as it collides with the wall, you must insure that r = distance of the particle from the wall, is always > 0 for SRD particles, or LAMMPS will generate an error. This means you cannot start your simulation with SRD particles at the wall position *coord* (r = 0) or with particles on the wrong side of the wall (r < 0).

NOTE: If you have 2 or more walls that come together at an edge or corner (e.g. walls in the x and y dimensions), then be sure to set the *overlap* keyword to *yes* in the fix srd command, since the walls effectively overlap when SRD particles collide with them. LAMMPS will issue a warning if you do not do this.

NOTE: The walls of this fix only interact with SRD particles, as defined by the fix srd command. If you are simulating a mixture containing other kinds of particles, then you should typically use another wall command to act on the other particles. Since SRD particles will be colliding both with the walls and the other particles, it is important to insure that the other particle's finite extent does not overlap an SRD wall. If you do not do this, you may generate errors when SRD particles end up "inside" another particle or a wall at the beginning of a collision step.

The *units* keyword determines the meaning of the distance units used to define a wall position, but only when a numeric constant is used. It is not relevant when EDGE or a variable is used to specify a face position.

A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacings.

Here are examples of variable definitions that move the wall position in a time-dependent fashion using equal-style variables.

```
variable ramp equal ramp(0,10)
fix 1 all wall/srd xlo v_ramp

variable linear equal vdisplace(0,20)
fix 1 all wall/srd xlo v_linear

variable wiggle equal swiggle(0.0,5.0,3.0)
fix 1 all wall/srd xlo v_wiggle

variable wiggle equal cwiggle(0.0,5.0,3.0)
fix 1 all wall/srd xlo v_wiggle
```

The ramp(lo,hi) function adjusts the wall position linearly from lo to hi over the course of a run. The displace(c0,velocity) function does something similar using the equation position = c0 + velocity*delta, where delta is the elapsed time.

The swiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, where omega = 2 PI / period:

```
position = c0 + A sin(omega*delta)
```

The cwiggle(c0,A,period) function causes the wall position to oscillate sinusoidally according to this equation, which will have an initial wall velocity of 0.0, and thus may impose a gentler perturbation on the particles:

```
position = c0 + A (1 - cos(omega*delta))
```

Restart, fix_modify, output, run start/stop, minimize info:

No information about this fix is written to binary restart files. None of the fix_modify options are relevant to this fix.

This fix computes a global array of values which can be accessed by various output commands. The number of rows in the array is equal to the number of walls defined by the fix. The number of columns is 3, for the x,y,z components of force on each wall.

Note that an outward normal force on a wall will be a negative value for *lo* walls and a positive value for *hi* walls. The array values calculated by this fix are "extensive".

No parameter of this fix can be used with the *start/stop* keywords of the run command. This fix is not invoked during energy minimization.

Restrictions:

Any dimension (xyz) that has an SRD wall must be non-periodic.

Related commands:

fix srd

Default: none

group command

Syntax:

```
group ID style args
```

- ID = user-defined name of the group
- style = *delete* or *region* or *type* or *id* or *molecule* or *variable* or *include* or *subtract* or *union* or *intersect* or *dynamic* or *static*

```
delete = no args
  clear = no args
  region args = region-ID
  type or id or molecule
    args = list of one or more atom types, atom IDs, or molecule IDs
      any entry in list can be a sequence formatted as A:B or A:B:C where
      A = starting index, B = ending index,
      C = increment between indices, 1 if not specified
    args = logical value
      logical = "" or ">=" or "==" or "!="
      value = an atom type or atom ID or molecule ID (depending on style)
    args = logical value1 value2
      logical = ""
      value1,value2 = atom types or atom IDs or molecule IDs (depending on style)
  variable args = variable-name
  include args = molecule
    molecule = add atoms to group with same molecule ID as atoms already in group
  subtract args = two or more group IDs
  union args = one or more group IDs
  intersect args = two or more group IDs
  dynamic args = parent-ID keyword value ...
    one or more keyword/value pairs may be appended
    keyword = region or var or every
      region value = region-ID
      var value = name of variable
      every value = N = update group every this many timesteps
  static = no args
```

Examples:

```
group edge region regstrip
group water type 3 4
group sub id 10 25 50
group sub id 10 25 50 500:1000
group sub id 100:10000:10
group sub id <= 150
group polyA molecule  50 250
group hienergy variable eng
group hienergy include molecule
group boundary subtract all a2 a3
group boundary union lower upper
group boundary intersect upper flow
group boundary delete
group mine dynamic all region myRegion every 100
```

Description:

Identify a collection of atoms as belonging to a group. The group ID can then be used in other commands such as fix, compute, dump, or velocity to act on those atoms together.

If the group ID already exists, the group command adds the specified atoms to the group.

NOTE: By default groups are static, meaning the atoms are permanently assigned to the group. For example, if the *region* style is used to assign atoms to a group, the atoms will remain in the group even if they later move out of the region. As explained below, the *dynamic* style can be used to make a group dynamic so that a periodic determination is made as to which atoms are in the group. Since many LAMMPS commands operate on groups of atoms, you should think carefully about whether making a group dynamic makes sense for your model.

A group with the ID *all* is predefined. All atoms belong to this group. This group cannot be deleted, or made dynamic.

The *delete* style removes the named group and un-assigns all atoms that were assigned to that group. Since there is a restriction (see below) that no more than 32 groups can be defined at any time, the *delete* style allows you to remove groups that are no longer needed, so that more can be specified. You cannot delete a group if it has been used to define a current fix or compute or dump.

The *clear* style un-assigns all atoms that were assigned to that group. This may be dangerous to do during a simulation run, e.g. using the run every command if a fix or compute or other operation expects the atoms in the group to remain constant, but LAMMPS does not check for this.

The *region* style puts all atoms in the region volume into the group. Note that this is a static one-time assignment. The atoms remain assigned (or not assigned) to the group even in they later move out of the region volume.

The *type*, *id*, and *molecule* styles put all atoms with the specified atom types, atom IDs, or molecule IDs into the group. These 3 styles can use arguments specified in one of two formats.

The first format is a list of values (types or IDs). For example, the 2nd command in the examples above puts all atoms of type 3 or 4 into the group named *water*. Each entry in the list can be a colon-separated sequence A:B or A:B:C, as in two of the examples above. A "sequence" generates a sequence of values (types or IDs), with an optional increment. The first example with 500:1000 has the default increment of 1 and would add all atom IDs from 500 to 1000 (inclusive) to the group sub, along with 10,25,50 since they also appear in the list of values. The second example with 100:10000:10 uses an increment of 10 and would thus would add atoms IDs 100,110,120, ... 9990,10000 to the group sub.

The second format is a *logical* followed by one or two values (type or ID). The 7 valid logicals are listed above. All the logicals except take a single argument. The 3rd example above adds all atoms with IDs from 1 to 150 to the group named *sub*. The logical means "between" and takes 2 arguments. The 4th example above adds all atoms belonging to molecules with IDs from 50 to 250 (inclusive) to the group named polyA.

The *variable* style evaluates a variable to determine which atoms to add to the group. It must be an atom-style variable previously defined in the input script. If the variable evaluates to a non-zero value for a particular atom, then that atom is added to the specified group.

Atom-style variables can specify formulas that include thermodynamic quantities, per-atom values such as atom coordinates, or per-atom quantities calculated by computes, fixes, or other variables. They can also include Boolean logic where 2 numeric values are compared to yield a 1 or 0 (effectively a true or false). Thus using the *variable* style, is a general way to flag specific atoms to include or exclude from a group.

For example, these lines define a variable "eatom" that calculates the potential energy of each atom and includes it

in the group if its potential energy is above the threshhold value -3.0.

```
compute         1 all pe/atom
compute         2 all reduce sum c_1
thermo_style    custom step temp pe c_2
run             0

variable        eatom atom "c_1 > -3.0"
group           hienergy variable eatom
```

Note that these lines

```
compute         2 all reduce sum c_1
thermo_style    custom step temp pe c_2
run             0
```

are necessary to insure that the "eatom" variable is current when the group command invokes it. Because the eatom variable computes the per-atom energy via the pe/atom compute, it will only be current if a run has been performed which evaluated pairwise energies, and the pe/atom compute was actually invoked during the run. Printing the thermodyanmic info for compute 2 insures that this is the case, since it sums the pe/atom compute values (in the reduce compute) to output them to the screen. See the "Variable Accuracy" section of the variable doc page for more details on insuring that variables are current when they are evaluated between runs.

The *include* style with its arg *molecule* adds atoms to a group that have the same molecule ID as atoms already in the group. The molecule ID = 0 is ignored in this operation, since it is assumed to flag isolated atoms that are not part of molecules. An example of where this operation is useful is if the *region* style has been used previously to add atoms to a group that are within a geometric region. If molecules straddle the region boundary, then atoms outside the region that are part of molecules with atoms inside the region will not be in the group. Using the group command a 2nd time with *include molecule* will add those atoms that are outside the region to the group.

NOTE: The *include molecule* operation is relatively expensive in a parallel sense. This is because it requires communication of relevant molecule IDs between all the processors and each processor to loop over its atoms once per processor, to compare its atoms to the list of molecule IDs from every other processor. Hence it scales as N, rather than N/P as most of the group operations do, where N is the number of atoms, and P is the number of processors.

The *subtract* style takes a list of two or more existing group names as arguments. All atoms that belong to the 1st group, but not to any of the other groups are added to the specified group.

The *union* style takes a list of one or more existing group names as arguments. All atoms that belong to any of the listed groups are added to the specified group.

The *intersect* style takes a list of two or more existing group names as arguments. Atoms that belong to every one of the listed groups are added to the specified group.

The *dynamic* style flags an existing or new group as dynamic. This means atoms will be (re)assigned to the group periodically as a simulation runs. This is in contrast to static groups where atoms are permanently assigned to the group. The way the assignment occurs is as follows. Only atoms in the group specified as the parent group via the parent-ID are assigned to the dynamic group before the following conditions are applied. If the *region* keyword is used, atoms not in the specified region are removed from the dynamic group. If the *var* keyword is used, the variable name must be an atom-style or atomfile-style variable. The variable is evaluated and atoms whose per-atom values are 0.0, are removed from the dynamic group.

The assignment of atoms to a dynamic group is done at the beginning of each run and on every timestep that is a multiple of *N*, which is the argument for the *every* keyword (N = 1 is the default). For an energy minimization, via the minimize command, an assignement is made at the beginning of the minimization, but not during the iterations of the minimizer.

The point in the timestep at which atoms are assigned to a dynamic group is after the initial stage of velocity Verlet time integration has been performed, and before neighbor lists or forces are computed. This is the point in the timestep where atom positions have just changed due to the time integration, so the region criterion should be accurate, if applied.

NOTE: If the *region* keyword is used to determine what atoms are in the dynamic group, atoms can move outside of the simulation box between reneighboring events. Thus if you want to include all atoms on the left side of the simulation box, you probably want to set the left boundary of the region to be outside the simulation box by some reasonable amount (e.g. up to the cutoff of the potential), else they may be excluded from the dynamic region.

Here is an example of using a dynamic group to shrink the set of atoms being integrated by using a spherical region with a variable radius (shrinking from 18 to 5 over the course of the run). This could be used to model a quench of the system, freezing atoms outside the shrinking sphere, then converting the remaining atoms to a static group and running further.

```
variable        nsteps equal 5000
variable        rad equal 18-(step/v_nsteps)*(18-5)
region          ss sphere 20 20 0 v_rad
group           mobile dynamic all region ss
fix             1 mobile nve
run             ${nsteps}
group           mobile static
run             ${nsteps}
```

NOTE: All fixes and computes take a group ID as an argument, but they do not all allow for use of a dynamic group. If you get an error message that this is not allowed, but feel that it should be for the fix or compute in question, then please post your reasoning to the LAMMPS mail list and we can change it.

The *static* style removes the setting for a dynamic group, converting it to a static group (the default). The atoms in the static group are those currently in the dynamic group.

Restrictions:

There can be no more than 32 groups defined at one time, including "all".

The parent group of a dynamic group cannot itself be a dynamic group.

Related commands:

dump, fix, region, velocity

Default:

All atoms belong to the "all" group.

group2ndx command

Syntax:

```
group2ndx file group-ID ...
```

- file = name of index file to write out
- zero or more group IDs may be appended

Examples:

```
group2ndx allindex.ndx
group2ndx someindex.ndx upper lower mobile
```

Description:

Write a Gromacs style index file in text format that associates atom IDs with the corresponding group definitions. This index file can be used with in combination with Gromacs analysis tools or to import group definitions into the fix colvars input file.

Without specifying any group IDs, all groups will be written to the index file. When specifying group IDs, only those groups will be written to the index file. In order to follow the Gromacs conventions, the group *all* will be renamed to *System* in the index file.

Restrictions:

This command requires that atoms have atom IDs, since this is the information that is written to the index file.

This fix is part of the USER-COLVARS package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

group, dump, fix colvars

Default: none

if command

Syntax:

```
if boolean then t1 t2 ... elif boolean f1 f2 ... elif boolean f1 f2 ... else e1 e2 ...
```

- boolean = a Boolean expression evaluated as TRUE or FALSE (see below)
- then = required word
- t1,t2,...,tN = one or more LAMMPS commands to execute if condition is met, each enclosed in quotes
- elif = optional word, can appear multiple times
- f1,f2,...,fN = one or more LAMMPS commands to execute if elif condition is met, each enclosed in quotes (optional arguments)
- else = optional argument
- e1,e2,...,eN = one or more LAMMPS commands to execute if no condition is met, each enclosed in quotes (optional arguments)

Examples:

```
if "${steps} > 1000" then quit
if "${myString} == a10" then quit
if "$x <= $y" then "print X is smaller = $x" else "print Y is smaller = $y"
if "(${eng} > 0.0) || ($n <1000)" then &
  "timestep 0.005" &
elif $n ${eng_previous}" then "jump file1" else "jump file2"
```

Description:

This command provides an if-then-else capability within an input script. A Boolean expression is evaluted and the result is TRUE or FALSE. Note that as in the examples above, the expression can contain variables, as defined by the variable command, which will be evaluated as part of the expression. Thus a user-defined formula that reflects the current state of the simulation can be used to issue one or more new commands.

If the result of the Boolean expression is TRUE, then one or more commands (t1, t2, ..., tN) are executed. If it is FALSE, then Boolean expressions associated with successive elif keywords are evaluated until one is found to be true, in which case its commands (f1, f2, ..., fN) are executed. If no Boolean expression is TRUE, then the commands associated with the else keyword, namely (e1, e2, ..., eN), are executed. The elif and else keywords and their associated commands are optional. If they aren't specified and the initial Boolean expression is FALSE, then no commands are executed.

The syntax for Boolean expressions is described below.

Each command (t1, f1, e1, etc) can be any valid LAMMPS input script command, except an include command, which is not allowed. If the command is more than one word, it must enclosed in quotes, so it will be treated as a single argument, as in the examples above.

NOTE: If a command itself requires a quoted argument (e.g. a print command), then double and single quotes can be used and nested in the usual manner, as in the examples above and below. See Section_commands 2 of the manual for more details on using quotes in arguments. Only one of level of nesting is allowed, but that should be sufficient for most use cases.

Note that by using the line continuation character "&", the if command can be spread across many lines, though it is still a single command:

```
if "$a <$b" then &
  "print 'Minimum value = $a'" &
  "run 1000" &
else &
  'print "Minimum value = $b"' &
  "minimize 0.001 0.001 1000 10000"
```

Note that if one of the commands to execute is quit, as in the first example above, then executing the command will cause LAMMPS to halt.

Note that by jumping to a label in the same input script, the if command can be used to break out of a loop. See the variable delete command for info on how to delete the associated loop variable, so that it can be re-used later in the input script.

Here is an example of a loop which checks every 1000 steps if the system temperature has reached a certain value, and if so, breaks out of the loop to finish the run. Note that any variable could be checked, so long as it is current on the timestep when the run completes. As explained on the variable doc page, this can be insured by includig the variable in thermodynamic output.

```
variable myTemp equal temp
label loop
variable a loop 1000
run 1000
if "${myTemp} <300.0" then "jump SELF break"
next a
jump SELF loop
label break
print "ALL DONE"
```

Here is an example of a double loop which uses the if and jump commands to break out of the inner loop when a condition is met, then continues iterating thru the outer loop.

```
label       loopa
variable    a loop 5
  label     loopb
  variable  b loop 5
  print     "A,B = $a,$b"
  run       10000
  if        "$b > 2" then "jump SELF break"
  next      b
  jump      in.script loopb
label       break
variable    b delete
next        a
jump        SELF loopa
```

The Boolean expressions for the if and elif keywords have a C-like syntax. Note that each expression is a single argument within the if command. Thus if you want to include spaces in the expression for clarity, you must enclose the entire expression in quotes.

An expression is built out of numbers (which start with a digit or period or minus sign) or strings (which start with a letter and can contain alphanumeric characters or underscores):

```
0.2, 100, 1.0e20, -15.4, etc
InP, myString, a123, ab_23_cd, etc
```

and Boolean operators:

```
A == B, A != B, A <B, A  <= B, A > B, A >= B, A && B, A || B, !A
```

Each A and B is a number or string or a variable reference like $a or ${abc}, or A or B can be another Boolean expression.

If a variable is used it can produce a number when evaluated, like an equal-style variable. Or it can produce a string, like an index-style variable. For an individual Boolean operator, A and B must both be numbers or must both be strings. You cannot compare a number to a string.

Expressions are evaluated left to right and have the usual C-style precedence: the unary logical NOT operator "!" has the highest precedence, the 4 relational operators "", and ">=" are next; the two remaining relational operators "==" and "!=" are next; then the logical AND operator "&&"; and finally the logical OR operator "||" has the lowest precedence. Parenthesis can be used to group one or more portions of an expression and/or enforce a different order of evaluation than what would occur with the default precedence.

When the 6 relational operators (first 6 in list above) compare 2 numbers, they return either a 1.0 or 0.0 depending on whether the relationship between A and B is TRUE or FALSE. When the 6 relational operators compare 2 strings, they also return a 1.0 or 0.0 for TRUE or FALSE, but the comparison is done by the C function strcmp().

When the 3 logical operators (last 3 in list above) compare 2 numbers, they also return either a 1.0 or 0.0 depending on whether the relationship between A and B is TRUE or FALSE (or just A). The logical AND operator will return 1.0 if both its arguments are non-zero, else it returns 0.0. The logical OR operator will return 1.0 if either of its arguments is non-zero, else it returns 0.0. The logical NOT operator returns 1.0 if its argument is 0.0, else it returns 0.0. The 3 logical operators can only be used to operate on numbers, not on strings.

The overall Boolean expression produces a TRUE result if the result is non-zero. If the result is zero, the expression result is FALSE.

Restrictions: none

Related commands:

variable, print

Default: none

improper_style class2 command

improper_style class2/omp command

Syntax:

```
improper_style class2
```

Examples:

```
improper_style class2
improper_coeff 1 100.0 0
improper_coeff * aa 0.0 0.0 0.0 115.06 130.01 115.06
```

Description:

The *class2* improper style uses the potential

$$
\begin{aligned}
E &= E_i + E_{aa} \\
E_i &= K[\frac{\chi_{ijkl} + \chi_{kjli} + \chi_{ljik}}{3} - \chi_0]^2 \\
E_{aa} &= M_1(\theta_{ijk} - \theta_1)(\theta_{kjl} - \theta_3) + \\
&\quad M_2(\theta_{ijk} - \theta_1)(\theta_{ijl} - \theta_2) + \\
&\quad M_3(\theta_{ijl} - \theta_2)(\theta_{kjl} - \theta_3)
\end{aligned}
$$

where Ei is the improper term and Eaa is an angle-angle term. The 3 X terms in Ei are an average over 3 out-of-plane angles.

The 4 atoms in an improper quadruplet (listed in the data file read by the read_data command) are ordered I,J,K,L. X_IJKL refers to the angle between the plane of I,J,K and the plane of J,K,L, and the bond JK lies in both planes. Similarly for X_KJLI and X_LJIK. Note that atom J appears in the common bonds (JI, JK, JL) of all 3 X terms. Thus J (the 2nd atom in the quadruplet) is the atom of symmetry in the 3 X angles.

The subscripts on the various theta's refer to different combinations of 3 atoms (I,J,K,L) used to form a particular angle. E.g. Theta_IJL is the angle formed by atoms I,J,L with J in the middle. Theta1, theta2, theta3 are the equilibrium positions of those angles. Again, atom J (the 2nd atom in the quadruplet) is the atom of symmetry in the theta angles, since it is always the center atom.

Since atom J is the atom of symmetry, normally the bonds J-I, J-K, J-L would exist for an improper to be defined between the 4 atoms, but this is not required.

See (Sun) for a description of the COMPASS class2 force field.

Coefficients for the Ei and Eaa formulas must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands.

These are the 2 coefficients for the Ei formula:

- K (energy/radian^2)
- X0 (degrees)

X0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K are in energy/radian^2.

For the Eaa formula, each line in a improper_coeff command in the input script lists 7 coefficients, the first of which is "aa" to indicate they are AngleAngle coefficients. In a data file, these coefficients should be listed under a "AngleAngle Coeffs" heading and you must leave out the "aa", i.e. only list 6 coefficients after the improper type.

- aa
- M1 (energy/distance)
- M2 (energy/distance)
- M3 (energy/distance)
- theta1 (degrees)
- theta2 (degrees)
- theta3 (degrees)

The theta values are specified in degrees, but LAMMPS converts them to radians internally; hence the units of M are in energy/radian^2.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This improper style can only be used if LAMMPS was built with the CLASS2 package. See the Making LAMMPS section for more info on packages.

Related commands:

improper_coeff

Default: none

(Sun) Sun, J Phys Chem B 102, 7338-7364 (1998).

improper_coeff command

Syntax:

```
improper_coeff N args
```

- N = improper type (see asterisk form below)
- args = coefficients for one or more improper types

Examples:

```
improper_coeff 1 300.0 0.0
improper_coeff * 80.2 -1 2
improper_coeff *4 80.2 -1 2
```

Description:

Specify the improper force field coefficients for one or more improper types. The number and meaning of the coefficients depends on the improper style. Improper coefficients can also be set in the data file read by the read_data command or in a restart file.

N can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to set the coefficients for multiple improper types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of improper types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

Note that using an improper_coeff command can override a previous setting for the same improper type. For example, these commands set the coeffs for all improper types, then overwrite the coeffs for just improper type 2:

```
improper_coeff * 300.0 0.0
improper_coeff 2 50.0 0.0
```

A line in a data file that specifies improper coefficients uses the exact same format as the arguments of the improper_coeff command in an input script, except that wild-card asterisks should not be used since coefficients for all N types must be listed in the file. For example, under the "Improper Coeffs" section of a data file, the line that corresponds to the 1st example above would be listed as

```
1 300.0 0.0
```

The improper_style class2 is an exception to this rule, in that an additional argument is used in the input script to allow specification of the cross-term coefficients. See its doc page for details.

Here is an alphabetic list of improper styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated improper_coeff command.

Note that there are also additional improper styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the improper section of this page.

- improper_style none - turn off improper interactions
- improper_style hybrid - define multiple styles of improper interactions

- improper_style class2 - COMPASS (class 2) improper
- improper_style cvff - CVFF improper
- improper_style harmonic - harmonic improper
- improper_style umbrella - DREIDING improper

Restrictions:

This command must come after the simulation box is defined by a read_data, read_restart, or create_box command.

An improper style must be defined before any improper coefficients are set, either in the input script or in a data file.

Related commands:

improper_style

Default: none

improper_style cossq command

improper_style cossq/omp command

Syntax:

```
improper_style cossq
```

Examples:

```
improper_style cossq
improper_coeff 1 4.0 0.0
```

Description:

The *cossq* improper style uses the potential

$$E = \frac{1}{2} K \cos^2 (\chi - \chi_0)$$

where x is the improper angle, x0 is its equilibrium value, and K is a prefactor.

If the 4 atoms in an improper quadruplet (listed in the data file read by the read_data command) are ordered I,J,K,L then X is the angle between the plane of I,J,K and the plane of J,K,L. Alternatively, you can think of atoms J,K,L as being in a plane, and atom I above the plane, and X as a measure of how far out-of-plane I is with respect to the other 3 atoms.

Note that defining 4 atoms to interact in this way, does not mean that bonds necessarily exist between I-J, J-K, or K-L, as they would in a linear dihedral. Normally, the bonds I-J, I-K, I-L would exist for an improper to be defined between the 4 atoms.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/radian^2)
- X0 (degrees)

X0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K are in energy/radian^2.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This improper style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

improper_coeff

Default: none

improper_style cvff command

improper_style cvff/intel command

improper_style cvff/omp command

Syntax:

```
improper_style cvff
```

Examples:

```
improper_style cvff
improper_coeff 1 80.0 -1 4
```

Description:

The *cvff* improper style uses the potential

$$E = K[1 + d\cos(n\phi)]$$

where phi is the improper dihedral angle.

If the 4 atoms in an improper quadruplet (listed in the data file read by the read_data command) are ordered I,J,K,L then the improper dihedral angle is between the plane of I,J,K and the plane of J,K,L. Note that because this is effectively a dihedral angle, the formula for this improper style is the same as for dihedral_style harmonic.

Note that defining 4 atoms to interact in this way, does not mean that bonds necessarily exist between I-J, J-K, or K-L, as they would in a linear dihedral. Normally, the bonds I-J, I-K, I-L would exist for an improper to be defined between the 4 atoms.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy)
- d (+1 or -1)
- n (0,1,2,3,4,6)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This improper style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

improper_coeff

Default: none

improper_style distance command

Syntax:

improper_style distance

Examples:

```
improper_style distance
improper_coeff 1 80.0 100.0
```

Description:

The *distance* improper style uses the potential

where d is the distance between the central atom and the plane formed by the other three atoms. If the 4 atoms in an improper quadruplet (listed in the data file read by the read_data command) are ordered I,J,K,L then the I-atom is assumed to be the central atom.

Note that defining 4 atoms to interact in this way, does not mean that bonds necessarily exist between I-J, J-K, or K-L, as they would in a linear dihedral. Normally, the bonds I-J, I-K, I-L would exist for an improper to be defined between the 4 atoms.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K_2 (energy/distance^2)
- K_4 (energy/distance^4)

Restrictions:

This improper style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

improper_coeff

Default: none

improper_style fourier command

improper_style fourier/omp command

Syntax:

```
improper_style fourier
```

Examples:

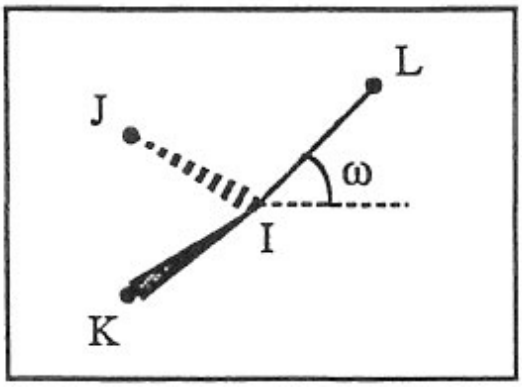
```
improper_style fourier
improper_coeff 1 100.0 180.0
```

Description:

The *fourier* improper style uses the following potential:

$$E = K[C_0 + C_1 \cos(\omega) + C_2 \cos(2\omega)]$$

where K is the force constant and omega is the angle between the IL axis and the IJK plane:



If all parameter (see bellow) is not zero, the all the three possible angles will taken in account.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy)
- C0 (real)
- C1 (real)
- C2 (real)
- all (integer >= 0)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in

Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This angle style can only be used if LAMMPS was built with the USER_MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

improper_coeff

Default: none

improper_style harmonic command

improper_style harmonic/intel command

improper_style harmonic/kk command

improper_style harmonic/omp command

Syntax:

```
improper_style harmonic
```

Examples:

```
improper_style harmonic
improper_coeff 1 100.0 0
```

Description:

The *harmonic* improper style uses the potential

$$E = K(\chi - \chi_0)^2$$

where X is the improper angle, X0 is its equilibrium value, and K is a prefactor. Note that the usual 1/2 factor is included in K.

If the 4 atoms in an improper quadruplet (listed in the data file read by the read_data command) are ordered I,J,K,L then X is the angle between the plane of I,J,K and the plane of J,K,L. Alternatively, you can think of atoms J,K,L as being in a plane, and atom I above the plane, and X as a measure of how far out-of-plane I is with respect to the other 3 atoms.

Note that defining 4 atoms to interact in this way, does not mean that bonds necessarily exist between I-J, J-K, or K-L, as they would in a linear dihedral. Normally, the bonds I-J, I-K, I-L would exist for an improper to be defined between the 4 atoms.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/radian^2)
- X0 (degrees)

X0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K are in energy/radian^2.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same

results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This improper style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

improper_coeff

Default: none

improper_style hybrid command

Syntax:

```
improper_style hybrid style1 style2 ...
```

- style1,style2 = list of one or more improper styles

Examples:

```
improper_style hybrid harmonic helix
improper_coeff 1 harmonic 120.0 30
improper_coeff 2 cvff 20.0 -1 2
```

Description:

The *hybrid* style enables the use of multiple improper styles in one simulation. An improper style is assigned to each improper type. For example, impropers in a polymer flow (of improper type 1) could be computed with a *harmonic* potential and impropers in the wall boundary (of improper type 2) could be computed with a *cvff* potential. The assignment of improper type to style is made via the improper_coeff command or in the data file.

In the improper_coeff command, the first coefficient sets the improper style and the remaining coefficients are those appropriate to that style. In the example above, the 2 improper_coeff commands would set impropers of improper type 1 to be computed with a *harmonic* potential with coefficients 120.0, 30 for K, X0. Improper type 2 would be computed with a *cvff* potential with coefficients 20.0, -1, 2 for K, d, n.

If the improper *class2* potential is one of the hybrid styles, it requires additional AngleAngle coefficients be specified in the data file. These lines must also have an additional "class2" argument added after the improper type. For improper types which are assigned to other hybrid styles, use the style name (e.g. "harmonic") appropriate to that style. The AngleAngle coeffs for that improper type will then be ignored.

An improper style of *none* can be specified as the 2nd argument to the improper_coeff command, if you desire to turn off certain improper types.

Restrictions:

This improper style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Unlike other improper styles, the hybrid improper style does not store improper coefficient info for individual sub-styles in a binary restart files. Thus when retarting a simulation from a restart file, you need to re-specify improper_coeff commands.

Related commands:

improper_coeff

Default: none

improper_style none command

Syntax:

```
improper_style none
```

Examples:

```
improper_style none
```

Description:

Using an improper style of none means improper forces are not computed, even if quadruplets of improper atoms were listed in the data file read by the read_data command.

Restrictions: none

Related commands: none

Default: none

improper_style ring command

improper_style ring/omp command

Syntax:

```
improper_style ring
```

Examples:

```
improper_style ring
improper_coeff 1 8000 70.5
```

Description:

The *ring* improper style uses the potential

$$
\begin{aligned}
E &= \frac{1}{6} K \left(\Delta_{ijl} + \Delta_{ijk} + \Delta_{kjl}\right)^6 \\
\Delta_{ijl} &= \cos\theta_{ijl} - \cos\theta_0 \\
\Delta_{ijk} &= \cos\theta_{ijk} - \cos\theta_0 \\
\Delta_{kjl} &= \cos\theta_{kjl} - \cos\theta_0
\end{aligned}
$$

where K is a prefactor, theta is the angle formed by the atoms specified by (i,j,k,l) indices and theta0 its equilibrium value.

If the 4 atoms in an improper quadruplet (listed in the data file read by the read_data command) are ordered i,j,k,l then theta_*ijl* is the angle between atoms i,j and l, theta_*ijk* is the angle between atoms i,j and k, theta_*kjl* is the angle between atoms j,k, and l.

The "ring" improper style implements the improper potential introduced by Destree et al., in Equation (9) of (Destree). This potential does not affect small amplitude vibrations but is used in an ad-hoc way to prevent the onset of accidentially large amplitude fluctuations leading to the occurrence of a planar conformation of the three bonds i-j, j-k and j-l, an intermediate conformation toward the chiral inversion of a methine carbon. In the "Impropers" section of data file four atoms: i, j, k and l are specified with i,j and l lying on the backbone of the chain and k specifying the chirality of j.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/radian^2)
- theta0 (degrees)

theta0 is specified in degrees, but LAMMPS converts it to radians internally; hence the units of K are in energy/radian^2.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This improper style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

improper_coeff

(Destree) M. Destree, F. Laupretre, A. Lyulin, and J.-P. Ryckaert, J Chem Phys, 112, 9632 (2000).

improper_style command

Syntax:

```
improper_style style
```

- style = *none* or *hybrid* or *class2* or *cvff* or *harmonic*

Examples:

```
improper_style harmonic
improper_style cvff
improper_style hybrid cvff harmonic
```

Description:

Set the formula(s) LAMMPS uses to compute improper interactions between quadruplets of atoms, which remain in force for the duration of the simulation. The list of improper quadruplets is read in by a read_data or read_restart command from a data or restart file. Note that the ordering of the 4 atoms in an improper quadruplet determines the the definition of the improper angle used in the formula for each style. See the doc pages of individual styles for details.

Hybrid models where impropers are computed using different improper potentials can be setup using the *hybrid* improper style.

The coefficients associated with an improper style can be specified in a data or restart file or via the improper_coeff command.

All improper potentials store their coefficient data in binary restart files which means improper_style and improper_coeff commands do not need to be re-specified in an input script that restarts a simulation. See the read_restart command for details on how to do this. The one exception is that improper_style *hybrid* only stores the list of sub-styles in the restart file; improper coefficients need to be re-specified.

NOTE: When both an improper and pair style is defined, the special_bonds command often needs to be used to turn off (or weight) the pairwise interaction that would otherwise exist between a group of 4 bonded atoms.

Here is an alphabetic list of improper styles defined in LAMMPS. Click on the style to display the formula it computes and coefficients specified by the associated improper_coeff command.

Note that there are also additional improper styles submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the improper section of this page.

- improper_style none - turn off improper interactions
- improper_style hybrid - define multiple styles of improper interactions

- improper_style class2 - COMPASS (class 2) improper
- improper_style cvff - CVFF improper
- improper_style harmonic - harmonic improper
- improper_style umbrella - DREIDING improper

Restrictions:

Improper styles can only be set for atom_style choices that allow impropers to be defined.

Most improper styles are part of the MOLECULE package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info on packages. The doc pages for individual improper potentials tell if it is part of a package.

Related commands:

improper_coeff

Default:

```
improper_style none
```

improper_style umbrella command

improper_style umbrella/omp command

Syntax:

```
improper_style umbrella
```

Examples:

```
improper_style umbrella
improper_coeff 1 100.0 180.0
```

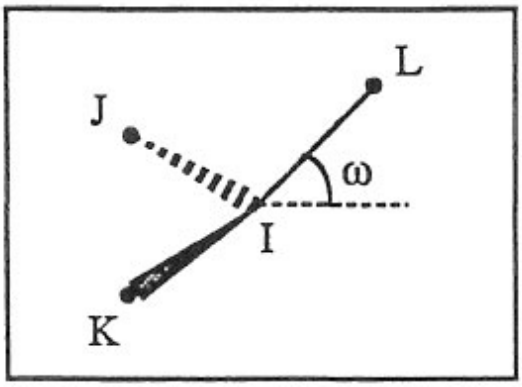
Description:

The *umbrella* improper style uses the following potential, which is commonly referred to as a classic inversion and used in the DREIDING force field:

$$E = \frac{1}{2}K\left(\frac{1+cos\omega_0}{sin\omega_0}\right)^2(cos\omega - cos\omega_0) \qquad \omega_0 \neq 0^o$$

$$E = K(1-cos\omega) \qquad \omega_0 = 0^o$$

where K is the force constant and omega is the angle between the IL axis and the IJK plane:



If omega0 = 0 the potential term has a minimum for the planar structure. Otherwise it has two minima at +/- omega0, with a barrier in between.

See (Mayo) for a description of the DREIDING force field.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy)
- omega0 (degrees)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This improper style can only be used if LAMMPS was built with the MOLECULE package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

improper_coeff

Default: none

(Mayo) Mayo, Olfason, Goddard III, J Phys Chem, 94, 8897-8909 (1990),

include command

Syntax:

```
include file
```

- file = filename of new input script to switch to

Examples:

```
include newfile
include in.run2
```

Description:

This command opens a new input script file and begins reading LAMMPS commands from that file. When the new file is finished, the original file is returned to. Include files can be nested as deeply as desired. If input script A includes script B, and B includes A, then LAMMPS could run for a long time.

If the filename is a variable (see the variable command), different processor partitions can run different input scripts.

Restrictions: none

Related commands:

variable, jump

Default: none

info command

Syntax:

```
info args
```

args = one or more of the following keywords: *out*, *all*, *system*, *communication*, *computes*, *dumps*, *fixes*, *groups*, *regions*, *variables*, *time*, or *configuration out* values = *screen*, *log*, *append* filename, *overwrite* filename:ul

Examples:

```
info system
info groups computes variables
info all out log
info all out append info.txt
```

Description:

Print out information about the current internal state of the running LAMMPS process. This can be helpful when debugging or validating complex input scripts. Several output categories are available and one or more output category may be requested.

The *out* flag controls where the output is sent. It can only be sent to one target. By default this is the screen, if it is active. The *log* argument selects the log file instead. With the *append* and *overwrite* option, followed by a filename, the output is written to that file, which is either appended to or overwritten, respectively.

The *all* flag activates printing all categories listed below.

The *system* category prints a general system overview listing. This includes the unit style, atom style, number of atoms, bonds, angles, dihedrals, and impropers and the number of the respective types, box dimensions and properties, force computing styles and more.

The *communication* category prints a variety of information about communication and parallelization: the MPI library version level, the number of MPI ranks and OpenMP threads, the communication style and layout, the processor grid dimensions, ghost atom communication mode, cutoff, and related settings.

The *computes* category prints a list of all currently defined computes, their IDs and styles and groups they operate on.

The *dumps* category prints a list of all currently active dumps, their IDs, styles, filenames, groups, and dump frequencies.

The *fixes* category prints a list of all currently defined fixes, their IDs and styles and groups they operate on.

The *groups* category prints a list of all currently defined groups.

The *regions* category prints a list of all currently defined regions, their IDs and styles and whether "inside" or "outside" atoms are selected.

The *variables* category prints a list of all currently defined variables, their names, styles, definition and last computed value, if available.

The *time* category prints the accumulated CPU and wall time for the process that writes output (usually MPI rank 0).

The *configuration* command prints some information about the LAMMPS version and architection and OS it is run on. Where supported, also information about the memory consumption provided by the OS is reported.

Restrictions: none

Related commands:

print

Default:

The *out* option has the default *screen*.

jump command

Syntax:

```
jump file label
```

- file = filename of new input script to switch to
- label = optional label within file to jump to

Examples:

```
jump newfile
jump in.run2 runloop
jump SELF runloop
```

Description:

This command closes the current input script file, opens the file with the specified name, and begins reading LAMMPS commands from that file. Unlike the include command, the original file is not returned to, although by using multiple jump commands it is possible to chain from file to file or back to the original file.

If the word "SELF" is used for the filename, then the current input script is re-opened and read again.

NOTE: The SELF option is not guaranteed to work when the current input script is being read through stdin (standard input), e.g.

```
lmp_g++ <in.script
```

since the SELF option invokes the C-library rewind() call, which may not be supported for stdin on some systems or by some MPI implementations. This can be worked around by using the -in command-line argument, e.g.

```
lmp_g++ -in in.script
```

or by using the -var command-line argument to pass the script name as a variable to the input script. In the latter case, a variable called "fname" could be used in place of SELF, e.g.

```
lmp_g++ -var fname in.script <in.script
```

The 2nd argument to the jump command is optional. If specified, it is treated as a label and the new file is scanned (without executing commands) until the label is found, and commands are executed from that point forward. This can be used to loop over a portion of the input script, as in this example. These commands perform 10 runs, each of 10000 steps, and create 10 dump files named file.1, file.2, etc. The next command is used to exit the loop after 10 iterations. When the "a" variable has been incremented for the tenth time, it will cause the next jump command to be skipped.

```
variable a loop 10
label loop
dump 1 all atom 100 file.$a
run 10000
undump 1
next a
jump in.lj loop
```

If the jump *file* argument is a variable, the jump command can be used to cause different processor partitions to run different input scripts. In this example, LAMMPS is run on 40 processors, with 4 partitions of 10 procs each. An in.file containing the example variable and jump command will cause each partition to run a different simulation.

```
mpirun -np 40 lmp_ibm -partition 4x10 -in in.file

variable f world script.1 script.2 script.3 script.4
jump $f
```

Here is an example of a loop which checks every 1000 steps if the system temperature has reached a certain value, and if so, breaks out of the loop to finish the run. Note that any variable could be checked, so long as it is current on the timestep when the run completes. As explained on the variable doc page, this can be insured by includig the variable in thermodynamic output.

```
variable myTemp equal temp
label loop
variable a loop 1000
run 1000
if "${myTemp} <300.0" then "jump SELF break"
next a
jump SELF loop
label break
print "ALL DONE"
```

Here is an example of a double loop which uses the if and jump commands to break out of the inner loop when a condition is met, then continues iterating thru the outer loop.

```
label       loopa
variable    a loop 5
  label     loopb
  variable  b loop 5
  print     "A,B = $a,$b"
  run       10000
  if        "$b > 2" then "jump SELF break"
  next      b
  jump      in.script loopb
label       break
variable    b delete
next        a
jump        SELF loopa
```

Restrictions:

If you jump to a file and it does not contain the specified label, LAMMPS will come to the end of the file and exit.

Related commands:

variable, include, label, next

Default: none

kspace_modify command

Syntax:

```
kspace_modify keyword value ...
```

- one or more keyword/value pairs may be listed

```
keyword = mesh or order or order/disp or mix/disp or overlap or minorder or force or gewald or
  mesh value = x y z
    x,y,z = grid size in each dimension for long-range Coulombics
  mesh/disp value = x y z
    x,y,z = grid size in each dimension for 1/r^6 dispersion
  order value = N
    N = extent of Gaussian for PPPM or MSM mapping of charge to grid
  order/disp value = N
    N = extent of Gaussian for PPPM mapping of dispersion term to grid
  mix/disp value = pair or geom or none
  overlap = yes or no = whether the grid stencil for PPPM is allowed to overlap into more than
  minorder value = M
    M = min allowed extent of Gaussian when auto-adjusting to minimize grid communication
  force value = accuracy (force units)
  gewald value = rinv (1/distance units)
    rinv = G-ewald parameter for Coulombics
  gewald/disp value = rinv (1/distance units)
    rinv = G-ewald parameter for dispersion
  slab value = volfactor or nozforce
    volfactor = ratio of the total extended volume used in the
      2d approximation compared with the volume of the simulation domain
  nozforce turns off kspace forces in the z direction
  compute value = yes or no
  cutoff/adjust value = yes or no
  pressure/scalar value = yes or no
  fftbench value = yes or no
  collective value = yes or no
  diff value = ad or ik = 2 or 4 FFTs for PPPM in smoothed or non-smoothed mode
  kmax/ewald value = kx ky kz
    kx,ky,kz = number of Ewald sum kspace vectors in each dimension
  force/disp/real value = accuracy (force units)
  force/disp/kspace value = accuracy (force units)
  splittol value = tol
    tol = relative size of two eigenvalues (see discussion below)
  disp/auto value = yes or no
```

Examples:

```
kspace_modify mesh 24 24 30 order 6
kspace_modify slab 3.0
```

Description:

Set parameters used by the kspace solvers defined by the kspace_style command. Not all parameters are relevant to all kspace styles.

The *mesh* keyword sets the grid size for kspace style *pppm* or *msm*. In the case of PPPM, this is the FFT mesh, and each dimension must be factorizable into powers of 2, 3, and 5. In the case of MSM, this is the finest scale real-space mesh, and each dimension must be factorizable into powers of 2. When this option is not set, the PPPM

or MSM solver chooses its own grid size, consistent with the user-specified accuracy and pairwise cutoff. Values for x,y,z of 0,0,0 unset the option.

The *mesh/disp* keyword sets the grid size for kspace style *pppm/disp*. This is the FFT mesh for long-range dispersion and ach dimension must be factorizable into powers of 2, 3, and 5. When this option is not set, the PPPM solver chooses its own grid size, consistent with the user-specified accuracy and pairwise cutoff. Values for x,y,z of 0,0,0 unset the option.

The *order* keyword determines how many grid spacings an atom's charge extends when it is mapped to the grid in kspace style *pppm* or *msm*. The default for this parameter is 5 for PPPM and 8 for MSM, which means each charge spans 5 or 8 grid cells in each dimension, respectively. For the LAMMPS implementation of MSM, the order can range from 4 to 10 and must be even. For PPPM, the minimum allowed setting is 2 and the maximum allowed setting is 7. The larger the value of this parameter, the smaller that LAMMPS will set the grid size, to achieve the requested accuracy. Conversely, the smaller the order value, the larger the grid size will be. Note that there is an inherent trade-off involved: a small grid will lower the cost of FFTs or MSM direct sum, but a larger order parameter will increase the cost of interpolating charge/fields to/from the grid.

The *order/disp* keyword determines how many grid spacings an atom's dispersion term extends when it is mapped to the grid in kspace style *pppm/disp*. It has the same meaning as the *order* setting for Coulombics.

The *overlap* keyword can be used in conjunction with the *minorder* keyword with the PPPM styles to adjust the amount of communication that occurs when values on the FFT grid are exchangeed between processors. This communication is distinct from the communication inherent in the parallel FFTs themselves, and is required because processors interpolate charge and field values using grid point values owned by neighboring processors (i.e. ghost point communication). If the *overlap* keyword is set to *yes* then this communication is allowed to extend beyond nearest-neighbor processors, e.g. when using lots of processors on a small problem. If it is set to *no* then the communication will be limited to nearest-neighbor processors and the *order* setting will be reduced if necessary, as explained by the *minorder* keyword discussion. The *overlap* keyword is always set to *yes* in MSM.

The *minorder* keyword allows LAMMPS to reduce the *order* setting if necessary to keep the communication of ghost grid point limited to exchanges between nearest-neighbor processors. See the discussion of the *overlap* keyword for details. If the *overlap* keyword is set to *yes*, which is the default, this is never needed. If it set to *no* and overlap occurs, then LAMMPS will reduce the order setting, one step at a time, until the ghost grid overlap only extends to nearest neighbor processors. The *minorder* keyword limits how small the *order* setting can become. The minimum allowed value for PPPM is 2, which is the default. If *minorder* is set to the same value as *order* then no reduction is allowed, and LAMMPS will generate an error if the grid communcation is non-nearest-neighbor and *overlap* is set to *no*. The *minorder* keyword is not currently supported in MSM.

The PPPM order parameter may be reset by LAMMPS when it sets up the FFT grid if the implied grid stencil extends beyond the grid cells owned by neighboring processors. Typically this will only occur when small problems are run on large numbers of processors. A warning will be generated indicating the order parameter is being reduced to allow LAMMPS to run the problem. Automatic adjustment of the order parameter is not supported in MSM.

The *force* keyword overrides the relative accuracy parameter set by the kspace_style command with an absolute accuracy. The accuracy determines the RMS error in per-atom forces calculated by the long-range solver and is thus specified in force units. A negative value for the accuracy setting means to use the relative accuracy parameter. The accuracy setting is used in conjunction with the pairwise cutoff to determine the number of K-space vectors for style *ewald*, the FFT grid size for style *pppm*, or the real space grid size for style *msm*.

The *gewald* keyword sets the value of the Ewald or PPPM G-ewald parameter for charge as *rinv* in reciprocal distance units. Without this setting, LAMMPS chooses the parameter automatically as a function of cutoff,

precision, grid spacing, etc. This means it can vary from one simulation to the next which may not be desirable for matching a KSpace solver to a pre-tabulated pairwise potential. This setting can also be useful if Ewald or PPPM fails to choose a good grid spacing and G-ewald parameter automatically. If the value is set to 0.0, LAMMPS will choose the G-ewald parameter automatically. MSM does not use the *gewald* parameter.

The *gewald/disp* keyword sets the value of the Ewald or PPPM G-ewald parameter for dispersion as *rinv* in reciprocal distance units. It has the same meaning as the *gewald* setting for Coulombics.

The *slab* keyword allows an Ewald or PPPM solver to be used for a systems that are periodic in x,y but non-periodic in z - a boundary setting of "boundary p p f". This is done by treating the system as if it were periodic in z, but inserting empty volume between atom slabs and removing dipole inter-slab interactions so that slab-slab interactions are effectively turned off. The volfactor value sets the ratio of the extended dimension in z divided by the actual dimension in z. The recommended value is 3.0. A larger value is inefficient; a smaller value introduces unwanted slab-slab interactions. The use of fixed boundaries in z means that the user must prevent particle migration beyond the initial z-bounds, typically by providing a wall-style fix. The methodology behind the *slab* option is explained in the paper by (Yeh). The *slab* option is also extended to non-neutral systems (Ballenegger). An alternative slab option can be invoked with the *nozforce* keyword in lieu of the volfactor. This turns off all kspace forces in the z direction. The *nozforce* option is not supported by MSM. For MSM, any combination of periodic, non-periodic, or shrink-wrapped boundaries can be set using boundary (the slab approximation in not needed). The *slab* keyword is not currently supported by Ewald or PPPM when using a triclinic simulation cell. The slab correction has also been extended to point dipole interactions (Klapp) in kspace_style *ewald/disp*.

The *compute* keyword allows Kspace computations to be turned off, even though a kspace_style is defined. This is not useful for running a real simulation, but can be useful for debugging purposes or for computing only partial forces that do not include the Kspace contribution. You can also do this by simply not defining a kspace_style, but a Kspace-compatible pair_style requires a kspace style to be defined. This keyword gives you that option.

The *cutoff/adjust* keyword applies only to MSM. If this option is turned on, the Coulombic cutoff will be automatically adjusted at the beginning of the run to give the desired estimated error. Other cutoffs such as LJ will not be affected. If the grid is not set using the *mesh* command, this command will also attempt to use the optimal grid that minimizes cost using an estimate given by (Hardy). Note that this cost estimate is not exact, somewhat experimental, and still may not yield the optimal parameters.

The *pressure/scalar* keyword applies only to MSM. If this option is turned on, only the scalar pressure (i.e. (Pxx + Pyy + Pzz)/3.0) will be computed, which can be used, for example, to run an isotropic barostat. Computing the full pressure tensor with MSM is expensive, and this option provides a faster alternative. The scalar pressure is computed using a relationship between the Coulombic energy and pressure (Hummer) instead of using the virial equation. This option cannot be used to access individual components of the pressure tensor, to compute per-atom virial, or with suffix kspace/pair styles of MSM, like OMP or GPU.

The *fftbench* keyword applies only to PPPM. It is on by default. If this option is turned off, LAMMPS will not take the time at the end of a run to give FFT benchmark timings, and will finish a few seconds faster than it would if this option were on.

The *collective* keyword applies only to PPPM. It is set to *no* by default, except on IBM BlueGene machines. If this option is set to *yes*, LAMMPS will use MPI collective operations to remap data for 3d-FFT operations instead of the default point-to-point communication. This is faster on IBM BlueGene machines, and may also be faster on other machines if they have an efficient implementation of MPI collective operations and adequate hardware.

The *diff* keyword specifies the differentiation scheme used by the PPPM method to compute forces on particles given electrostatic potentials on the PPPM mesh. The *ik* approach is the default for PPPM and is the original

formulation used in (Hockney). It performs differentiation in Kspace, and uses 3 FFTs to transfer each component of the computed fields back to real space for total of 4 FFTs per timestep.

The analytic differentiation *ad* approach uses only 1 FFT to transfer information back to real space for a total of 2 FFTs per timestep. It then performs analytic differentiation on the single quantity to generate the 3 components of the electric field at each grid point. This is sometimes referred to as "smoothed" PPPM. This approach requires a somewhat larger PPPM mesh to achieve the same accuracy as the *ik* method. Currently, only the *ik* method (default) can be used for a triclinic simulation cell with PPPM. The *ad* method is always used for MSM.

NOTE: Currently, not all PPPM styles support the *ad* option. Support for those PPPM variants will be added later.

The *kmax/ewald* keyword sets the number of kspace vectors in each dimension for kspace style *ewald*. The three values must be positive integers, or else (0,0,0), which unsets the option. When this option is not set, the Ewald sum scheme chooses its own kspace vectors, consistent with the user-specified accuracy and pairwise cutoff. In any case, if kspace style *ewald* is invoked, the values used are printed to the screen and the log file at the start of the run.

With the *mix/disp* keyword one can select the mixing rule for the dispersion coefficients. With *pair*, the dispersion coefficients of unlike types are computed as indicated with pair_modify. With *geom*, geometric mixing is enforced on the dispersion coefficients in the kspace coefficients. When using the arithmetic mixing rule, this will speed-up the simulations but introduces some error in the force computations, as shown in (Wennberg). With *none*, it is assumed that no mixing rule is applicable. Splitting of the dispersion coefficients will be performed as described in (Isele-Holder). This splitting can be influenced with the *splittol* keywords. Only the eigenvalues that are larger than tol compared to the largest eigenvalues are included. Using this keywords the original matrix of dispersion coefficients is approximated. This leads to faster computations, but the accuracy in the reciprocal space computations of the dispersion part is decreased.

The *force/disp/real* and *force/disp/kspace* keywords set the force accuracy for the real and space computations for the dispersion part of pppm/disp. As shown in (Isele-Holder), optimal performance and accuracy in the results is obtained when these values are different.

The *disp/auto* option controlls whether the pppm/disp is allowed to generate PPPM parameters automatically. If set to *no*, parameters have to be specified using the *gewald/disp*, *mesh/disp*, *force/disp/real* or *force/disp/kspace* keywords, or the code will stop with an error message. When this option is set to *yes*, the error message will not appear and the simulation will start. For a typical application, using the automatic parameter generation will provide simulations that are either inaccurate or slow. Using this option is thus not recommended. For guidelines on how to obtain good parameters, see the How-To discussion.

Restrictions: none

Related commands:

kspace_style, boundary

Default:

The option defaults are mesh = mesh/disp = 0 0 0, order = order/disp = 5 (PPPM), order = 10 (MSM), minorder = 2, overlap = yes, force = -1.0, gewald = gewald/disp = 0.0, slab = 1.0, compute = yes, cutoff/adjust = yes (MSM), pressure/scalar = yes (MSM), fftbench = yes (PPPM), diff = ik (PPPM), mix/disp = pair, force/disp/real = -1.0, force/disp/kspace = -1.0, split = 0, tol = 1.0e-6, and disp/auto = no.

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kspace_style command

Syntax:

```
kspace_style style value
```

- style = *none* or *ewald* or *ewald/disp* or *ewald/omp* or *pppm* or *pppm/cg* or *pppm/disp* or *pppm/tip4p* or *pppm/stagger* or *pppm/disp/tip4p* or *pppm/gpu* or *pppm/omp* or *pppm/cg/omp* or *pppm/tip4p/omp* or *msm* or *msm/cg* or *msm/omp* or *msm/cg/omp*

```
none value = none
  ewald value = accuracy
    accuracy = desired relative error in forces
  ewald/disp value = accuracy
    accuracy = desired relative error in forces
  ewald/omp value = accuracy
    accuracy = desired relative error in forces
  pppm value = accuracy
    accuracy = desired relative error in forces
  pppm/cg value = accuracy (smallq)
    accuracy = desired relative error in forces
    smallq = cutoff for charges to be considered (optional) (charge units)
  pppm/disp value = accuracy
    accuracy = desired relative error in forces
  pppm/tip4p value = accuracy
    accuracy = desired relative error in forces
  pppm/disp/tip4p value = accuracy
    accuracy = desired relative error in forces
  pppm/gpu value = accuracy
    accuracy = desired relative error in forces
  pppm/omp value = accuracy
    accuracy = desired relative error in forces
  pppm/cg/omp value = accuracy
    accuracy = desired relative error in forces
  pppm/tip4p/omp value = accuracy
    accuracy = desired relative error in forces
  pppm/stagger value = accuracy
    accuracy = desired relative error in forces
  msm value = accuracy
    accuracy = desired relative error in forces
  msm/cg value = accuracy (smallq)
    accuracy = desired relative error in forces
    smallq = cutoff for charges to be considered (optional) (charge units)
  msm/omp value = accuracy
    accuracy = desired relative error in forces
  msm/cg/omp value = accuracy (smallq)
    accuracy = desired relative error in forces
    smallq = cutoff for charges to be considered (optional) (charge units)
```

Examples:

```
kspace_style pppm 1.0e-4
kspace_style pppm/cg 1.0e-5 1.0e-6
kspace style msm 1.0e-4
kspace_style none
```

Description:

Define a long-range solver for LAMMPS to use each timestep to compute long-range Coulombic interactions or long-range 1/r^6 interactions. Most of the long-range solvers perform their computation in K-space, hence the name of this command.

When such a solver is used in conjunction with an appropriate pair style, the cutoff for Coulombic or 1/r^N interactions is effectively infinite. If the Coulombic case, this means each charge in the system interacts with charges in an infinite array of periodic images of the simulation domain.

Note that using a long-range solver requires use of a matching pair style to perform consistent short-range pairwise calculations. This means that the name of the pair style contains a matching keyword to the name of the KSpace style, as in this table:

Pair style	KSpace style
coul/long	ewald or pppm
coul/msm	msm
lj/long or buck/long	disp (for dispersion)
tip4p/long	tip4p

The *ewald* style performs a standard Ewald summation as described in any solid-state physics text.

The *ewald/disp* style adds a long-range dispersion sum option for 1/r^6 potentials and is useful for simulation of interfaces (Veld). It also performs standard Coulombic Ewald summations, but in a more efficient manner than the *ewald* style. The 1/r^6 capability means that Lennard-Jones or Buckingham potentials can be used without a cutoff, i.e. they become full long-range potentials. The *ewald/disp* style can also be used with point-dipoles (Toukmaji) and is currently the only kspace solver in LAMMPS with this capability.

The *pppm* style invokes a particle-particle particle-mesh solver (Hockney) which maps atom charge to a 3d mesh, uses 3d FFTs to solve Poisson's equation on the mesh, then interpolates electric fields on the mesh points back to the atoms. It is closely related to the particle-mesh Ewald technique (PME) (Darden) used in AMBER and CHARMM. The cost of traditional Ewald summation scales as N^(3/2) where N is the number of atoms in the system. The PPPM solver scales as Nlog(N) due to the FFTs, so it is almost always a faster choice (Pollock).

The *pppm/cg* style is identical to the *pppm* style except that it has an optimization for systems where most particles are uncharged. Similarly the *msm/cg* style implements the same optimization for *msm*. The optional *smallq* argument defines the cutoff for the absolute charge value which determines whether a particle is considered charged or not. Its default value is 1.0e-5.

The *pppm/tip4p* style is identical to the *pppm* style except that it adds a charge at the massless 4th site in each TIP4P water molecule. It should be used with pair styles with a *tip4p/long* in their style name.

The *pppm/stagger* style performs calculations using two different meshes, one shifted slightly with respect to the other. This can reduce force aliasing errors and increase the accuracy of the method for a given mesh size. Or a coarser mesh can be used for the same target accuracy, which saves CPU time. However, there is a trade-off since FFTs on two meshes are now performed which increases the compuation required. See (Cerutti), (Neelov), and (Hockney) for details of the method.

For high relative accuracy, using staggered PPPM allows the mesh size to be reduced by a factor of 2 in each dimension as compared to regular PPPM (for the same target accuracy). This can give up to a 4x speedup in the KSpace time (8x less mesh points, 2x more expensive). However, for low relative accuracy, the staggered PPPM mesh size may be essentially the same as for regular PPPM, which means the method will be up to 2x slower in the KSpace time (simply 2x more expensive). For more details and timings, see Section_accelerate.

NOTE: Using *pppm/stagger* may not give the same increase in the accuracy of energy and pressure as it does in forces, so some caution must be used if energy and/or pressure are quantities of interest, such as when using a barostat.

The *pppm/disp* and *pppm/disp/tip4p* styles add a mesh-based long-range dispersion sum option for 1/r^6 potentials (Isele-Holder), similar to the *ewald/disp* style. The 1/r^6 capability means that Lennard-Jones or Buckingham potentials can be used without a cutoff, i.e. they become full long-range potentials.

For these styles, you will possibly want to adjust the default choice of parameters by using the kspace_modify command. This can be done by either choosing the Ewald and grid parameters, or by specifying separate accuracies for the real and kspace calculations. When not making any settings, the simulation will stop with an error message. Further information on the influence of the parameters and how to choose them is described in (Isele-Holder), (Isele-Holder2) and the How-To discussion.

NOTE: All of the PPPM styles can be used with single-precision FFTs by using the compiler switch -DFFT_SINGLE for the FFT_INC setting in your lo-level Makefile. This setting also changes some of the PPPM operations (e.g. mapping charge to mesh and interpolating electric fields to particles) to be performed in single precision. This option can speed-up long-range calulations, particularly in parallel or on GPUs. The use of the -DFFT_SINGLE flag is discussed in this section of the manual. MSM does not currently support the -DFFT_SINGLE compiler switch.

The *msm* style invokes a multi-level summation method MSM solver, (Hardy) or (Hardy2), which maps atom charge to a 3d mesh, and uses a multi-level hierarchy of coarser and coarser meshes on which direct coulomb solves are done. This method does not use FFTs and scales as N. It may therefore be faster than the other K-space solvers for relatively large problems when running on large core counts. MSM can also be used for non-periodic boundary conditions and for mixed periodic and non-periodic boundaries.

MSM is most competitive versus Ewald and PPPM when only relatively low accuracy forces, about 1e-4 relative error or less accurate, are needed. Note that use of a larger coulomb cutoff (i.e. 15 angstroms instead of 10 angstroms) provides better MSM accuracy for both the real space and grid computed forces.

Currently calculation of the full pressure tensor in MSM is expensive. Using the kspace_modify *pressure/scalar yes* command provides a less expensive way to compute the scalar pressure (Pxx + Pyy + Pzz)/3.0. The scalar pressure can be used, for example, to run an isotropic barostat. If the full pressure tensor is needed, then calculating the pressure at every timestep or using a fixed pressure simulation with MSM will cause the code to run slower.

The specified *accuracy* determines the relative RMS error in per-atom forces calculated by the long-range solver. It is set as a dimensionless number, relative to the force that two unit point charges (e.g. 2 monovalent ions) exert on each other at a distance of 1 Angstrom. This reference value was chosen as representative of the magnitude of electrostatic forces in atomic systems. Thus an accuracy value of 1.0e-4 means that the RMS error will be a factor of 10000 smaller than the reference force.

The accuracy setting is used in conjunction with the pairwise cutoff to determine the number of K-space vectors for style *ewald* or the grid size for style *pppm* or *msm*.

Note that style *pppm* only computes the grid size at the beginning of a simulation, so if the length or triclinic tilt of the simulation cell increases dramatically during the course of the simulation, the accuracy of the simulation may degrade. Likewise, if the kspace_modify slab option is used with shrink-wrap boundaries in the z-dimension, and the box size changes dramatically in z. For example, for a triclinic system with all three tilt factors set to the maximum limit, the PPPM grid should be increased roughly by a factor of 1.5 in the y direction and 2.0 in the z direction as compared to the same system using a cubic orthogonal simulation cell. One way to ensure the

accuracy requirement is being met is to run a short simulation at the maximum expected tilt or length, note the required grid size, and then use the kspace_modify *mesh* command to manually set the PPPM grid size to this value.

RMS force errors in real space for *ewald* and *pppm* are estimated using equation 18 of (Kolafa), which is also referenced as equation 9 of (Petersen). RMS force errors in K-space for *ewald* are estimated using equation 11 of (Petersen), which is similar to equation 32 of (Kolafa). RMS force errors in K-space for *pppm* are estimated using equation 38 of (Deserno). RMS force errors for *msm* are estimated using ideas from chapter 3 of (Hardy), with equation 3.197 of particular note. When using *msm* with non-periodic boundary conditions, it is expected that the error estimation will be too pessimistic. RMS force errors for dipoles when using *ewald/disp* are estimated using equations 33 and 46 of (Wang).

See the kspace_modify command for additional options of the K-space solvers that can be set, including a *force* option for setting an absoulte RMS error in forces, as opposed to a relative RMS error.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

More specifically, the *pppm/gpu* style performs charge assignment and force interpolation calculations on the GPU. These processes are performed either in single or double precision, depending on whether the -DFFT_SINGLE setting was specified in your lo-level Makefile, as discussed above. The FFTs themselves are still calculated on the CPU. If *pppm/gpu* is used with a GPU-enabled pair style, part of the PPPM calculation can be performed concurrently on the GPU while other calculations for non-bonded and bonded force calculation are performed on the CPU.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP, and OPT packages respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

Note that the long-range electrostatic solvers in LAMMPS assume conducting metal (tinfoil) boundary conditions for both charge and dipole interactions. Vacuum boundary conditions are not currently supported.

The *ewald/disp*, *ewald*, *pppm*, and *msm* styles support non-orthogonal (triclinic symmetry) simulation boxes. However, triclinic simulation cells may not yet be supported by suffix versions of these styles (such as *pppm/cuda*).

All of the kspace styles are part of the KSPACE package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info. Note that the KSPACE package is installed by default.

For MSM, a simulation must be 3d and one can use any combination of periodic, non-periodic, or shrink-wrapped boundaries (specified using the boundary command).

For Ewald and PPPM, a simulation must be 3d and periodic in all dimensions. The only exception is if the slab option is set with kspace_modify, in which case the xy dimensions must be periodic and the z dimension must be non-periodic.

Related commands:

kspace_modify, pair_style lj/cut/coul/long, pair_style lj/charmm/coul/long, pair_style lj/long/coul/long, pair_style buck/coul/long

Default:

```
kspace_style none
```

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label command

Syntax:

```
label ID
```

- ID = string used as label name

Examples:

```
label xyz
label loop
```

Description:

Label this line of the input script with the chosen ID. Unless a jump command was used previously, this does nothing. But if a jump command was used with a label argument to begin invoking this script file, then all command lines in the script prior to this line will be ignored. I.e. execution of the script will begin at this line. This is useful for looping over a section of the input script as discussed in the jump command.

Restrictions: none

Related commands: none

Default: none

lattice command

Syntax:

```
lattice style scale keyword values ...
```

- style = *none* or *sc* or *bcc* or *fcc* or *hcp* or *diamond* or *sq* or *sq2* or *hex* or *custom*
- scale = scale factor between lattice and simulation box

```
  scale = reduced density rho* (for LJ units)
  scale = lattice constant in distance units (for all other units)
```

- zero or more keyword/value pairs may be appended
- keyword = *origin* or *orient* or *spacing* or *a1* or *a2* or *a3* or *basis*

```
  origin values = x y z
    x,y,z = fractions of a unit cell (0 <= x,y,z <1)
  orient values = dim i j k
    dim = x or y or z
    i,j,k = integer lattice directions
  spacing values = dx dy dz
    dx,dy,dz = lattice spacings in the x,y,z box directions
  a1,a2,a3 values = x y z
    x,y,z = primitive vector components that define unit cell
  basis values = x y z
    x,y,z = fractional coords of a basis atom (0  <= x,y,z <1)
```

Examples:

```
lattice fcc 3.52
lattice hex 0.85
lattice sq 0.8 origin 0.0 0.5 0.0 orient x 1 1 0 orient y -1 1 0
lattice custom 3.52 a1 1.0 0.0 0.0 a2 0.5 1.0 0.0 a3 0.0 0.0 0.5 &
                    basis 0.0 0.0 0.0 basis 0.5 0.5 0.5
lattice none 2.0
```

Description:

Define a lattice for use by other commands. In LAMMPS, a lattice is simply a set of points in space, determined by a unit cell with basis atoms, that is replicated infinitely in all dimensions. The arguments of the lattice command can be used to define a wide variety of crystallographic lattices.

A lattice is used by LAMMPS in two ways. First, the create_atoms command creates atoms on the lattice points inside the simulation box. Note that the create_atoms command allows different atom types to be assigned to different basis atoms of the lattice. Second, the lattice spacing in the x,y,z dimensions implied by the lattice, can be used by other commands as distance units (e.g. create_box, region and velocity), which are often convenient to use when the underlying problem geometry is atoms on a lattice.

The lattice style must be consistent with the dimension of the simulation - see the dimension command. Styles *sc* or *bcc* or *fcc* or *hcp* or *diamond* are for 3d problems. Styles *sq* or *sq2* or *hex* are for 2d problems. Style *custom* can be used for either 2d or 3d problems.

A lattice consists of a unit cell, a set of basis atoms within that cell, and a set of transformation parameters (scale, origin, orient) that map the unit cell into the simulation box. The vectors a1,a2,a3 are the edge vectors of the unit cell. This is the nomenclature for "primitive" vectors in solid-state crystallography, but in LAMMPS the unit cell

they determine does not have to be a "primitive cell" of minimum volume.

Note that the lattice command can be used multiple times in an input script. Each time it is invoked, the lattice attributes are re-defined and are used for all subsequent commands (that use lattice attributes). For example, a sequence of lattice, region, and create_atoms commands can be repeated multiple times to build a poly-crystalline model with different geometric regions populated with atoms in different lattice orientations.

A lattice of style *none* does not define a unit cell and basis set, so it cannot be used with the create_atoms command. However it does define a lattice spacing via the specified scale parameter. As explained above the lattice spacings in x,y,z can be used by other commands as distance units. No additional keyword/value pairs can be specified for the *none* style. By default, a "lattice none 1.0" is defined, which means the lattice spacing is the same as one distance unit, as defined by the units command.

Lattices of style *sc*, *fcc*, *bcc*, and *diamond* are 3d lattices that define a cubic unit cell with edge length = 1.0. This means a1 = 1 0 0, a2 = 0 1 0, and a3 = 0 0 1. Style *hcp* has a1 = 1 0 0, a2 = 0 sqrt(3) 0, and a3 = 0 0 sqrt(8/3). The placement of the basis atoms within the unit cell are described in any solid-state physics text. A *sc* lattice has 1 basis atom at the lower-left-bottom corner of the cube. A *bcc* lattice has 2 basis atoms, one at the corner and one at the center of the cube. A *fcc* lattice has 4 basis atoms, one at the corner and 3 at the cube face centers. A *hcp* lattice has 4 basis atoms, two in the z = 0 plane and 2 in the z = 0.5 plane. A *diamond* lattice has 8 basis atoms.

Lattices of style *sq* and *sq2* are 2d lattices that define a square unit cell with edge length = 1.0. This means a1 = 1 0 0 and a2 = 0 1 0. A *sq* lattice has 1 basis atom at the lower-left corner of the square. A *sq2* lattice has 2 basis atoms, one at the corner and one at the center of the square. A *hex* style is also a 2d lattice, but the unit cell is rectangular, with a1 = 1 0 0 and a2 = 0 sqrt(3) 0. It has 2 basis atoms, one at the corner and one at the center of the rectangle.

A lattice of style *custom* allows you to specify a1, a2, a3, and a list of basis atoms to put in the unit cell. By default, a1 and a2 and a3 are 3 orthogonal unit vectors (edges of a unit cube). But you can specify them to be of any length and non-orthogonal to each other, so that they describe a tilted parallelepiped. Via the *basis* keyword you add atoms, one at a time, to the unit cell. Its arguments are fractional coordinates (0.0 <= x,y,z < 1.0). The position vector x of a basis atom within the unit cell is thus a linear combination of the the unit cell's 3 edge vectors, i.e. x = bx a1 + by a2 + bz a3, where bx,by,bz are the 3 values specified for the *basis* keyword.

This sub-section discusses the arguments that determine how the idealized unit cell is transformed into a lattice of points within the simulation box.

The *scale* argument determines how the size of the unit cell will be scaled when mapping it into the simulation box. I.e. it determines a multiplicative factor to apply to the unit cell, to convert it to a lattice of the desired size and distance units in the simulation box. The meaning of the *scale* argument depends on the units being used in your simulation.

For all unit styles except *lj*, the scale argument is specified in the distance units defined by the unit style. For example, in *real* or *metal* units, if the unit cell is a unit cube with edge length 1.0, specifying scale = 3.52 would create a cubic lattice with a spacing of 3.52 Angstroms. In *cgs* units, the spacing would be 3.52 cm.

For unit style *lj*, the scale argument is the Lennard-Jones reduced density, typically written as rho*. LAMMPS converts this value into the multiplicative factor via the formula "factor^dim = rho/rho*", where rho = N/V with V = the volume of the lattice unit cell and N = the number of basis atoms in the unit cell (described below), and dim = 2 or 3 for the dimensionality of the simulation. Effectively, this means that if LJ particles of size sigma = 1.0 are used in the simulation, the lattice of particles will be at the desired reduced density.

The *origin* option specifies how the unit cell will be shifted or translated when mapping it into the simulation box. The x,y,z values are fractional values (0.0 <= x,y,z < 1.0) meaning shift the lattice by a fraction of the lattice spacing in each dimension. The meaning of "lattice spacing" is discussed below.

The *orient* option specifies how the unit cell will be rotated when mapping it into the simulation box. The *dim* argument is one of the 3 coordinate axes in the simulation box. The other 3 arguments are the crystallographic direction in the lattice that you want to orient along that axis, specified as integers. E.g. "orient x 2 1 0" means the x-axis in the simulation box will be the [210] lattice direction, and similarly for y and z. The 3 lattice directions you specify do not have to be unit vectors, but they must be mutually orthogonal and obey the right-hand rule, i.e. (X cross Y) points in the Z direction.

NOTE: The preceding paragraph describing lattice directions is only valid for orthogonal cubic unit cells (or square in 2d). If you are using a *hcp* or *hex* lattice or the more general lattice style *custom* with non-orthogonal a1,a2,a3 vectors, then you should think of the 3 *orient* vectors as creating a 3x3 rotation matrix which is applied to a1,a2,a3 to rotate the original unit cell to a new orientation in the simulation box.

Several LAMMPS commands have the option to use distance units that are inferred from "lattice spacings" in the x,y,z box directions. E.g. the region command can create a block of size 10x20x20, where 10 means 10 lattice spacings in the x direction.

NOTE: Though they are called lattice spacings, all the commands that have a "units lattice" option, simply use the 3 values as scale factors on the distance units defined by the units command. Thus if you do not like the lattice spacings computed by LAMMPS (e.g. for a non-orthogonal or rotated unit cell), you can define the 3 values to be whatever you wish, via the *spacing* option.

If the *spacing* option is not specified, the lattice spacings are computed by LAMMPS in the following way. A unit cell of the lattice is mapped into the simulation box (scaled and rotated), so that it now has (perhaps) a modified size and orientation. The lattice spacing in X is defined as the difference between the min/max extent of the x coordinates of the 8 corner points of the modified unit cell (4 in 2d). Similarly, the Y and Z lattice spacings are defined as the difference in the min/max of the y and z coordinates.

Note that if the unit cell is orthogonal with axis-aligned edges (no rotation via the *orient* keyword), then the lattice spacings in each dimension are simply the scale factor (described above) multiplied by the length of a1,a2,a3. Thus a *hex* style lattice with a scale factor of 3.0 Angstroms, would have a lattice spacing of 3.0 in x and 3*sqrt(3.0) in y.

NOTE: For non-orthogonal unit cells and/or when a rotation is applied via the *orient* keyword, then the lattice spacings computed by LAMMPS are typically less intuitive. In particular, in these cases, there is no guarantee that a particular lattice spacing is an integer multiple of the periodicity of the lattice in that direction. Thus, if you create an orthogonal periodic simulation box whose size in a dimension is a multiple of the lattice spacing, and then fill it with atoms via the create_atoms command, you will NOT necessarily create a periodic system. I.e. atoms may overlap incorrectly at the faces of the simulation box.

The *spacing* option sets the 3 lattice spacings directly. All must be non-zero (use 1.0 for dz in a 2d simulation). The specified values are multiplied by the multiplicative factor described above that is associated with the scale factor. Thus a spacing of 1.0 means one unit cell edge length independent of the scale factor. As mentioned above, this option can be useful if the spacings LAMMPS computes are inconvenient to use in subsequent commands, which can be the case for non-orthogonal or rotated lattices.

Note that whenever the lattice command is used, the values of the lattice spacings LAMMPS calculates are printed out. Thus their effect in commands that use the spacings should be decipherable.

Example commands for generating a Wurtzite crystal (courtesy of Aidan Thompson), with its 8 atom unit cell.

```
variable a equal  4.340330
variable b equal  $a*sqrt(3.0)
variable c equal  $a*sqrt(8.0/3.0)

variable 1_3 equal 1.0/3.0
variable 2_3 equal 2.0/3.0
variable 1_6 equal 1.0/6.0
variable 5_6 equal 5.0/6.0
variable 1_12 equal 1.0/12.0
variable 5_12 equal 5.0/12/0

lattice custom    1.0     &
        a1      $a      0.0     0.0     &
        a2      0.0     $b      0.0     &
        a3      0.0     0.0     $c      &
        basis   0.0     0.0     0.0     &
        basis   0.5     0.5     0.0     &
        basis   ${1_3}  0.0     0.5     &
        basis   ${5_6}  0.5     0.5     &
        basis   0.0     0.0     0.625   &
        basis   0.5     0.5     0.625   &
        basis   ${1_3}  0.0     0.125   &
        basis   ${5_6}  0.5     0.125

region myreg block 0 1 0 1 0 1
create_box      2 myreg
create_atoms    1 box
```

Restrictions:

The *a1,a2,a3,basis* keywords can only be used with style *custom*.

Related commands:

dimension, create_atoms, region

Default:

```
lattice none 1.0
```

For other lattice styles, the option defaults are origin = 0.0 0.0 0.0, orient = x 1 0 0, orient = y 0 1 0, orient = z 0 0 1, a1 = 1 0 0, a2 = 0 1 0, and a3 = 0 0 1.

log command

Syntax:

```
log file keyword
```

- file = name of new logfile
- keyword = *append* if output should be appended to logfile (optional)

Examples:

```
log log.equil
log log.equil append
```

Description:

This command closes the current LAMMPS log file, opens a new file with the specified name, and begins logging information to it. If the specified file name is *none*, then no new log file is opened. If the optional keyword *append* is specified, then output will be appended to an existing log file, instead of overwriting it.

If multiple processor partitions are being used, the file name should be a variable, so that different processors do not attempt to write to the same log file.

The file "log.lammps" is the default log file for a LAMMPS run. The name of the initial log file can also be set by the command-line switch -log. See Section_start 6 for details.

Restrictions: none

Related commands: none

Default:

The default LAMMPS log file is named log.lammps

mass command

Syntax:

```
mass I value
```

- I = atom type (see asterisk form below)
- value = mass

Examples:

```
mass 1 1.0
mass * 62.5
mass 2* 62.5
```

Description:

Set the mass for all atoms of one or more atom types. Per-type mass values can also be set in the read_data data file using the "Masses" keyword. See the units command for what mass units to use.

The I index can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to set the mass for multiple atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive).

A line in a data file that follows the "Masses" keyword specifies mass using the same format as the arguments of the mass command in an input script, except that no wild-card asterisk can be used. For example, under the "Masses" section of a data file, the line that corresponds to the 1st example above would be listed as

```
1 1.0
```

Note that the mass command can only be used if the atom style requires per-type atom mass to be set. Currently, all but the *sphere* and *ellipsoid* and *peri* styles do. They require mass to be set for individual particles, not types. Per-atom masses are defined in the data file read by the read_data command, or set to default values by the create_atoms command. Per-atom masses can also be set to new values by the set mass or set density commands.

Also note that pair_style eam and pair_style bop commands define the masses of atom types in their respective potential files, in which case the mass command is normally not used.

If you define a hybrid atom style which includes one (or more) sub-styles which require per-type mass and one (or more) sub-styles which require per-atom mass, then you must define both. However, in this case the per-type mass will be ignored; only the per-atom mass will be used by LAMMPS.

Restrictions:

This command must come after the simulation box is defined by a read_data, read_restart, or create_box command.

All masses must be defined before a simulation is run. They must also all be defined before a velocity or fix shake command is used.

The mass assigned to any type or atom must be > 0.0.

Related commands: none

Default: none

min_modify command

Syntax:

```
min_modify keyword values ...
```

- one or more keyword/value pairs may be listed

```
keyword = dmax or line
  dmax value = max
    max = maximum distance for line search to move (distance units)
  line value = backtrack or quadratic or forcezero
    backtrack,quadratic,forcezero = style of linesearch to use
```

Examples:

```
min_modify dmax 0.2
```

Description:

This command sets parameters that affect the energy minimization algorithms selected by the min_style command. The various settings may affect the convergence rate and overall number of force evaluations required by a minimization, so users can experiment with these parameters to tune their minimizations.

The *cg* and *sd* minimization styles have an outer iteration and an inner iteration which is steps along a one-dimensional line search in a particular search direction. The *dmax* parameter is how far any atom can move in a single line search in any dimension (x, y, or z). For the *quickmin* and *fire* minimization styles, the *dmax* setting is how far any atom can move in a single iteration (timestep). Thus a value of 0.1 in real units means no atom will move further than 0.1 Angstroms in a single outer iteration. This prevents highly overlapped atoms from being moved long distances (e.g. through another atom) due to large forces.

The choice of line search algorithm for the *cg* and *sd* minimization styles can be selected via the *line* keyword. The default *quadratic* line search algorithm starts out using the robust backtracking method described below. However, once the system gets close to a local minimum and the linesearch steps get small, so that the energy is approximately quadratic in the step length, it uses the estimated location of zero gradient as the linesearch step, provided the energy change is downhill. This becomes more efficient than backtracking for highly-converged relaxations. The *forcezero* line search algorithm is similar to *quadratic*. It may be more efficient than *quadratic* on some systems.

The backtracking search is robust and should always find a local energy minimum. However, it will "converge" when it can no longer reduce the energy of the system. Individual atom forces may still be larger than desired at this point, because the energy change is measured as the difference of two large values (energy before and energy after) and that difference may be smaller than machine epsilon even if atoms could move in the gradient direction to reduce forces further.

Restrictions: none

Related commands:

min_style, minimize

Default:

The option defaults are dmax = 0.1 and line = quadratic.

min_style command

Syntax:

```
min_style style
```

- style = *cg* or *hftn* or *sd* or *quickmin* or *fire*

Examples:

```
min_style cg
min_style fire
```

Description:

Choose a minimization algorithm to use when a minimize command is performed.

Style *cg* is the Polak-Ribiere version of the conjugate gradient (CG) algorithm. At each iteration the force gradient is combined with the previous iteration information to compute a new search direction perpendicular (conjugate) to the previous search direction. The PR variant affects how the direction is chosen and how the CG method is restarted when it ceases to make progress. The PR variant is thought to be the most effective CG choice for most problems.

Style *hftn* is a Hessian-free truncated Newton algorithm. At each iteration a quadratic model of the energy potential is solved by a conjugate gradient inner iteration. The Hessian (second derivatives) of the energy is not formed directly, but approximated in each conjugate search direction by a finite difference directional derivative. When close to an energy minimum, the algorithm behaves like a Newton method and exhibits a quadratic convergence rate to high accuracy. In most cases the behavior of *hftn* is similar to *cg*, but it offers an alternative if *cg* seems to perform poorly. This style is not affected by the min_modify command.

Style *sd* is a steepest descent algorithm. At each iteration, the search direction is set to the downhill direction corresponding to the force vector (negative gradient of energy). Typically, steepest descent will not converge as quickly as CG, but may be more robust in some situations.

Style *quickmin* is a damped dynamics method described in (Sheppard), where the damping parameter is related to the projection of the velocity vector along the current force vector for each atom. The velocity of each atom is initialized to 0.0 by this style, at the beginning of a minimization.

Style *fire* is a damped dynamics method described in (Bitzek), which is similar to *quickmin* but adds a variable timestep and alters the projection operation to maintain components of the velocity non-parallel to the current force vector. The velocity of each atom is initialized to 0.0 by this style, at the beginning of a minimization.

Either the *quickmin* and *fire* styles are useful in the context of nudged elastic band (NEB) calculations via the neb command.

NOTE: The damped dynamic minimizers use whatever timestep you have defined via the timestep command. Often they will converge more quickly if you use a timestep about 10x larger than you would normally use for dynamics simulations.

NOTE: The *quickmin* and *fire* styles do not yet support the use of the fix box/relax command or minimizations

involving the electron radius in eFF models.

Restrictions: none

Related commands:

min_modify, minimize, neb

Default:

```
min_style cg
```

(Sheppard) Sheppard, Terrell, Henkelman, J Chem Phys, 128, 134106 (2008). See ref 1 in this paper for original reference to Qmin in Jonsson, Mills, Jacobsen.

(Bitzek) Bitzek, Koskinen, Gahler, Moseler, Gumbsch, Phys Rev Lett, 97, 170201 (2006).

minimize command

Syntax:

```
minimize etol ftol maxiter maxeval
```

- etol = stopping tolerance for energy (unitless)
- ftol = stopping tolerance for force (force units)
- maxiter = max iterations of minimizer
- maxeval = max number of force/energy evaluations

Examples:

```
minimize 1.0e-4 1.0e-6 100 1000
minimize 0.0 1.0e-8 1000 100000
```

Description:

Perform an energy minimization of the system, by iteratively adjusting atom coordinates. Iterations are terminated when one of the stopping criteria is satisfied. At that point the configuration will hopefully be in local potential energy minimum. More precisely, the configuration should approximate a critical point for the objective function (see below), which may or may not be a local minimum.

The minimization algorithm used is set by the min_style command. Other options are set by the min_modify command. Minimize commands can be interspersed with run commands to alternate between relaxation and dynamics. The minimizers bound the distance atoms move in one iteration, so that you can relax systems with highly overlapped atoms (large energies and forces) by pushing the atoms off of each other.

Alternate means of relaxing a system are to run dynamics with a small or limited timestep. Or dynamics can be run using fix viscous to impose a damping force that slowly drains all kinetic energy from the system. The pair_style soft potential can be used to un-overlap atoms while running dynamics.

Note that you can minimize some atoms in the system while holding the coordiates of other atoms fixed by applying fix setforce to the other atoms. See a fuller discussion of using fixes while minimizing below.

The minimization styles *cg*, *sd*, and *hftn* involves an outer iteration loop which sets the search direction along which atom coordinates are changed. An inner iteration is then performed using a line search algorithm. The line search typically evaluates forces and energies several times to set new coordinates. Currently, a backtracking algorithm is used which may not be optimal in terms of the number of force evaulations performed, but appears to be more robust than previous line searches we've tried. The backtracking method is described in Nocedal and Wright's Numerical Optimization (Procedure 3.1 on p 41).

The minimization styles *quickmin* and *fire* perform damped dynamics using an Euler integration step. Thus they require a timestep be defined.

NOTE: The damped dynamic minimizers use whatever timestep you have defined via the timestep command. Often they will converge more quickly if you use a timestep about 10x larger than you would normally use for dynamics simulations.

In all cases, the objective function being minimized is the total potential energy of the system as a function of the

N atom coordinates:

$$E(r_1, r_2, \ldots, r_N) = \sum_{i,j} E_{pair}(r_i, r_j) + \sum_{ij} E_{bond}(r_i, r_j) + \sum_{ijk} E_{angle}(r_i, r_j, r_k) + \sum_{ijkl} E_{dihedral}(r_i, r_j, r_k, r_l) + \sum_{ijkl} E_{improper}(r_i, r_j, r_k, r_l) + \sum_{i} E$$

where the first term is the sum of all non-bonded pairwise interactions including long-range Coulombic interactions, the 2nd thru 5th terms are bond, angle, dihedral, and improper interactions respectively, and the last term is energy due to fixes which can act as constraints or apply force to atoms, such as thru interaction with a wall. See the discussion below about how fix commands affect minimization.

The starting point for the minimization is the current configuration of the atoms.

The minimization procedure stops if any of several criteria are met:

- the change in energy between outer iterations is less than *etol*
- the 2-norm (length) of the global force vector is less than the *ftol*
- the line search fails because the step distance backtracks to 0.0
- the number of outer iterations or timesteps exceeds *maxiter*
- the number of total force evaluations exceeds *maxeval*

For the first criterion, the specified energy tolerance *etol* is unitless; it is met when the energy change between successive iterations divided by the energy magnitude is less than or equal to the tolerance. For example, a setting of 1.0e-4 for *etol* means an energy tolerance of one part in 10^4. For the damped dynamics minimizers this check is not performed for a few steps after velocities are reset to 0, otherwise the minimizer would prematurely converge.

For the second criterion, the specified force tolerance *ftol* is in force units, since it is the length of the global force vector for all atoms, e.g. a vector of size 3N for N atoms. Since many of the components will be near zero after minimization, you can think of *ftol* as an upper bound on the final force on any component of any atom. For example, a setting of 1.0e-4 for *ftol* means no x, y, or z component of force on any atom will be larger than 1.0e-4 (in force units) after minimization.

Either or both of the *etol* and *ftol* values can be set to 0.0, in which case some other criterion will terminate the minimization.

During a minimization, the outer iteration count is treated as a timestep. Output is triggered by this timestep, e.g. thermodynamic output or dump and restart files.

Using the thermo_style custom command with the *fmax* or *fnorm* keywords can be useful for monitoring the progress of the minimization. Note that these outputs will be calculated only from forces on the atoms, and will not include any extra degrees of freedom, such as from the fix box/relax command.

Following minimization, a statistical summary is printed that lists which convergence criterion caused the minimizer to stop, as well as information about the energy, force, final line search, and iteration counts. An example is as follows:

```
Minimization stats:
  Stopping criterion = max iterations
  Energy initial, next-to-last, final =
       -0.626828169302     -2.82642039062     -2.82643549739
  Force two-norm initial, final = 2052.1 91.9642
  Force max component initial, final = 346.048 9.78056
  Final line search alpha, max atom move = 2.23899e-06 2.18986e-05
  Iterations, force evaluations = 2000 12724
```

The 3 energy values are for before and after the minimization and on the next-to-last iteration. This is what the *etol* parameter checks.

The two-norm force values are the length of the global force vector before and after minimization. This is what the *ftol* parameter checks.

The max-component force values are the absolute value of the largest component (x,y,z) in the global force vector, i.e. the infinity-norm of the force vector.

The alpha parameter for the line-search, when multiplied by the max force component (on the last iteration), gives the max distance any atom moved during the last iteration. Alpha will be 0.0 if the line search could not reduce the energy. Even if alpha is non-zero, if the "max atom move" distance is tiny compared to typical atom coordinates, then it is possible the last iteration effectively caused no atom movement and thus the evaluated energy did not change and the minimizer terminated. Said another way, even with non-zero forces, it's possible the effect of those forces is to move atoms a distance less than machine precision, so that the energy cannot be further reduced.

The iterations and force evaluation values are what is checked by the *maxiter* and *maxeval* parameters.

NOTE: There are several force fields in LAMMPS which have discontinuities or other approximations which may prevent you from performing an energy minimization to high tolerances. For example, you should use a pair style that goes to 0.0 at the cutoff distance when performing minimization (even if you later change it when running dynamics). If you do not do this, the total energy of the system will have discontinuities when the relative distance between any pair of atoms changes from cutoff+epsilon to cutoff-epsilon and the minimizer may behave poorly. Some of the manybody potentials use splines and other internal cutoffs that inherently have this problem. The long-range Coulombic styles (PPPM, Ewald) are approximate to within the user-specified tolerance, which means their energy and forces may not agree to a higher precision than the Kspace-specified tolerance. In all these cases, the minimizer may give up and stop before finding a minimum to the specified energy or force tolerance.

Note that a cutoff Lennard-Jones potential (and others) can be shifted so that its energy is 0.0 at the cutoff via the pair_modify command. See the doc pages for inidividual pair styles for details. Note that Coulombic potentials always have a cutoff, unless versions with a long-range component are used (e.g. pair_style lj/cut/coul/long). The CHARMM potentials go to 0.0 at the cutoff (e.g. pair_style lj/charmm/coul/charmm), as do the GROMACS potentials (e.g. pair_style lj/gromacs).

If a soft potential (pair_style soft) is used the Astop value is used for the prefactor (no time dependence).

The fix box/relax command can be used to apply an external pressure to the simulation box and allow it to shrink/expand during the minimization.

Only a few other fixes (typically those that apply force constraints) are invoked during minimization. See the doc pages for individual fix commands to see which ones are relevant. Current examples of fixes that can be used include:

- fix addforce

- fix addtorque
- fix efield
- fix enforce2d
- fix indent
- fix lineforce
- fix planeforce
- fix setforce
- fix spring
- fix spring/self
- fix viscous
- fix wall
- fix wall/region

NOTE: Some fixes which are invoked during minimization have an associated potential energy. For that energy to be included in the total potential energy of the system (the quantity being minimized), you MUST enable the fix_modify *energy* option for that fix. The doc pages for individual fix commands specify if this should be done.

Restrictions:

Features that are not yet implemented are listed here, in case someone knows how they could be coded:

It is an error to use fix shake with minimization because it turns off bonds that should be included in the potential energy of the system. The effect of a fix shake can be approximated during a minimization by using stiff spring constants for the bonds and/or angles that would normally be constrained by the SHAKE algorithm.

Fix rigid is also not supported by minimization. It is not an error to have it defined, but the energy minimization will not keep the defined body(s) rigid during the minimization. Note that if bonds, angles, etc internal to a rigid body have been turned off (e.g. via neigh_modify exclude), they will not contribute to the potential energy which is probably not what is desired.

Pair potentials that produce torque on a particle (e.g. granular potentials or the GayBerne potential for ellipsoidal particles) are not relaxed by a minimization. More specifically, radial relaxations are induced, but no rotations are induced by a minimization, so such a system will not fully relax.

Related commands:

min_modify, min_style, run_style

Default: none

molecule command

Syntax:

```
molecule ID file1 keyword values ... file2 keyword values ... fileN ...
```

- ID = user-assigned name for the molecule template
- file1,file2,... = names of files containing molecule descriptions
- zero or more keyword/value pairs may be appended after each file
- keyword = *offset* or *toff* or *boff* or *aoff* or *doff* or *ioff* or *scale*

```
offset values = Toff Boff Aoff Doff Ioff
    Toff = offset to add to atom types
    Boff = offset to add to bond types
    Aoff = offset to add to angle types
    Doff = offset to add to dihedral types
    Ioff = offset to add to improper types
  toff value = Toff
    Toff = offset to add to atom types
  boff value = Boff
    Boff = offset to add to bond types
  aoff value = Aoff
    Aoff = offset to add to angle types
  doff value = Doff
    Doff = offset to add to dihedral types
  ioff value = Ioff
    Ioff = offset to add to improper types
  scale value = sfactor
    sfactor = scale factor to apply to the size and mass of the molecule
```

Examples:

```
molecule 1 mymol.txt
molecule 1 co2.txt h2o.txt
molecule CO2 co2.txt boff 3 aoff 2
molecule 1 mymol.txt offset 6 9 18 23 14
molecule objects file.1 scale 1.5 file.1 scale 2.0 file.2 scale 1.3
```

Description:

Define a molecule template that can be used as part of other LAMMPS commands, typically to define a collection of particles as a bonded molecule or a rigid body. Commands that currently use molecule templates include:

- fix deposit
- fix pour
- fix rigid/small
- fix shake
- fix gcmc
- create_atoms
- atom_style template

The ID of a molecule template can only contain alphanumeric characters and underscores.

A single template can contain multiple molecules, listed one per file. Some of the commands listed above currently use only the first molecule in the template, and will issue a warning if the template contains multiple molecules. The atom_style template command allows multiple-molecule templates to define a system with more than one templated molecule.

Each filename can be followed by optional keywords which are applied only to the molecule in the file as used in this template. This is to make it easy to use the same molecule file in different molecule templates or in different simulations. You can specify the same file multiple times with different optional keywords.

The *offset*, *toff*, *aoff*, *doff*, *ioff* keywords add the specified offset values to the atom types, bond types, angle types, dihedral types, and/or improper types as they are read from the molecule file. E.g. if *toff* = 2, and the file uses atom types 1,2,3, then each created molecule will have atom types 3,4,5. For the *offset* keyword, all five offset values must be specified, but individual values will be ignored if the molecule template does not use that attribute (e.g. no bonds).

The *scale* keyword scales the size of the molecule. This can be useful for modeling polydisperse granular rigid bodies. The scale factor is applied to each of these properties in the molecule file, if they are defined: the individual particle coordinates (Coords section), the individual mass of each particle (Masses section), the individual diameters of each particle (Diameters section), the total mass of the molecule (header keyword = mass), the center-of-mass of the molecule (header keyword = com), and the moments of inertia of the molecule (header keyword = inertia).

NOTE: The molecule command can be used to define molecules with bonds, angles, dihedrals, imporopers, or special bond lists of neighbors within a molecular topology, so that you can later add the molecules to your simulation, via one or more of the commands listed above. If such molecules do not already exist when LAMMPS creates the simulation box, via the create_box or read_data command, when you later add them you may overflow the pre-allocated data structures which store molecular topology information with each atom, and an error will be generated. Both the create_box command and the data files read by the read_data command have "extra" options which insure space is allocated for storing topology info for molecules that are added later.

The format of an individual molecule file is similar to the data file read by the read_data commands, and is as follows.

A molecule file has a header and a body. The header appears first. The first line of the header is always skipped; it typically contains a description of the file. Then lines are read one at a time. Lines can have a trailing comment starting with '#' that is ignored. If the line is blank (only whitespace after comment is deleted), it is skipped. If the line contains a header keyword, the corresponding value(s) is read from the line. If it doesn't contain a header keyword, the line begins the body of the file.

The body of the file contains zero or more sections. The first line of a section has only a keyword. The next line is skipped. The remaining lines of the section contain values. The number of lines depends on the section keyword as described below. Zero or more blank lines can be used between sections. Sections can appear in any order, with a few exceptions as noted below.

These are the recognized header keywords. Header lines can come in any order. The numeric value(s) are read from the beginning of the line. The keyword should appear at the end of the line. All these settings have default values, as explained below. A line need only appear if the value(s) are different than the default.

- N *atoms* = # of atoms N in molecule, default = 0
- Nb *bonds* = # of bonds Nb in molecule, default = 0
- Na *angles* = # of angles Na in molecule, default = 0
- Nd *dihedrals* = # of dihedrals Nd in molecule, default = 0

- Ni *impropers* = # of impropers Ni in molecule, default = 0
- Mtotal *mass* = total mass of molecule
- Xc Yc Zc *com* = coordinates of center-of-mass of molecule
- Ixx Iyy Izz Ixy Ixz Iyz *inertia* = 6 components of inertia tensor of molecule

For *mass*, *com*, and *inertia*, the default is for LAMMPS to calculate this quantity itself if needed, assuming the molecules consists of a set of point particles or finite-size particles (with a non-zero diameter) that do not overlap. If finite-size particles in the molecule do overlap, LAMMPS will not account for the overlap effects when calculating any of these 3 quantities, so you should pre-compute them yourself and list the values in the file.

The mass and center-of-mass coordinates (Xc,Yc,Zc) are self-explanatory. The 6 moments of inertia (ixx,iyy,izz,ixy,ixz,iyz) should be the values consistent with the current orientation of the rigid body around its center of mass. The values are with respect to the simulation box XYZ axes, not with respect to the prinicpal axes of the rigid body itself. LAMMPS performs the latter calculation internally.

These are the allowed section keywords for the body of the file.

- *Coords, Types, Charges, Diameters, Masses* = atom-property sections
- *Bonds, Angles, Dihedrals, Impropers* = molecular topology sections
- *Special Bond Counts, Special Bonds* = special neighbor info
- *Shake Flags, Shake Atoms, Shake Bond Types* = SHAKE info

If a Bonds section is specified then the Special Bond Counts and Special Bonds sections can also be used, if desired, to explicitly list the 1-2, 1-3, 1-4 neighbors within the molecule topology (see details below). This is optional since if these sections are not included, LAMMPS will auto-generate this information. Note that LAMMPS uses this info to properly exclude or weight bonded pairwise interactions between bonded atoms. See the special_bonds command for more details. One reason to list the special bond info explicitly is for the thermalized Drude oscillator model which treats the bonds between nuclear cores and Drude electrons in a different manner.

NOTE: Whether a section is required depends on how the molecule template is used by other LAMMPS commands. For example, to add a molecule via the fix deposit command, the Coords and Types sections are required. To add a rigid body via the fix pour command, the Bonds (Angles, etc) sections are not required, since the molecule will be treated as a rigid body. Some sections are optional. For example, the fix pour command can be used to add "molecules" which are clusters of finite-size granular particles. If the Diameters section is not specified, each particle in the molecule will have a default diameter of 1.0. See the doc pages for LAMMPS commands that use molecule templates for more details.

Each section is listed below in alphabetic order. The format of each section is described including the number of lines it must contain and rules (if any) for whether it can appear in the data file. In each case the ID is ignored; it is simply included for readability, and should be a number from 1 to Nlines for the section, indicating which atom (or bond, etc) the entry applies to. The lines are assumed to be listed in order from 1 to Nlines, but LAMMPS does not check for this.

Coords section:

- one line per atom
- line syntax: ID x y z
- x,y,z = coordinate of atom

Types section:

- one line per atom
- line syntax: ID type
- type = atom type of atom

Charges section:

- one line per atom
- line syntax: ID q
- q = charge on atom

This section is only allowed for atom styles that support charge. If this section is not included, the default charge on each atom in the molecule is 0.0.

Diameters section:

- one line per atom
- line syntax: ID diam
- diam = diameter of atom

This section is only allowed for atom styles that support finite-size spherical particles, e.g. atom_style sphere. If not listed, the default diameter of each atom in the molecule is 1.0.

Masses section:

- one line per atom
- line syntax: ID mass
- mass = mass of atom

This section is only allowed for atom styles that support per-atom mass, as opposed to per-type mass. See the mass command for details. If this section is not included, the default mass for each atom is derived from its volume (see Diameters section) and a default density of 1.0, in units of mass/volume.

Bonds section:

- one line per bond
- line syntax: ID type atom1 atom2
- type = bond type (1-Nbondtype)
- atom1,atom2 = IDs of atoms in bond

The IDs for the two atoms in each bond should be values from 1 to Natoms, where Natoms = # of atoms in the molecule.

Angles section:

- one line per angle
- line syntax: ID type atom1 atom2 atom3
- type = angle type (1-Nangletype)
- atom1,atom2,atom3 = IDs of atoms in angle

The IDs for the three atoms in each angle should be values from 1 to Natoms, where Natoms = # of atoms in the molecule. The 3 atoms are ordered linearly within the angle. Thus the central atom (around which the angle is computed) is the atom2 in the list.

Dihedrals section:

- one line per dihedral
- line syntax: ID type atom1 atom2 atom3 atom4
- type = dihedral type (1-Ndihedraltype)
- atom1,atom2,atom3,atom4 = IDs of atoms in dihedral

The IDs for the four atoms in each dihedral should be values from 1 to Natoms, where Natoms = # of atoms in the molecule. The 4 atoms are ordered linearly within the dihedral.

Impropers section:

- one line per improper
- line syntax: ID type atom1 atom2 atom3 atom4
- type = improper type (1-Nimpropertype)
- atom1,atom2,atom3,atom4 = IDs of atoms in improper

The IDs for the four atoms in each improper should be values from 1 to Natoms, where Natoms = # of atoms in the molecule. The ordering of the 4 atoms determines the definition of the improper angle used in the formula for the defined improper style. See the doc pages for individual styles for details.

Special Bond Counts section:

- one line per atom
- line syntax: ID N1 N2 N3
- N1 = # of 1-2 bonds
- N2 = # of 1-3 bonds
- N3 = # of 1-4 bonds

N1, N2, N3 are the number of 1-2, 1-3, 1-4 neighbors respectively of this atom within the topology of the molecule. See the special_bonds doc page for more discussion of 1-2, 1-3, 1-4 neighbors. If this section appears, the Special Bonds section must also appear. If this section is not specied, the atoms in the molecule will have no special bonds.

Special Bonds section:

- one line per atom
- line syntax: ID a b c d ...
- a,b,c,d,... = IDs of atoms in N1+N2+N3 special bonds

A, b, c, d, etc are the IDs of the n1+n2+n3 atoms that are 1-2, 1-3, 1-4 neighbors of this atom. The IDs should be values from 1 to Natoms, where Natoms = # of atoms in the molecule. The first N1 values should be the 1-2 neighbors, the next N2 should be the 1-3 neighbors, the last N3 should be the 1-4 neighbors. No atom ID should appear more than once. See the special_bonds doc page for more discussion of 1-2, 1-3, 1-4 neighbors. If this section appears, the Special Bond Counts section must also appear. If this section is not specied, the atoms in the molecule will have no special bonds.

Shake Flags section:

- one line per atom
- line syntax: ID flag

- flag = 0,1,2,3,4

This section is only needed when molecules created using the template will be constrained by SHAKE via the "fix shake" command. The other two Shake sections must also appear in the file, following this one.

The meaning of the flag for each atom is as follows. See the fix shake doc page for a further description of SHAKE clusters.

- 0 = not part of a SHAKE cluster
- 1 = part of a SHAKE angle cluster (two bonds and the angle they form)
- 2 = part of a 2-atom SHAKE cluster with a single bond
- 3 = part of a 3-atom SHAKE cluster with two bonds
- 4 = part of a 4-atom SHAKE cluster with three bonds

Shake Atoms section:

- one line per atom
- line syntax: ID a b c d
- a,b,c,d = IDs of atoms in cluster

This section is only needed when molecules created using the template will be constrained by SHAKE via the "fix shake" command. The other two Shake sections must also appear in the file.

The a,b,c,d values are atom IDs (from 1 to Natoms) for all the atoms in the SHAKE cluster that this atom belongs to. The number of values that must appear is determined by the shake flag for the atom (see the Shake Flags section above). All atoms in a particular cluster should list their a,b,c,d values identically.

If flag = 0, no a,b,c,d values are listed on the line, just the (ignored) ID.

If flag = 1, a,b,c are listed, where a = ID of central atom in the angle, and b,c the other two atoms in the angle.

If flag = 2, a,b are listed, where a = ID of atom in bond with the the lowest ID, and b = ID of atom in bond with the highest ID.

If flag = 3, a,b,c are listed, where a = ID of central atom, and b,c = IDs of other two atoms bonded to the central atom.

If flag = 4, a,b,c,d are listed, where a = ID of central atom, and b,c,d = IDs of other three atoms bonded to the central atom.

See the fix shake doc page for a further description of SHAKE clusters.

Shake Bond Types section:

- one line per atom
- line syntax: ID a b c
- a,b,c = bond types (or angle type) of bonds (or angle) in cluster

This section is only needed when molecules created using the template will be constrained by SHAKE via the "fix shake" command. The other two Shake sections must also appear in the file.

The a,b,c values are bond types (from 1 to Nbondtypes) for all bonds in the SHAKE cluster that this atom belongs to. The number of values that must appear is determined by the shake flag for the atom (see the Shake Flags section above). All atoms in a particular cluster should list their a,b,c values identically.

If flag = 0, no a,b,c values are listed on the line, just the (ignored) ID.

If flag = 1, a,b,c are listed, where a = bondtype of the bond between the central atom and the first non-central atom (value b in the Shake Atoms section), b = bondtype of the bond between the central atom and the 2nd non-central atom (value c in the Shake Atoms section), and c = the angle type (1 to Nangletypes) of the angle between the 3 atoms.

If flag = 2, only a is listed, where a = bondtype of the bond between the 2 atoms in the cluster.

If flag = 3, a,b are listed, where a = bondtype of the bond between the central atom and the first non-central atom (value b in the Shake Atoms section), and b = bondtype of the bond between the central atom and the 2nd non-central atom (value c in the Shake Atoms section).

If flag = 4, a,b,c are listed, where a = bondtype of the bond between the central atom and the first non-central atom (value b in the Shake Atoms section), b = bondtype of the bond between the central atom and the 2nd non-central atom (value c in the Shake Atoms section), and c = bondtype of the bond between the central atom and the 3rd non-central atom (value d in the Shake Atoms section).

See the fix shake doc page for a further description of SHAKE clusters.

Restrictions: none

Related commands:

fix deposit, fix pour, fix_gcmc

Default:

The default keywords values are offset 0 0 0 0 0 and scale = 1.0.

neb command

Syntax:

```
neb etol ftol N1 N2 Nevery file-style arg
```

- etol = stopping tolerance for energy (energy units)
- ftol = stopping tolerance for force (force units)
- N1 = max # of iterations (timesteps) to run initial NEB
- N2 = max # of iterations (timesteps) to run barrier-climbing NEB
- Nevery = print replica energies and reaction coordinates every this many timesteps
- file-style= *final* or *each* or *none*

```
final arg = filename
    filename = file with initial coords for final replica
      coords for intermediate replicas are linearly interpolated between first and last replic
  each arg = filename
    filename = unique filename for each replica (except first) with its initial coords
  none arg = no argument
    all replicas assumed to already have their initial coords
```

Examples:

```
neb 0.1 0.0 1000 500 50 final coords.final
neb 0.0 0.001 1000 500 50 each coords.initial.$i
neb 0.0 0.001 1000 500 50 none
```

Description:

Perform a nudged elastic band (NEB) calculation using multiple replicas of a system. Two or more replicas must be used; the first and last are the end points of the transition path.

NEB is a method for finding both the atomic configurations and height of the energy barrier associated with a transition state, e.g. for an atom to perform a diffusive hop from one energy basin to another in a coordinated fashion with its neighbors. The implementation in LAMMPS follows the discussion in these 3 papers: (Henkelman1), (Henkelman2), and (Nakano).

Each replica runs on a partition of one or more processors. Processor partitions are defined at run-time using the -partition command-line switch; see Section_start 7 of the manual. Note that if you have MPI installed, you can run a multi-replica simulation with more replicas (partitions) than you have physical processors, e.g you can run a 10-replica simulation on just one or two processors. You will simply not get the performance speed-up you would see with one or more physical processors per replica. See this section of the manual for further discussion.

NOTE: The current NEB implementation in LAMMPS only allows there to be one processor per replica.

NOTE: As explained below, a NEB calculation perfoms a damped dynamics minimization across all the replicas. The mimimizer uses whatever timestep you have defined in your input script, via the timestep command. Often NEB will converge more quickly if you use a timestep about 10x larger than you would normally use for dynamics simulations.

When a NEB calculation is performed, it is assumed that each replica is running the same system, though LAMMPS does not check for this. I.e. the simulation domain, the number of atoms, the interaction potentials, and

the starting configuration when the neb command is issued should be the same for every replica.

In a NEB calculation each atom in a replica is connected to the same atom in adjacent replicas by springs, which induce inter-replica forces. These forces are imposed by the fix neb command, which must be used in conjunction with the neb command. The group used to define the fix neb command defines the NEB atoms which are the only ones that inter-replica springs are applied to. If the group does not include all atoms, then non-NEB atoms have no inter-replica springs and the forces they feel and their motion is computed in the usual way due only to other atoms within their replica. Conceptually, the non-NEB atoms provide a background force field for the NEB atoms. They can be allowed to move during the NEB minimiation procedure (which will typically induce different coordinates for non-NEB atoms in different replicas), or held fixed using other LAMMPS commands such as fix setforce. Note that the partition command can be used to invoke a command on a subset of the replicas, e.g. if you wish to hold NEB or non-NEB atoms fixed in only the end-point replicas.

The initial atomic configuration for each of the replicas can be specified in different manners via the *file-style* setting, as discussed below. Only atoms whose initial coordinates should differ from the current configuration need be specified.

Conceptually, the initial configuration for the first replica should be a state with all the atoms (NEB and non-NEB) having coordinates on one side of the energy barrier. A perfect energy minimum is not required, since atoms in the first replica experience no spring forces from the 2nd replica. Thus the damped dynamics minimizaiton will drive the first replica to an energy minimum if it is not already there. However, you will typically get better convergence if the initial state is already at a minimum. For example, for a system with a free surface, the surface should be fully relaxed before attempting a NEB calculation.

Likewise, the initial configuration of the final replica should be a state with all the atoms (NEB and non-NEB) on the other side of the energy barrier. Again, a perfect energy minimum is not required, since the atoms in the last replica also experience no spring forces from the next-to-last replica, and thus the damped dynamics minimization will drive it to an energy minimum.

As explained below, the initial configurations of intermediate replicas can be atomic coordinates interpolated in a linear fashion between the first and last replicas. This is often adequate state for simple transitions. For more complex transitions, it may lead to slow convergence or even bad results if the minimum energy path (MEP, see below) of states over the barrier cannot be correctly converged to from such an initial configuration. In this case, you will want to generate initial states for the intermediate replicas that are geometrically closer to the MEP and read them in.

For a *file-style* setting of *final*, a filename is specified which contains atomic coordinates for zero or more atoms, in the format described below. For each atom that appears in the file, the new coordinates are assigned to that atom in the final replica. Each intermediate replica also assigns a new position to that atom in an interpolated manner. This is done by using the current position of the atom as the starting point and the read-in position as the final point. The distance between them is calculated, and the new position is assigned to be a fraction of the distance. E.g. if there are 10 replicas, the 2nd replica will assign a position that is 10% of the distance along a line between the starting and final point, and the 9th replica will assign a position that is 90% of the distance along the line. Note that this procedure to produce consistent coordinates across all the replicas, the current coordinates need to be the same in all replicas. LAMMPS does not check for this, but invalid initial configurations will likely result if it is not the case.

NOTE: The "distance" between the starting and final point is calculated in a minimum-image sense for a periodic simulation box. This means that if the two positions are on opposite sides of a box (periodic in that dimension), the distance between them will be small, because the periodic image of one of the atoms is close to the other. Similarly, even if the assigned position resulting from the interpolation is outside the periodic box, the atom will be wrapped back into the box when the NEB calculation begins.

For a *file-style* setting of *each*, a filename is specified which is assumed to be unique to each replica. This can be done by using a variable in the filename, e.g.

```
variable i equal part
neb 0.0 0.001 1000 500 50 each coords.initial.$i
```

which in this case will substitute the partition ID (0 to N-1) for the variable I, which is also effectively the replica ID. See the variable command for other options, such as using world-, universe-, or uloop-style variables.

Each replica (except the first replica) will read its file, formatted as described below, and for any atom that appears in the file, assign the specified coordinates to its atom. The various files do not need to contain the same set of atoms.

For a *file-style* setting of *none*, no filename is specified. Each replica is assumed to already be in its initial configuration at the time the neb command is issued. This allows each replica to define its own configuration by reading a replica-specific data or restart or dump file, via the read_data, read_restart, or read_dump commands. The replica-specific names of these files can be specified as in the discussion above for the *each* file-style. Also see the section below for how a NEB calculation can produce restart files, so that a long calculation can be restarted if needed.

NOTE: None of the *file-style* settings change the initial configuration of any atom in the first replica. The first replica must thus be in the correct initial configuration at the time the neb command is issued.

A NEB calculation proceeds in two stages, each of which is a minimization procedure, performed via damped dynamics. To enable this, you must first define a damped dynamics min_style, such as *quickmin* or *fire*. The *cg*, *sd*, and *hftn* styles cannot be used, since they perform iterative line searches in their inner loop, which cannot be easily synchronized across multiple replicas.

The minimizer tolerances for energy and force are set by *etol* and *ftol*, the same as for the minimize command.

A non-zero *etol* means that the NEB calculation will terminate if the energy criterion is met by every replica. The energies being compared to *etol* do not include any contribution from the inter-replica forces, since these are non-conservative. A non-zero *ftol* means that the NEB calculation will terminate if the force criterion is met by every replica. The forces being compared to *ftol* include the inter-replica forces between an atom and its images in adjacent replicas.

The maximum number of iterations in each stage is set by *N1* and *N2*. These are effectively timestep counts since each iteration of damped dynamics is like a single timestep in a dynamics run. During both stages, the potential energy of each replica and its normalized distance along the reaction path (reaction coordinate RD) will be printed to the screen and log file every *Nevery* timesteps. The RD is 0 and 1 for the first and last replica. For intermediate replicas, it is the cumulative distance (normalized by the total cumulative distance) between adjacent replicas, where "distance" is defined as the length of the 3N-vector of differences in atomic coordinates, where N is the number of NEB atoms involved in the transition. These outputs allow you to monitor NEB's progress in finding a good energy barrier. *N1* and *N2* must both be multiples of *Nevery*.

In the first stage of NEB, the set of replicas should converge toward the minimum energy path (MEP) of conformational states that transition over the barrier. The MEP for a barrier is defined as a sequence of 3N-dimensional states that cross the barrier at its saddle point, each of which has a potential energy gradient parallel to the MEP itself. The replica states will also be roughly equally spaced along the MEP due to the inter-replica spring force added by the fix neb command.

In the second stage of NEB, the replica with the highest energy is selected and the inter-replica forces on it are converted to a force that drives its atom coordinates to the top or saddle point of the barrier, via the

barrier-climbing calculation described in (Henkelman2). As before, the other replicas rearrange themselves along the MEP so as to be roughly equally spaced.

When both stages are complete, if the NEB calculation was successful, one of the replicas should be an atomic configuration at the top or saddle point of the barrier, the potential energies for the set of replicas should represent the energy profile of the barrier along the MEP, and the configurations of the replicas should be a sequence of configurations along the MEP.

A few other settings in your input script are required or advised to perform a NEB calculation. See the NOTE about the choice of timestep at the beginning of this doc page.

An atom map must be defined which it is not by default for atom_style atomic problems. The atom_modify map command can be used to do this.

The "atom_modify sort 0 0.0" command should be used to turn off atom sorting.

NOTE: This sorting restriction will be removed in a future version of NEB in LAMMPS.

The minimizers in LAMMPS operate on all atoms in your system, even non-NEB atoms, as defined above. To prevent non-NEB atoms from moving during the minimization, you should use the fix setforce command to set the force on each of those atoms to 0.0. This is not required, and may not even be desired in some cases, but if those atoms move too far (e.g. because the initial state of your system was not well-minimized), it can cause problems for the NEB procedure.

The damped dynamics minimizers, such as *quickmin* and *fire*), adjust the position and velocity of the atoms via an Euler integration step. Thus you must define an appropriate timestep to use with NEB. As mentioned above, NEB will often converge more quickly if you use a timestep about 10x larger than you would normally use for dynamics simulations.

Each file read by the neb command containing atomic coordinates used to initialize one or more replicas must be formatted as follows.

The file can be ASCII text or a gzipped text file (detected by a .gz suffix). The file can contain initial blank lines or comment lines starting with "#" which are ignored. The first non-blank, non-comment line should list N = the number of lines to follow. The N successive lines contain the following information:

```
ID1 x1 y1 z1
ID2 x2 y2 z2
...
IDN xN yN zN
```

The fields are the the atom ID, followed by the x,y,z coordinates. The lines can be listed in any order. Additional trailing information on the line is OK, such as a comment.

Note that for a typical NEB calculation you do not need to specify initial coordinates for very many atoms to produce differing starting and final replicas whose intermediate replicas will converge to the energy barrier. Typically only new coordinates for atoms geometrically near the barrier need be specified.

Also note there is no requirement that the atoms in the file correspond to the NEB atoms in the group defined by the fix neb command. Not every NEB atom need be in the file, and non-NEB atoms can be listed in the file.

Four kinds of output can be generated during a NEB calculation: energy barrier statistics, thermodynamic output by each replica, dump files, and restart files.

When running with multiple partitions (each of which is a replica in this case), the print-out to the screen and master log.lammps file contains a line of output, printed once every *Nevery* timesteps. It contains the timestep, the maximum force per replica, the maximum force per atom (in any replica), potential gradients in the initial, final, and climbing replicas, the forward and backward energy barriers, the total reaction coordinate (RDT), and the normalized reaction coordinate and potential energy of each replica.

The "maximum force per replica" is the two-norm of the 3N-length force vector for the atoms in each replica, maximized across replicas, which is what the *ftol* setting is checking against. In this case, N is all the atoms in each replica. The "maximum force per atom" is the maximum force component of any atom in any replica. The potential gradients are the two-norm of the 3N-length force vector solely due to the interaction potential i.e. without adding in inter-replica forces. Note that inter-replica forces are zero in the initial and final replicas, and only affect the direction in the climbing replica. For this reason, the "maximum force per replica" is often equal to the potential gradient in the climbing replica. In the first stage of NEB, there is no climbing replica, and so the potential gradient in the highest energy replica is reported, since this replica will become the climbing replica in the second stage of NEB.

The "reaction coordinate" (RD) for each replica is the two-norm of the 3N-length vector of distances between its atoms and the preceding replica's atoms, added to the RD of the preceding replica. The RD of the first replica RD1 = 0.0; the RD of the final replica RDN = RDT, the total reaction coordinate. The normalized RDs are divided by RDT, so that they form a monotonically increasing sequence from zero to one. When computing RD, N only includes the atoms being operated on by the fix neb command.

The forward (reverse) energy barrier is the potential energy of the highest replica minus the energy of the first (last) replica.

When running on multiple partitions, LAMMPS produces additional log files for each partition, e.g. log.lammps.0, log.lammps.1, etc. For a NEB calculation, these contain the thermodynamic output for each replica.

If dump commands in the input script define a filename that includes a *universe* or *uloop* style variable, then one dump file (per dump command) will be created for each replica. At the end of the NEB calculation, the final snapshot in each file will contain the sequence of snapshots that transition the system over the energy barrier. Earlier snapshots will show the convergence of the replicas to the MEP.

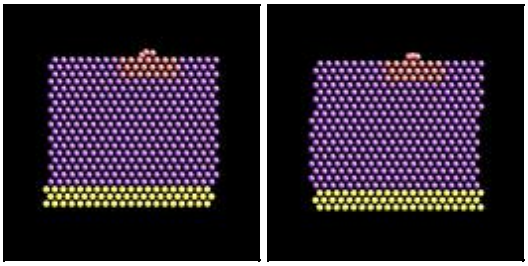
Likewise, restart filenames can be specified with a *universe* or *uloop* style variable, to generate restart files for each replica. These may be useful if the NEB calculation fails to converge properly to the MEP, and you wish to restart the calculation from an intermediate point with altered parameters.

There are 2 Python scripts provided in the tools/python directory, neb_combine.py and neb_final.py, which are useful in analyzing output from a NEB calculation. Assume a NEB simulation with M replicas, and the NEB atoms labelled with a specific atom type.

The neb_combine.py script extracts atom coords for the NEB atoms from all M dump files and creates a single dump file where each snapshot contains the NEB atoms from all the replicas and one copy of non-NEB atoms from the first replica (presumed to be identical in other replicas). This can be visualized/animated to see how the NEB atoms relax as the NEB calculation proceeds.

The neb_final.py script extracts the final snapshot from each of the M dump files to create a single dump file with M snapshots. This can be visualized to watch the system make its transition over the energy barrier.

To illustrate, here are images from the final snapshot produced by the neb_combine.py script run on the dump files produced by the two example input scripts in examples/neb. Click on them to see a larger image.



Restrictions:

This command can only be used if LAMMPS was built with the REPLICA package. See the Making LAMMPS section for more info on packages.

Related commands:

prd, temper, fix langevin, fix viscous

Default: none

(Henkelman1) Henkelman and Jonsson, J Chem Phys, 113, 9978-9985 (2000).

(Henkelman2) Henkelman, Uberuaga, Jonsson, J Chem Phys, 113, 9901-9904 (2000).

(Nakano) Nakano, Comp Phys Comm, 178, 280-289 (2008).

neigh_modify command

Syntax:

```
neigh_modify keyword values ...
```

- one or more keyword/value pairs may be listed

```
keyword = delay or every or check or once or cluster or include or exclude or page or one or
  delay value = N
    N = delay building until this many steps since last build
  every value = M
    M = build neighbor list every this many steps
  check value = yes or no
    yes = only build if some atom has moved half the skin distance or more
    no = always build on 1st step that every and delay are satisfied
  once
    yes = only build neighbor list once at start of run and never rebuild
    no = rebuild neighbor list according to other settings
  cluster
    yes = check bond,angle,etc neighbor list for nearby clusters
    no = do not check bond,angle,etc neighbor list for nearby clusters
  include value = group-ID
    group-ID = only build pair neighbor lists for atoms in this group
  exclude values:
    type M N
      M,N = exclude if one atom in pair is type M, other is type N
    group group1-ID group2-ID
      group1-ID,group2-ID = exclude if one atom is in 1st group, other in 2nd
    molecule group-ID
      groupname = exclude if both atoms are in the same molecule and in the same group
    none
      delete all exclude settings
  page value = N
    N = number of pairs stored in a single neighbor page
  one value = N
    N = max number of neighbors of one atom
  binsize value = size
    size = bin size for neighbor list construction (distance units)
```

Examples:

```
neigh_modify every 2 delay 10 check yes page 100000
neigh_modify exclude type 2 3
neigh_modify exclude group frozen frozen check no
neigh_modify exclude group residue1 chain3
neigh_modify exclude molecule rigid
```

Description:

This command sets parameters that affect the building and use of pairwise neighbor lists. Depending on what pair interactions and other commands are defined, a simulation may require one or more neighbor lists.

The *every*, *delay*, *check*, and *once* options affect how often lists are built as a simulation runs. The *delay* setting means never build new lists until at least N steps after the previous build. The *every* setting means build lists every M steps (after the delay has passed). If the *check* setting is *no*, the lists are built on the first step that satisfies the *delay* and *every* settings. If the *check* setting is *yes*, then the *every* and *delay* settings determine when a build

may possibly be performed, but an actual build only occurs if some atom has moved more than half the skin distance (specified in the neighbor command) since the last build.

If the *once* setting is yes, then the neighbor list is only built once at the beginning of each run, and never rebuilt, except on steps when a restart file is written, or steps when a fix forces a rebuild to occur (e.g. fixes that create or delete atoms, such as fix deposit or fix evaporate). This setting should only be made if you are certain atoms will not move far enough that the neighbor list should be rebuilt, e.g. running a simulation of a cold crystal. Note that it is not that expensive to check if neighbor lists should be rebuilt.

When the rRESPA integrator is used (see the run_style command), the *every* and *delay* parameters refer to the longest (outermost) timestep.

The *cluster* option does a sanity test every time neighbor lists are built for bond, angle, dihedral, and improper interactions, to check that each set of 2, 3, or 4 atoms is a cluster of nearby atoms. It does this by computing the distance between pairs of atoms in the interaction and insuring they are not further apart than half the periodic box length. If they are, an error is generated, since the interaction would be computed between far-away atoms instead of their nearby periodic images. The only way this should happen is if the pairwise cutoff is so short that atoms that are part of the same interaction are not communicated as ghost atoms. This is an unusual model (e.g. no pair interactions at all) and the problem can be fixed by use of the comm_modify cutoff command. Note that to save time, the default *cluster* setting is *no*, so that this check is not performed.

The *include* option limits the building of pairwise neighbor lists to atoms in the specified group. This can be useful for models where a large portion of the simulation is particles that do not interact with other particles or with each other via pairwise interactions. The group specified with this option must also be specified via the atom_modify first command.

The *exclude* option turns off pairwise interactions between certain pairs of atoms, by not including them in the neighbor list. These are sample scenarios where this is useful:

- In crack simulations, pairwise interactions can be shut off between 2 slabs of atoms to effectively create a crack.
- When a large collection of atoms is treated as frozen, interactions between those atoms can be turned off to save needless computation. E.g. Using the fix setforce command to freeze a wall or portion of a bio-molecule.
- When one or more rigid bodies are specified, interactions within each body can be turned off to save needless computation. See the fix rigid command for more details.

The *exclude type* option turns off the pairwise interaction if one atom is of type M and the other of type N. M can equal N. The *exclude group* option turns off the interaction if one atom is in the first group and the other is the second. Group1-ID can equal group2-ID. The *exclude molecule* option turns off the interaction if both atoms are in the specified group and in the same molecule, as determined by their molecule ID.

Each of the exclude options can be specified multiple times. The *exclude type* option is the most efficient option to use; it requires only a single check, no matter how many times it has been specified. The other exclude options are more expensive if specified multiple times; they require one check for each time they have been specified.

Note that the exclude options only affect pairwise interactions; see the delete_bonds command for information on turning off bond interactions.

NOTE: Excluding pairwise interactions will not work correctly when also using a long-range solver via the kspace_style command. LAMMPS will give a warning to this effect. This is because the short-range pairwise interaction needs to subtract off a term from the total energy for pairs whose short-range interaction is excluded,

to compensate for how the long-range solver treats the interaction. This is done correctly for pairwise interactions that are excluded (or weighted) via the special_bonds command. But it is not done for interactions that are excluded via these neigh_modify exclude options.

The *page* and *one* options affect how memory is allocated for the neighbor lists. For most simulations the default settings for these options are fine, but if a very large problem is being run or a very long cutoff is being used, these parameters can be tuned. The indices of neighboring atoms are stored in "pages", which are allocated one after another as they fill up. The size of each page is set by the *page* value. A new page is allocated when the next atom's neighbors could potentially overflow the list. This threshold is set by the *one* value which tells LAMMPS the maximum number of neighbor's one atom can have.

NOTE: LAMMPS can crash without an error message if the number of neighbors for a single particle is larger than the *page* setting, which means it is much, much larger than the *one* setting. This is because LAMMPS doesn't error check these limits for every pairwise interaction (too costly), but only after all the particle's neighbors have been found. This problem usually means something is very wrong with the way you've setup your problem (particle spacing, cutoff length, neighbor skin distance, etc). If you really expect that many neighbors per particle, then boost the *one* and *page* settings accordingly.

The *binsize* option allows you to specify what size of bins will be used in neighbor list construction to sort and find neighboring atoms. By default, for neighbor style bin, LAMMPS uses bins that are 1/2 the size of the maximum pair cutoff. For neighbor style multi, the bins are 1/2 the size of the minimum pair cutoff. Typically these are good values values for minimizing the time for neighbor list construction. This setting overrides the default. If you make it too big, there is little overhead due to looping over bins, but more atoms are checked. If you make it too small, the optimal number of atoms is checked, but bin overhead goes up. If you set the binsize to 0.0, LAMMPS will use the default binsize of 1/2 the cutoff.

Restrictions:

If the "delay" setting is non-zero, then it must be a multiple of the "every" setting.

The exclude molecule option can only be used with atom styles that define molecule IDs.

The value of the *page* setting must be at least 10x larger than the *one* setting. This insures neighbor pages are not mostly empty space.

Related commands:

neighbor, delete_bonds

Default:

The option defaults are delay = 10, every = 1, check = yes, once = no, cluster = no, include = all, exclude = none, page = 100000, one = 2000, and binsize = 0.0.

neighbor command

Syntax:

```
neighbor skin style
```

- skin = extra distance beyond force cutoff (distance units)
- style = *bin* or *nsq* or *multi*

Examples:

```
neighbor 0.3 bin
neighbor 2.0 nsq
```

Description:

This command sets parameters that affect the building of pairwise neighbor lists. All atom pairs within a neighbor cutoff distance equal to the their force cutoff plus the *skin* distance are stored in the list. Typically, the larger the skin distance, the less often neighbor lists need to be built, but more pairs must be checked for possible force interactions every timestep. The default value for *skin* depends on the choice of units for the simulation; see the default values below.

The *skin* distance is also used to determine how often atoms migrate to new processors if the *check* option of the neigh_modify command is set to *yes*. Atoms are migrated (communicated) to new processors on the same timestep that neighbor lists are re-built.

The *style* value selects what algorithm is used to build the list. The *bin* style creates the list by binning which is an operation that scales linearly with N/P, the number of atoms per processor where N = total number of atoms and P = number of processors. It is almost always faster than the *nsq* style which scales as (N/P)^2. For unsolvated small molecules in a non-periodic box, the *nsq* choice can sometimes be faster. Either style should give the same answers.

The *multi* style is a modified binning algorithm that is useful for systems with a wide range of cutoff distances, e.g. due to different size particles. For the *bin* style, the bin size is set to 1/2 of the largest cutoff distance between any pair of atom types and a single set of bins is defined to search over for all atom types. This can be inefficient if one pair of types has a very long cutoff, but other type pairs have a much shorter cutoff. For style *multi* the bin size is set to 1/2 of the shortest cutoff distance and multiple sets of bins are defined to search over for different atom types. This imposes some extra setup overhead, but the searches themselves may be much faster for the short-cutoff cases. See the comm_modify mode multi command for a communication option option that may also be beneficial for simulations of this kind.

The neigh_modify command has additional options that control how often neighbor lists are built and which pairs are stored in the list.

When a run is finished, counts of the number of neighbors stored in the pairwise list and the number of times neighbor lists were built are printed to the screen and log file. See this section for details.

Restrictions: none

Related commands:

neigh_modify, units, comm_modify

Default:

0.3 bin for units = lj, skin = 0.3 sigma
2.0 bin for units = real or metal, skin = 2.0 Angstroms
0.001 bin for units = si, skin = 0.001 meters = 1.0 mm
0.1 bin for units = cgs, skin = 0.1 cm = 1.0 mm

newton command

Syntax:

```
newton flag
newton flag1 flag2
```

- flag = *on* or *off* for both pairwise and bonded interactions
- flag1 = *on* or *off* for pairwise interactions
- flag2 = *on* or *off* for bonded interactions

Examples:

```
newton off
newton on off
```

Description:

This command turns Newton's 3rd law *on* or *off* for pairwise and bonded interactions. For most problems, setting Newton's 3rd law to *on* means a modest savings in computation at the cost of two times more communication. Whether this is faster depends on problem size, force cutoff lengths, a machine's compute/communication ratio, and how many processors are being used.

Setting the pairwise newton flag to *off* means that if two interacting atoms are on different processors, both processors compute their interaction and the resulting force information is not communicated. Similarly, for bonded interactions, newton *off* means that if a bond, angle, dihedral, or improper interaction contains atoms on 2 or more processors, the interaction is computed by each processor.

LAMMPS should produce the same answers for any newton flag settings, except for round-off issues.

With run_style *respa* and only bonded interactions (bond, angle, etc) computed in the innermost timestep, it may be faster to turn newton *off* for bonded interactions, to avoid extra communication in the innermost loop.

Restrictions:

The newton bond setting cannot be changed after the simulation box is defined by a read_data or create_box command.

Related commands:

run_style respa

Default:

```
newton on
```

next command

Syntax:

```
next variables
```

- variables = one or more variable names

Examples:

```
next x
next a t x myTemp
```

Description:

This command is used with variables defined by the variable command. It assigns the next value to the variable from the list of values defined for that variable by the variable command. Thus when that variable is subsequently substituted for in an input script command, the new value is used.

See the variable command for info on how to define and use different kinds of variables in LAMMPS input scripts. If a variable name is a single lower-case character from "a" to "z", it can be used in an input script command as $a or $z. If it is multiple letters, it can be used as ${myTemp}.

If multiple variables are used as arguments to the *next* command, then all must be of the same variable style: *index*, *loop*, *file*, *universe*, or *uloop*. An exception is that *universe*- and *uloop*-style variables can be mixed in the same *next* command.

All the variables specified with the next command are incremented by one value from their respective list of values. A *file*-style variable reads the next line from its associated file. An *atomfile*-style variable reads the next set of lines (one per atom) from its associated file. *String*- or *atom*- or *equal*- or *world*-style variables cannot be used with the the next command, since they only store a single value.

When any of the variables in the next command has no more values, a flag is set that causes the input script to skip the next jump command encountered. This enables a loop containing a next command to exit. As explained in the variable command, the variable that has exhausted its values is also deleted. This allows it to be used and re-defined later in the input script. *File*-style and *atomfile*-style variables are exhausted when the end-of-file is reached.

When the next command is used with *index*- or *loop*-style variables, the next value is assigned to the variable for all processors. When the next command is used with *file*-style variables, the next line is read from its file and the string assigned to the variable. When the next command is used with *atomfile*-style variables, the next set of per-atom values is read from its file and assigned to the variable.

When the next command is used with *universe*- or *uloop*-style variables, all *universe*- or *uloop*-style variables must be listed in the next command. This is because of the manner in which the incrementing is done, using a single lock file for all variables. The next value (for each variable) is assigned to whichever processor partition executes the command first. All processors in the partition are assigned the same value(s). Running LAMMPS on multiple partitions of processors via the "-partition" command-line switch is described in this section of the manual. *Universe*- and *uloop*-style variables are incremented using the files "tmp.lammps.variable" and "tmp.lammps.variable.lock" which you will see in your directory during and after such a LAMMPS run.

Here is an example of running a series of simulations using the next command with an *index*-style variable. If this input script is named in.polymer, 8 simulations would be run using data files from directories run1 thru run8.

```
variable d index run1 run2 run3 run4 run5 run6 run7 run8
shell cd $d
read_data data.polymer
run 10000
shell cd ..
clear
next d
jump in.polymer
```

If the variable "d" were of style *universe*, and the same in.polymer input script were run on 3 partitions of processors, then the first 3 simulations would begin, one on each set of processors. Whichever partition finished first, it would assign variable "d" the 4th value and run another simulation, and so forth until all 8 simulations were finished.

Jump and next commands can also be nested to enable multi-level loops. For example, this script will run 15 simulations in a double loop.

```
variable i loop 3
  variable j loop 5
  clear
  ...
  read_data data.polymer.$i$j
  print Running simulation $i.$j
  run 10000
  next j
  jump in.script
next i
jump in.script
```

Here is an example of a double loop which uses the if and jump commands to break out of the inner loop when a condition is met, then continues iterating thru the outer loop.

```
label       loopa
variable    a loop 5
  label     loopb
  variable  b loop 5
  print     "A,B = $a,$b"
  run       10000
  if        $b > 2 then "jump in.script break"
  next      b
  jump      in.script loopb
label       break
variable    b delete

next        a
jump        in.script loopa
```

Restrictions:

As described above.

Related commands:

jump, include, shell, variable,

Default: none

package command

Syntax:

```
package style args
```

- style = *cuda* or *gpu* or *intel* or *kokkos* or *omp*
- args = arguments specific to the style

```
cuda args = Ngpu keyword value ...
    Ngpu = # of GPUs per node
    zero or more keyword/value pairs may be appended
    keywords = newton or gpuID or timing or test or thread
      newton = off or on
        off = set Newton pairwise and bonded flags off (default)
        on = set Newton pairwise and bonded flags on
      gpuID values = gpu1 .. gpuN
        gpu1 .. gpuN = IDs of the Ngpu GPUs to use
      timing values = none
      test values = id
        id = atom-ID of a test particle
      thread = auto or tpa or bpa
        auto = test whether tpa or bpa is faster
        tpa = one thread per atom
        bpa = one block per atom
  gpu args = Ngpu keyword value ...
    Ngpu = # of GPUs per node
    zero or more keyword/value pairs may be appended
    keywords = neigh or newton or binsize or split or gpuID or tpa or device or blocksize
      neigh value = yes or no
        yes = neighbor list build on GPU (default)
        no = neighbor list build on CPU
      newton = off or on
        off = set Newton pairwise flag off (default and required)
        on = set Newton pairwise flag on (currently not allowed)
      binsize value = size
        size = bin size for neighbor list construction (distance units)
      split = fraction
        fraction = fraction of atoms assigned to GPU (default = 1.0)
      gpuID values = first last
        first = ID of first GPU to be used on each node
        last = ID of last GPU to be used on each node
      tpa value = Nthreads
        Nthreads = # of GPU threads used per atom
      device value = device_type
        device_type = kepler or fermi or cypress or generic
      blocksize value = size
        size = thread block size for pair force computation
  intel args = NPhi keyword value ...
    Nphi = # of coprocessors per node
    zero or more keyword/value pairs may be appended
    keywords = omp or mode or balance or ghost or tpc or tptask or no_affinity
      omp value = Nthreads
        Nthreads = number of OpenMP threads to use on CPU (default = 0)
      mode value = single or mixed or double
        single = perform force calculations in single precision
        mixed = perform force calculations in mixed precision
        double = perform force calculations in double precision
      balance value = split
        split = fraction of work to offload to coprocessor, -1 for dynamic
```

```
      ghost value = yes or no
        yes = include ghost atoms for offload
        no = do not include ghost atoms for offload
      tpc value = Ntpc
        Ntpc = max number of coprocessor threads per coprocessor core (default = 4)
      tptask value = Ntptask
        Ntptask = max number of coprocessor threads per MPI task (default = 240)
      no_affinity values = none
  kokkos args = keyword value ...
    zero or more keyword/value pairs may be appended
    keywords = neigh or newton or binsize or comm or comm/exchange or comm/forward
      neigh value = full or half/thread or half or n2 or full/cluster
        full = full neighbor list
        half/thread = half neighbor list built in thread-safe manner
        half = half neighbor list, not thread-safe, only use when 1 thread/MPI task
        n2 = non-binning neighbor list build, O(N^2) algorithm
        full/cluster = full neighbor list with clustered groups of atoms
      newton = off or on
        off = set Newton pairwise and bonded flags off (default)
        on = set Newton pairwise and bonded flags on
      binsize value = size
        size = bin size for neighbor list construction (distance units)
      comm value = no or host or device
        use value for both comm/exchange and comm/forward
      comm/exchange value = no or host or device
      comm/forward value = no or host or device
        no = perform communication pack/unpack in non-KOKKOS mode
        host = perform pack/unpack on host (e.g. with OpenMP threading)
        device = perform pack/unpack on device (e.g. on GPU)
  omp args = Nthreads keyword value ...
    Nthread = # of OpenMP threads to associate with each MPI process
    zero or more keyword/value pairs may be appended
    keywords = neigh
      neigh value = yes or no
        yes = threaded neighbor list build (default)
        no = non-threaded neighbor list build
```

Examples:

```
package gpu 1
package gpu 1 split 0.75
package gpu 2 split -1.0
package cuda 2 gpuID 0 2
package cuda 1 test 3948
package kokkos neigh half/thread comm device
package omp 0 neigh no
package omp 4
package intel 1
package intel 2 omp 4 mode mixed balance 0.5
```

Description:

This command invokes package-specific settings for the various accelerator packages available in LAMMPS. Currently the following packages use settings from this command: USER-CUDA, GPU, USER-INTEL, KOKKOS, and USER-OMP.

If this command is specified in an input script, it must be near the top of the script, before the simulation box has been defined. This is because it specifies settings that the accelerator packages use in their intialization, before a simultion is defined.

This command can also be specified from the command-line when launching LAMMPS, using the "-pk" command-line switch. The syntax is exactly the same as when used in an input script.

Note that all of the accelerator packages require the package command to be specified (except the OPT package), if the package is to be used in a simulation (LAMMPS can be built with an accelerator package without using it in a particular simulation). However, in all cases, a default version of the command is typically invoked by other accelerator settings.

The USER-CUDA and KOKKOS packages require a "-c on" or "-k on" command-line switch respectively, which invokes a "package cuda" or "package kokkos" command with default settings.

For the GPU, USER-INTEL, and USER-OMP packages, if a "-sf gpu" or "-sf intel" or "-sf omp" command-line switch is used to auto-append accelerator suffixes to various styles in the input script, then those switches also invoke a "package gpu", "package intel", or "package omp" command with default settings.

NOTE: A package command for a particular style can be invoked multiple times when a simulation is setup, e.g. by the "-c on", "-k on", "-sf", and "-pk" command-line switches, and by using this command in an input script. Each time it is used all of the style options are set, either to default values or to specified settings. I.e. settings from previous invocations do not persist across multiple invocations.

See the Section Accelerate section of the manual for more details about using the various accelerator packages for speeding up LAMMPS simulations.

The *cuda* style invokes settings associated with the use of the USER-CUDA package.

The *Ngpus* argument sets the number of GPUs per node. There must be exactly one MPI task per GPU, as set by the mpirun or mpiexec command.

Optional keyword/value pairs can also be specified. Each has a default value as listed below.

The *newton* keyword sets the Newton flags for pairwise and bonded interactions to *off* or *on*, the same as the newton command allows. The default is *off* because this will almost always give better performance for the USER-CUDA package. This means more computation is done, but less communication.

The *gpuID* keyword allows selection of which GPUs on each node will be used for a simulation. GPU IDs range from 0 to N-1 where N is the physical number of GPUs/node. An ID is specified for each of the Ngpus being used. For example if you have three GPUs on a machine, one of which is used for the X-Server (the GPU with the ID 1) while the others (with IDs 0 and 2) are used for computations you would specify:

```
package cuda 2 gpuID 0 2
```

The purpose of the *gpuID* keyword is to allow two (or more) simulations to be run on one workstation. In that case one could set the first simulation to use GPU 0 and the second to use GPU 1. This is not necessary however, if the GPUs are in what is called *compute exclusive* mode. Using that setting, every process will get its own GPU automatically. This *compute exclusive* mode can be set as root using the *nvidia-smi* tool which is part of the CUDA installation.

Also note that if the *gpuID* keyword is not used, the USER-CUDA package sorts existing GPUs on each node according to their number of multiprocessors. This way, compute GPUs will be priorized over X-Server GPUs.

If the *timing* keyword is specified, detailed timing information for various subroutines will be output.

If the *test* keyword is specified, information for the specified atom with atom-ID will be output at several points during each timestep. This is mainly usefull for debugging purposes. Note that the simulation slow down dramatically if this option is used.

The *thread* keyword can be used to specify how GPU threads are assigned work during pair style force evaluation. If the value = *tpa*, one thread per atom is used. If the value = *bpa*, one block per atom is used. If the value = *auto*, a short test is performed at the beginning of each run to determing where *tpa* or *bpa* mode is faster. The result of this test is output. Since *auto* is the default value, it is usually not necessary to use this keyword.

The *gpu* style invokes settings associated with the use of the GPU package.

The *Ngpu* argument sets the number of GPUs per node. There must be at least as many MPI tasks per node as GPUs, as set by the mpirun or mpiexec command. If there are more MPI tasks (per node) than GPUs, multiple MPI tasks will share each GPU.

Optional keyword/value pairs can also be specified. Each has a default value as listed below.

The *neigh* keyword specifies where neighbor lists for pair style computation will be built. If *neigh* is *yes*, which is the default, neighbor list building is performed on the GPU. If *neigh* is *no*, neighbor list building is performed on the CPU. GPU neighbor list building currently cannot be used with a triclinic box. GPU neighbor list calculation currently cannot be used with hybrid pair styles. GPU neighbor lists are not compatible with comannds that are not GPU-enabled. When a non-GPU enabled command requires a neighbor list, it will also be built on the CPU. In these cases, it will typically be more efficient to only use CPU neighbor list builds.

The *newton* keyword sets the Newton flags for pairwise (not bonded) interactions to *off* or *on*, the same as the newton command allows. Currently, only an *off* value is allowed, since all the GPU package pair styles require this setting. This means more computation is done, but less communication. In the future a value of *on* may be allowed, so the *newton* keyword is included as an option for compatibility with the package command for other accelerator styles. Note that the newton setting for bonded interactions is not affected by this keyword.

The *binsize* keyword sets the size of bins used to bin atoms in neighbor list builds performed on the GPU, if *neigh* = *yes* is set. If *binsize* is set to 0.0 (the default), then bins = the size of the pairwise cutoff + neighbor skin distance. This is 2x larger than the LAMMPS default used for neighbor list building on the CPU. This will be close to optimal for the GPU, so you do not normally need to use this keyword. Note that if you use a longer-than-usual pairwise cutoff, e.g. to allow for a smaller fraction of KSpace work with a long-range Coulombic solver because the GPU is faster at performing pairwise interactions, then it may be optimal to make the *binsize* smaller than the default. For example, with a cutoff of 20*sigma in LJ units and a neighbor skin distance of sigma, a *binsize* = 5.25*sigma can be more efficient than the default.

The *split* keyword can be used for load balancing force calculations between CPU and GPU cores in GPU-enabled pair styles. If 0 < *split* < 1.0, a fixed fraction of particles is offloaded to the GPU while force calculation for the other particles occurs simulataneously on the CPU. If *split* < 0.0, the optimal fraction (based on CPU and GPU timings) is calculated every 25 timesteps, i.e. dynamic load-balancing across the CPU and GPU is performed. If *split* = 1.0, all force calculations for GPU accelerated pair styles are performed on the GPU. In this case, other hybrid pair interactions, bond, angle, dihedral, improper, and long-range calculations can be performed on the CPU while the GPU is performing force calculations for the GPU-enabled pair style. If all CPU force computations complete before the GPU completes, LAMMPS will block until the GPU has finished before continuing the timestep.

As an example, if you have two GPUs per node and 8 CPU cores per node, and would like to run on 4 nodes (32 cores) with dynamic balancing of force calculation across CPU and GPU cores, you could specify

```
mpirun -np 32 -sf gpu -in in.script    # launch command
```

```
package gpu 2 split -1                  # input script command
```

In this case, all CPU cores and GPU devices on the nodes would be utilized. Each GPU device would be shared by 4 CPU cores. The CPU cores would perform force calculations for some fraction of the particles at the same time the GPUs performed force calculation for the other particles.

The *gpuID* keyword allows selection of which GPUs on each node will be used for a simulation. The *first* and *last* values specify the GPU IDs to use (from 0 to Ngpu-1). By default, first = 0 and last = Ngpu-1, so that all GPUs are used, assuming Ngpu is set to the number of physical GPUs. If you only wish to use a subset, set Ngpu to a smaller number and first/last to a sub-range of the available GPUs.

The *tpa* keyword sets the number of GPU thread per atom used to perform force calculations. With a default value of 1, the number of threads will be chosen based on the pair style, however, the value can be set explicitly with this keyword to fine-tune performance. For large cutoffs or with a small number of particles per GPU, increasing the value can improve performance. The number of threads per atom must be a power of 2 and currently cannot be greater than 32.

The *device* keyword can be used to tune parameters optimized for a specific accelerator, when using OpenCL. For CUDA, the *device* keyword is ignored. Currently, the device type is limited to NVIDIA Kepler, NVIDIA Fermi, AMD Cypress, or a generic device. More devices may be added later. The default device type can be specified when building LAMMPS with the GPU library, via settings in the lib/gpu/Makefile that is used.

The *blocksize* keyword allows you to tweak the number of threads used per thread block. This number should be a multiple of 32 (for GPUs) and its maximum depends on the specific GPU hardware. Typical choices are 64, 128, or 256. A larger blocksize increases occupancy of individual GPU cores, but reduces the total number of thread blocks, thus may lead to load imbalance.

The *intel* style invokes settings associated with the use of the USER-INTEL package. All of its settings, except the *omp* and *mode* keywords, are ignored if LAMMPS was not built with Xeon Phi coprocessor support. All of its settings, including the *omp* and *mode* keyword are applicable if LAMMPS was built with coprocessor support.

The *Nphi* argument sets the number of coprocessors per node. This can be set to any value, including 0, if LAMMPS was not built with coprocessor support.

Optional keyword/value pairs can also be specified. Each has a default value as listed below.

The *omp* keyword determines the number of OpenMP threads allocated for each MPI task when any portion of the interactions computed by a USER-INTEL pair style are run on the CPU. This can be the case even if LAMMPS was built with coprocessor support; see the *balance* keyword discussion below. If you are running with less MPI tasks/node than there are CPUs, it can be advantageous to use OpenMP threading on the CPUs.

NOTE: The *omp* keyword has nothing to do with coprocessor threads on the Xeon Phi; see the *tpc* and *tptask* keywords below for a discussion of coprocessor threads.

The *Nthread* value for the *omp* keyword sets the number of OpenMP threads allocated for each MPI task. Setting *Nthread* = 0 (the default) instructs LAMMPS to use whatever value is the default for the given OpenMP environment. This is usually determined via the *OMP_NUM_THREADS* environment variable or the compiler runtime, which is usually a value of 1.

For more details, including examples of how to set the OMP_NUM_THREADS environment variable, see the discussion of the *Nthreads* setting on this doc page for the "package omp" command. Nthreads is a required argument for the USER-OMP package. Its meaning is exactly the same for the USER-INTEL pacakge.

NOTE: If you build LAMMPS with both the USER-INTEL and USER-OMP packages, be aware that both packages allow setting of the *Nthreads* value via their package commands, but there is only a single global *Nthreads* value used by OpenMP. Thus if both package commands are invoked, you should insure the two values are consistent. If they are not, the last one invoked will take precedence, for both packages. Also note that if the "-sf hybrid intel omp" command-line"> switch is used, it invokes a "package intel" command, followed by a "package omp" command, both with a setting of *Nthreads* = 0.

The *mode* keyword determines the precision mode to use for computing pair style forces, either on the CPU or on the coprocessor, when using a USER-INTEL supported pair style. It can take a value of *single*, *mixed* which is the default, or *double*. *Single* means single precision is used for the entire force calculation. *Mixed* means forces between a pair of atoms are computed in single precision, but accumulated and stored in double precision, including storage of forces, torques, energies, and virial quantities. *Double* means double precision is used for the entire force calculation.

The *balance* keyword sets the fraction of pair style work offloaded to the coprocessor for split values between 0.0 and 1.0 inclusive. While this fraction of work is running on the coprocessor, other calculations will run on the host, including neighbor and pair calculations that are not offloaded, as well as angle, bond, dihedral, kspace, and some MPI communications. If *split* is set to -1, the fraction of work is dynamically adjusted automatically throughout the run. This typically give performance within 5 to 10 percent of the optimal fixed fraction.

The *ghost* keyword determines whether or not ghost atoms, i.e. atoms at the boundaries of proessor sub-domains, are offloaded for neighbor and force calculations. When the value = "no", ghost atoms are not offloaded. This option can reduce the amount of data transfer with the coprocessor and can also overlap MPI communication of forces with computation on the coprocessor when the newton pair setting is "on". When the value = "yes", ghost atoms are offloaded. In some cases this can provide better performance, especially if the *balance* fraction is high.

The *tpc* keyword sets the max # of coprocessor threads *Ntpc* that will run on each core of the coprocessor. The default value = 4, which is the number of hardware threads per core supported by the current generation Xeon Phi chips.

The *tptask* keyword sets the max # of coprocessor threads (Ntptask assigned to each MPI task. The default value = 240, which is the total # of threads an entire current generation Xeon Phi chip can run (240 = 60 cores * 4 threads/core). This means each MPI task assigned to the Phi will enough threads for the chip to run the max allowed, even if only 1 MPI task is assigned. If 8 MPI tasks are assigned to the Phi, each will run with 30 threads. If you wish to limit the number of threads per MPI task, set *tptask* to a smaller value. E.g. for *tptask* = 16, if 8 MPI tasks are assigned, each will run with 16 threads, for a total of 128.

Note that the default settings for *tpc* and *tptask* are fine for most problems, regardless of how many MPI tasks you assign to a Phi.

The *no_affinity* keyword will turn off automatic setting of core affinity for MPI tasks and OpenMP threads on the host when using offload to a coprocessor. Affinity settings are used when possible to prevent MPI tasks and OpenMP threads from being on separate NUMA domains and to prevent offload threads from interfering with other processes/threads used for LAMMPS.

The *kokkos* style invokes settings associated with the use of the KOKKOS package.

All of the settings are optional keyword/value pairs. Each has a default value as listed below.

The *neigh* keyword determines how neighbor lists are built. A value of *half* uses half-neighbor lists, the same as used by most pair styles in LAMMPS. A value of *half/thread* uses a thread-safe variant of the half-neighbor list. It should be used instead of *half* when running with more than 1 threads per MPI task on a CPU. A value of *n2* uses

an O(N^2) algorithm to build the neighbor list without binning, where N = # of atoms on a processor. It is typically slower than the other methods, which use binning.

A value of *full* uses a full neighbor lists and is the default. This performs twice as much computation as the *half* option, however that is often a win because it is thread-safe and doesn't require atomic operations in the calculation of pair forces. For that reason, *full* is the default setting. However, when running in MPI-only mode with 1 thread per MPI task, *half* neighbor lists will typically be faster, just as it is for non-accelerated pair styles.

A value of *full/cluster* is an experimental neighbor style, where particles interact with all particles within a small cluster, if at least one of the clusters particles is within the neighbor cutoff range. This potentially allows for better vectorization on architectures such as the Intel Phi. If also reduces the size of the neighbor list by roughly a factor of the cluster size, thus reducing the total memory footprint considerably.

The *newton* keyword sets the Newton flags for pairwise and bonded interactions to *off* or *on*, the same as the newton command allows. The default is *off* because this will almost always give better performance for the KOKKOS package. This means more computation is done, but less communication. However, when running in MPI-only mode with 1 thread per MPI task, a value of *on* will typically be faster, just as it is for non-accelerated pair styles.

The *binsize* keyword sets the size of bins used to bin atoms in neighbor list builds. The same value can be set by the neigh_modify binsize command. Making it an option in the package kokkos command allows it to be set from the command line. The default value is 0.0, which means the LAMMPS default will be used, which is bins = 1/2 the size of the pairwise cutoff + neighbor skin distance. This is fine when neighbor lists are built on the CPU. For GPU builds, a 2x larger binsize equal to the pairwise cutoff + neighbor skin, is often faster, which can be set by this keyword. Note that if you use a longer-than-usual pairwise cutoff, e.g. to allow for a smaller fraction of KSpace work with a long-range Coulombic solver because the GPU is faster at performing pairwise interactions, then this rule of thumb may give too large a binsize.

The *comm* and *comm/exchange* and *comm/forward* keywords determine whether the host or device performs the packing and unpacking of data when communicating per-atom data between processors. "Exchange" communication happens only on timesteps that neighbor lists are rebuilt. The data is only for atoms that migrate to new processors. "Forward" communication happens every timestep. The data is for atom coordinates and any other atom properties that needs to be updated for ghost atoms owned by each processor.

The *comm* keyword is simply a short-cut to set the same value for both the *comm/exchange* and *comm/forward* keywords.

The value options for all 3 keywords are *no* or *host* or *device*. A value of *no* means to use the standard non-KOKKOS method of packing/unpacking data for the communication. A value of *host* means to use the host, typically a multi-core CPU, and perform the packing/unpacking in parallel with threads. A value of *device* means to use the device, typically a GPU, to perform the packing/unpacking operation.

The optimal choice for these keywords depends on the input script and the hardware used. The *no* value is useful for verifying that the Kokkos-based *host* and *device* values are working correctly. It may also be the fastest choice when using Kokkos styles in MPI-only mode (i.e. with a thread count of 1).

When running on CPUs or Xeon Phi, the *host* and *device* values work identically. When using GPUs, the *device* value will typically be optimal if all of your styles used in your input script are supported by the KOKKOS package. In this case data can stay on the GPU for many timesteps without being moved between the host and GPU, if you use the *device* value. This requires that your MPI is able to access GPU memory directly. Currently that is true for OpenMPI 1.8 (or later versions), Mvapich2 1.9 (or later), and CrayMPI. If your script uses styles (e.g. fixes) which are not yet supported by the KOKKOS package, then data has to be move between the host and

device anyway, so it is typically faster to let the host handle communication, by using the *host* value. Using *host* instead of *no* will enable use of multiple threads to pack/unpack communicated data.

The *omp* style invokes settings associated with the use of the USER-OMP package.

The *Nthread* argument sets the number of OpenMP threads allocated for each MPI task. For example, if your system has nodes with dual quad-core processors, it has a total of 8 cores per node. You could use two MPI tasks per node (e.g. using the -ppn option of the mpirun command in MPICH or -npernode in OpenMPI), and set *Nthreads* = 4. This would use all 8 cores on each node. Note that the product of MPI tasks * threads/task should not exceed the physical number of cores (on a node), otherwise performance will suffer.

Setting *Nthread* = 0 instructs LAMMPS to use whatever value is the default for the given OpenMP environment. This is usually determined via the *OMP_NUM_THREADS* environment variable or the compiler runtime. Note that in most cases the default for OpenMP capable compilers is to use one thread for each available CPU core when *OMP_NUM_THREADS* is not explicitly set, which can lead to poor performance.

Here are examples of how to set the environment variable when launching LAMMPS:

```
env OMP_NUM_THREADS=4 lmp_machine -sf omp -in in.script
env OMP_NUM_THREADS=2 mpirun -np 2 lmp_machine -sf omp -in in.script
mpirun -x OMP_NUM_THREADS=2 -np 2 lmp_machine -sf omp -in in.script
```

or you can set it permanently in your shell's start-up script. All three of these examples use a total of 4 CPU cores.

Note that different MPI implementations have different ways of passing the OMP_NUM_THREADS environment variable to all MPI processes. The 2nd example line above is for MPICH; the 3rd example line with -x is for OpenMPI. Check your MPI documentation for additional details.

What combination of threads and MPI tasks gives the best performance is difficult to predict and can depend on many components of your input. Not all features of LAMMPS support OpenMP threading via the USER-OMP packaage and the parallel efficiency can be very different, too.

Optional keyword/value pairs can also be specified. Each has a default value as listed below.

The *neigh* keyword specifies whether neighbor list building will be multi-threaded in addition to force calculations. If *neigh* is set to *no* then neighbor list calculation is performed only by MPI tasks with no OpenMP threading. If *mode* is *yes* (the default), a multi-threaded neighbor list build is used. Using *neigh* = *yes* is almost always faster and should produce idential neighbor lists at the expense of using more memory. Specifically, neighbor list pages are allocated for all threads at the same time and each thread works within its own pages.

Restrictions:

This command cannot be used after the simulation box is defined by a read_data or create_box command.

The cuda style of this command can only be invoked if LAMMPS was built with the USER-CUDA package. See the Making LAMMPS section for more info.

The gpu style of this command can only be invoked if LAMMPS was built with the GPU package. See the Making LAMMPS section for more info.

The intel style of this command can only be invoked if LAMMPS was built with the USER-INTEL package. See the Making LAMMPS section for more info.

The kk style of this command can only be invoked if LAMMPS was built with the KOKKOS package. See the Making LAMMPS section for more info.

The omp style of this command can only be invoked if LAMMPS was built with the USER-OMP package. See the Making LAMMPS section for more info.

Related commands:

suffix, "-pk" command-line setting

Default:

For the USER-CUDA package, the default is Ngpu = 1 and the option defaults are newton = off, gpuID = 0 to Ngpu-1, timing = not enabled, test = not enabled, and thread = auto. These settings are made automatically by the required "-c on" command-line switch. You can change them bu using the package cuda command in your input script or via the "-pk cuda" command-line switch.

For the GPU package, the default is Ngpu = 1 and the option defaults are neigh = yes, newton = off, binsize = 0.0, split = 1.0, gpuID = 0 to Ngpu-1, tpa = 1, and device = not used. These settings are made automatically if the "-sf gpu" command-line switch is used. If it is not used, you must invoke the package gpu command in your input script or via the "-pk gpu" command-line switch.

For the USER-INTEL package, the default is Nphi = 1 and the option defaults are omp = 0, mode = mixed, balance = -1, tpc = 4, tptask = 240. The default ghost option is determined by the pair style being used. This value is output to the screen in the offload report at the end of each run. Note that all of these settings, except "omp" and "mode", are ignored if LAMMPS was not built with Xeon Phi coprocessor support. These settings are made automatically if the "-sf intel" command-line switch is used. If it is not used, you must invoke the package intel command in your input script or or via the "-pk intel" command-line switch.

For the KOKKOS package, the option defaults neigh = full, newton = off, binsize = 0.0, and comm = device. These settings are made automatically by the required "-k on" command-line switch. You can change them bu using the package kokkos command in your input script or via the "-pk kokkos" command-line switch.

For the OMP package, the default is Nthreads = 0 and the option defaults are neigh = yes. These settings are made automatically if the "-sf omp" command-line switch is used. If it is not used, you must invoke the package omp command in your input script or via the "-pk omp" command-line switch.

pair_style adp command

pair_style adp/omp command

Syntax:

```
pair_style adp
```

Examples:

```
pair_style adp
pair_coeff * * Ta.adp Ta
pair_coeff * * ../potentials/AlCu.adp Al Al Cu
```

Description:

Style *adp* computes pairwise interactions for metals and metal alloys using the angular dependent potential (ADP) of (Mishin), which is a generalization of the embedded atom method (EAM) potential. The LAMMPS implementation is discussed in (Singh). The total energy Ei of an atom I is given by

$$
\begin{aligned}
E_i &= F_\alpha \left(\sum_{j \neq i} \rho_\beta(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij}) + \frac{1}{2} \sum_s (\mu_i^s)^2 + \frac{1}{2} \sum_{s,t} (\lambda_i^{st})^2 - \frac{1}{6} \nu_i^2 \\
\mu_i^s &= \sum_{j \neq i} u_{\alpha\beta}(r_{ij}) r_{ij}^s \\
\lambda_i^{st} &= \sum_{j \neq i} w_{\alpha\beta}(r_{ij}) r_{ij}^s r_{ij}^t \\
\nu_i &= \sum_s \lambda_i^{ss}
\end{aligned}
$$

where F is the embedding energy which is a function of the atomic electron density rho, phi is a pair potential interaction, alpha and beta are the element types of atoms I and J, and s and t = 1,2,3 and refer to the cartesian coordinates. The mu and lambda terms represent the dipole and quadruple distortions of the local atomic environment which extend the original EAM framework by introducing angular forces.

Note that unlike for other potentials, cutoffs for ADP potentials are not set in the pair_style or pair_coeff command; they are specified in the ADP potential files themselves. Likewise, the ADP potential files list atomic masses; thus you do not need to use the mass command to specify them.

The NIST WWW site distributes and documents ADP potentials:

```
http://www.ctcms.nist.gov/potentials
```

Note that these must be converted into the extended DYNAMO *setfl* format discussed below.

The NIST site is maintained by Chandler Becker (cbecker at nist.gov) who is good resource for info on interatomic potentials and file formats.

Only a single pair_coeff command is used with the *adp* style which specifies an extended DYNAMO *setfl* file, which contains information for M elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of extended *setfl* elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file.

As an example, the potentials/AlCu.adp file, included in the potentials directory of the LAMMPS distrbution, is an extended *setfl* file which has tabulated ADP values for w elements and their alloy interactions: Cu and Al. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Al, and the 4th to be Cu, you would use the following pair_coeff command:

```
pair_coeff * * AlCu.adp Al Al Al Cu
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Al arguments map LAMMPS atom types 1,2,3 to the Al element in the extended *setfl* file. The final Cu argument maps LAMMPS atom type 4 to the Al element in the extended *setfl* file. Note that there is no requirement that your simulation use all the elements specified by the extended *setfl* file.

If a mapping value is specified as NULL, the mapping is not performed. This can be used when an *adp* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Adp files in the *potentials* directory of the LAMMPS distribution have an ".adp" suffix. A DYNAMO *setfl* file extended for ADP is formatted as follows. Basically it is the standard *setfl* format with additional tabulated functions u and w added to the file after the tabulated pair potentials. See the pair_eam command for further details on the *setfl* format.

- lines 1,2,3 = comments (ignored)
- line 4: Nelements Element1 Element2 ... ElementN
- line 5: Nrho, drho, Nr, dr, cutoff

Following the 5 header lines are Nelements sections, one for each element, each with the following format:

- line 1 = atomic number, mass, lattice constant, lattice type (e.g. FCC)
- embedding function F(rho) (Nrho values)
- density function rho(r) (Nr values)

Following the Nelements sections, Nr values for each pair potential phi(r) array are listed for all i,j element pairs in the same format as other arrays. Since these interactions are symmetric (i,j = j,i) only phi arrays with i >= j are listed, in the following order: i,j = (1,1), (2,1), (2,2), (3,1), (3,2), (3,3), (4,1), ..., (Nelements, Nelements). The tabulated values for each phi function are listed as r*phi (in units of eV-Angstroms), since they are for atom pairs, the same as for other EAM files.

After the phi(r) arrays, each of the u(r) arrays are listed in the same order with the same assumptions of symmetry. Directly following the u(r), the w(r) arrays are listed. Note that phi(r) is the only array tabulated with a scaling by

r.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, no special mixing rules are needed, since the ADP potential files specify alloy interactions explicitly.

This pair style does not support the pair_modify shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in tabulated potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default).

Related commands:

pair_coeff, pair_eam

Default: none

(Mishin) Mishin, Mehl, and Papaconstantopoulos, Acta Mater, 53, 4029 (2005).

(Singh) Singh and Warner, Acta Mater, 58, 5797-5805 (2010),

pair_style airebo command

pair_style airebo/omp command

pair_style rebo command

pair_style rebo/omp command

Syntax:

```
pair_style style cutoff LJ_flag TORSION_flag
```

- style = *airebo* or *rebo*
- cutoff = LJ cutoff (sigma scale factor) (AIREBO only)
- LJ_flag = 0/1 to turn off/on the LJ term (AIREBO only, optional)
- TORSION_flag = 0/1 to turn off/on the torsion term (AIREBO only, optional)

Examples:

```
pair_style airebo 3.0
pair_style airebo 2.5 1 0
pair_coeff * * ../potentials/CH.airebo H C

pair_style rebo
pair_coeff * * ../potentials/CH.airebo H C
```

Description:

The *airebo* pair style computes the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) Potential of (Stuart) for a system of carbon and/or hydrogen atoms. Note that this is the initial formulation of AIREBO from 2000, not the later formulation. The *rebo* pair style computes the Reactive Empirical Bond Order (REBO) Potential of (Brenner). Note that this is the so-called 2nd generation REBO from 2002, not the original REBO from 1990. As discussed below, 2nd generation REBO is closely related to the intial AIREBO; it is just a subset of the potential energy terms.

The AIREBO potential consists of three terms:

$$E = \frac{1}{2} \sum_i \sum_{j \neq i} \left[E_{ij}^{REBO} + E_{ij}^{LJ} + \sum_{k \neq i,j} \sum_{l \neq i,j,k} E_{kijl}^{TORSION} \right]$$

By default, all three terms are included. For the *airebo* style, if the two optional flag arguments to the pair_style command are included, the LJ and torsional terms can be turned off. Note that both or neither of the flags must be included. If both of the LJ an torsional terms are turned off, it becomes the 2nd-generation REBO potential, with a small caveat on the spline fitting procedure mentioned below. This can be specified directly as pair_style rebo with no additional arguments.

The detailed formulas for this potential are given in (Stuart); here we provide only a brief description.

The E_REBO term has the same functional form as the hydrocarbon REBO potential developed in (Brenner). The coefficients for E_REBO in AIREBO are essentially the same as Brenner's potential, but a few fitted spline values are slightly different. For most cases the E_REBO term in AIREBO will produce the same energies, forces and statistical averages as the original REBO potential from which it was derived. The E_REBO term in the AIREBO potential gives the model its reactive capabilities and only describes short-ranged C-C, C-H and H-H interactions (r < 2 Angstroms). These interactions have strong coordination-dependence through a bond order parameter, which adjusts the attraction between the I,J atoms based on the position of other nearby atoms and thus has 3- and 4-body dependence.

The E_LJ term adds longer-ranged interactions (2 < r < cutoff) using a form similar to the standard Lennard Jones potential. The E_LJ term in AIREBO contains a series of switching functions so that the short-ranged LJ repulsion (1/r^12) does not interfere with the energetics captured by the E_REBO term. The extent of the E_LJ interactions is determined by the *cutoff* argument to the pair_style command which is a scale factor. For each type pair (C-C, C-H, H-H) the cutoff is obtained by multiplying the scale factor by the sigma value defined in the potential file for that type pair. In the standard AIREBO potential, sigma_CC = 3.4 Angstroms, so with a scale factor of 3.0 (the argument in pair_style), the resulting E_LJ cutoff would be 10.2 Angstroms.

The E_TORSION term is an explicit 4-body potential that describes various dihedral angle preferences in hydrocarbon configurations.

Only a single pair_coeff command is used with the *airebo* or *rebo* style which specifies an AIREBO potential file with parameters for C and H. Note that the *rebo* style in LAMMPS uses the same AIREBO-formatted potential file. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of AIREBO elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file.

As an example, if your LAMMPS simulation has 4 atom types and you want the 1st 3 to be C, and the 4th to be H, you would use the following pair_coeff command:

```
pair_coeff * * CH.airebo C C C H
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three C arguments map LAMMPS atom types 1,2,3 to the C element in the AIREBO file. The final H argument maps LAMMPS atom type 4 to the H element in the SW file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *airebo* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

The parameters/coefficients for the AIREBO potentials are listed in the CH.airebo file to agree with the original (Stuart) paper. Thus the parameters are specific to this potential and the way it was fit, so modifying the file should be done cautiously.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support the pair_modify mix, shift, table, and tail options.

These pair styles do not write their information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.

Restrictions:

These pair styles are part of the MANYBODY package. They are only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

These pair potentials require the newton setting to be "on" for pair interactions.

The CH.airebo potential file provided with LAMMPS (see the potentials directory) is parameterized for metal units. You can use the AIREBO or REBO potential with any LAMMPS units, but you would need to create your own AIREBO potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

Related commands:

pair_coeff

Default: none

(Stuart) Stuart, Tutein, Harrison, J Chem Phys, 112, 6472-6486 (2000).

(Brenner) Brenner, Shenderova, Harrison, Stuart, Ni, Sinnott, J Physics: Condensed Matter, 14, 783-802 (2002).

pair_style awpmd/cut command

Syntax:

```
pair_style awpmd/cut Rc keyword value ...
```

- Rc = global cutoff, -1 means cutoff of half the shortest box length
- zero or more keyword/value pairs may be appended
- keyword = *hartree* or *dproduct* or *uhf* or *free* or *pbc* or *fix* or *harm* or *ermscale* or *flex_press*

```
hartree value = none
  dproduct value = none
  uhf value = none
  free value = none
  pbc value = Plen
    Plen = periodic width of electron = -1 or positive value (distance units)
  fix value = Flen
    Flen = fixed width of electron = -1 or positive value (distance units)
  harm value = width
    width = harmonic width constraint
  ermscale value = factor
    factor = scaling between electron mass and width variable mass
  flex_press value = none
```

Examples:

```
pair_style awpmd/cut -1
pair_style awpmd/cut 40.0 uhf free
pair_coeff * *
pair_coeff 2 2 20.0
```

Description:

This pair style contains an implementation of the Antisymmetrized Wave Packet Molecular Dynamics (AWPMD) method. Need citation here. Need basic formulas here. Could be links to other documents.

Rc is the cutoff.

The pair_style command allows for several optional keywords to be specified.

The *hartree*, *dproduct*, and *uhf* keywords specify the form of the initial trial wave function for the system. If the *hartree* keyword is used, then a Hartree multielectron trial wave function is used. If the *dproduct* keyword is used, then a trial function which is a product of two determinants for each spin type is used. If the *uhf* keyword is used, then an unrestricted Hartree-Fock trial wave function is used.

The *free*, *pbc*, and *fix* keywords specify a width constraint on the electron wavepackets. If the *free* keyword is specified, then there is no constraint. If the *pbc* keyword is used and *Plen* is specified as -1, then the maximum width is half the shortest box length. If *Plen* is a positive value, then the value is the maximum width. If the *fix* keyword is used and *Flen* is specified as -1, then electrons have a constant width that is read from the data file. If *Flen* is a positive value, then the constant width for all electrons is set to *Flen*.

The *harm* keyword allow oscillations in the width of the electron wavepackets. More details are needed.

The *ermscale* keyword specifies a unitless scaling factor between the electron masses and the width variable mass. More details needed.

If the *flex_press* keyword is used, then a contribution from the electrons is added to the total virial and pressure of the system.

This potential is designed to be used with atom_style wavepacket definitions, in order to handle the description of systems with interacting nuclei and explicit electrons.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- cutoff (distance units)

For *awpmd/cut*, the cutoff coefficient is optional. If it is not used (as in some of the examples above), the default global value specified in the pair_style command is used.

Mixing, shift, table, tail correction, restart, rRESPA info:

The pair_modify mix, shift, table, and tail options are not relevant for this pair style.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions: none

Related commands:

pair_coeff

Default:

These are the defaults for the pair_style keywords: *hartree* for the initial wavefunction, *free* for the wavepacket width.

pair_style beck command

pair_style beck/gpu command

pair_style beck/omp command

Syntax:

```
pair_style beck Rc
```

- Rc = cutoff for interactions (distance units)

Examples:

```
pair_style beck 8.0
pair_coeff * * 399.671876712 0.0000867636112694 0.675 4.390 0.0003746
pair_coeff 1 1 399.671876712 0.0000867636112694 0.675 4.390 0.0003746 6.0
```

Description:

Style *beck* computes interactions based on the potential by (Beck), originally designed for simulation of Helium. It includes truncation at a cutoff distance Rc.

$$E\left(r\right) = A \exp\left[-\alpha r - \beta r^6\right] - \frac{B}{\left(r^2+a^2\right)^3}\left(1 + \frac{2.709+3a^2}{r^2+a^2}\right) \qquad r < R_c$$

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands.

- A (energy units)
- B (energy-distance^6 units)
- a (distance units)
- alpha (1/distance units)
- beta (1/distance^6 units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global cutoff Rc is used.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, coeffiecients must be specified. No default mixing rules are used.

This pair style does not support the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions: none

Related commands:

pair_coeff

Default: none

(Beck) Beck, Molecular Physics, 14, 311 (1968).

pair_style body command

Syntax:

```
pair_style body cutoff
```

cutoff = global cutoff for interactions (distance units)

Examples:

```
pair_style body 3.0
pair_coeff * * 1.0 1.0
pair_coeff 1 1 1.0 1.5 2.5
```

Description:

Style *body* is for use with body particles and calculates pairwise body/body interactions as well as interactions between body and point-particles. See Section_howto 14 of the manual and the body doc page for more details on using body particles.

This pair style is designed for use with the "nparticle" body style, which is specified as an argument to the "atom-style body" command. See the body doc page for more details about the body styles LAMMPS supports. The "nparticle" style treats a body particle as a rigid body composed of N sub-particles.

The coordinates of a body particle are its center-of-mass (COM). If the COMs of a pair of body particles are within the cutoff (global or type-specific, as specified above), then all interactions between pairs of sub-particles in the two body particles are computed. E.g. if the first body particle has 3 sub-particles, and the second has 10, then 30 interactions are computed and summed to yield the total force and torque on each body particle.

NOTE: In the example just described, all 30 interactions are computed even if the distance between a particular pair of sub-particles is greater than the cutoff. Likewise, no interaction between two body particles is computed if the two COMs are further apart than the cutoff, even if the distance between some pairs of their sub-particles is within the cutoff. Thus care should be used in defining the cutoff distances for body particles, depending on their shape and size.

Similar rules apply for a body particle interacting with a point particle. The distance between the two particles is calculated using the COM of the body particle and the position of the point particle. If the distance is within the cutoff and the body particle has N sub-particles, then N interactions with the point particle are computed and summed. If the distance is not within the cutoff, no interactions between the body and point particle are computed.

The interaction between two sub-particles, or a sub-particle and point particle, or betwee two point particles is computed as a Lennard-Jones interaction, using the standard formula

$$E = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \qquad r < r_c$$

where Rc is the cutoff. As explained above, an interaction involving one or two body sub-particles may be computed even for r > Rc.

For style *body*, the following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- epsilon (energy units)
- sigma (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global cutoff is used.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of this pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style does not support the pair_modify shift, table, and tail options.

This pair style does not write its information to binary restart files.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This style is part of the BODY package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Defining particles to be bodies so they participate in body/body or body/particle interactions requires the use of the atom_style body command.

Related commands:

pair_coeff, fix_rigid

Default: none

pair_style bop command

Syntax:

```
pair_style bop keyword ...
```

- zero or more keywords may be appended
- keyword = *save*

```
save = pre-compute and save some values
```

Examples:

```
pair_style bop
pair_coeff * * ../potentials/CdTe_bop Cd Te
pair_style bop save
pair_coeff * * ../potentials/CdTe.bop.table Cd Te Te
comm_modify cutoff 14.70
```

Description:

The *bop* pair style computes Bond-Order Potentials (BOP) based on quantum mechanical theory incorporating both sigma and pi bondings. By analytically deriving the BOP from quantum mechanical theory its transferability to different phases can approach that of quantum mechanical methods. This potential is similar to the original BOP developed by Pettifor (Pettifor_1, Pettifor_2, Pettifor_3) and later updated by Murdick, Zhou, and Ward (Murdick, Ward). Currently, BOP potential files for these systems are provided with LAMMPS: AlCu, CCu, CdTe, CdTeSe, CdZnTe, CuH, GaAs. A sysstem with only a subset of these elements, including a single element (e.g. C or Cu or Al or Ga or Zn or CdZn), can also be modeled by using the appropriate alloy file and assigning all atom types to the singleelement or subset of elements via the pair_coeff command, as discussed below.

The BOP potential consists of three terms:

$$E = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=i_1}^{i_N}\phi_{ij}\left(r_{ij}\right) - \sum_{i=1}^{N}\sum_{j=i_1}^{i_N}\beta_{\sigma,ij}\left(r_{ij}\right)\cdot\Theta_{\sigma,ij} - \sum_{i=1}^{N}\sum_{j=i_1}^{i_N}\beta_{\pi,ij}\left(r_{ij}\right)\cdot\Theta_{\pi,ij} + U_{pr}$$

where phi_ij(r_ij) is a short-range two-body function representing the repulsion between a pair of ion cores, beta_(sigma,ij)(r_ij) and beta_(sigma,ij)(r_ij) are respectively sigma and pi bond ingtegrals, THETA_(sigma,ij) and THETA_(pi,ij) are sigma and pi bond-orders, and U_prom is the promotion energy for sp-valent systems.

The detailed formulas for this potential are given in Ward (Ward); here we provide only a brief description.

The repulsive energy phi_ij(r_ij) and the bond integrals beta_(sigma,ij)(r_ij) and beta_(phi,ij)(r_ij) are functions of the interatomic distance r_ij between atom i and j. Each of these potentials has a smooth cutoff at a radius of r_(cut,ij). These smooth cutoffs ensure stable behavior at situations with high sampling near the cutoff such as melts and surfaces.

The bond-orders can be viewed as environment-dependent local variables that are ij bond specific. The maximum value of the sigma bond-order (THETA_sigma) is 1, while that of the pi bond-order (THETA_pi) is 2, attributing to a maximum value of the total bond-order (THETA_sigma+THETA_pi) of 3. The sigma and pi bond-orders reflect the ubiquitous single-, double-, and triple- bond behavior of chemistry. Their analytical expressions can be derived from tight- binding theory by recursively expanding an inter-site Green's function as a continued fraction. To accurately represent the bonding with a computationally efficient potential formulation suitable for MD simulations, the derived BOP only takes (and retains) the first two levels of the recursive representations for both the sigma and the pi bond-orders. Bond-order terms can be understood in terms of molecular orbital hopping paths based upon the Cyrot-Lackmann theorem (Pettifor_1). The sigma bond-order with a half-full valence shell is used to interpolate the bond-order expressiont that incorporated explicite valance band filling. This pi bond-order expression also contains also contains a three-member ring term that allows implementation of an asymmetric density of states, which helps to either stabilize or destabilize close-packed structures. The pi bond-order includes hopping paths of length 4. This enables the incorporation of dihedral angles effects.

NOTE: Note that unlike for other potentials, cutoffs for BOP potentials are not set in the pair_style or pair_coeff command; they are specified in the BOP potential files themselves. Likewise, the BOP potential files list atomic masses; thus you do not need to use the mass command to specify them. Note that for BOP potentials with hydrogen, you will likely want to set the mass of H atoms to be 10x or 20x larger to avoid having to use a tiny timestep. You can do this by using the mass command after using the pair_coeff command to read the BOP potential file.

One option can be specified as a keyword with the pair_style command.

The *save* keyword gives you the option to calculate in advance and store a set of distances, angles, and derivatives of angles. The default is to not do this, but to calculate them on-the-fly each time they are needed. The former may be faster, but takes more memory. The latter requires less memory, but may be slower. It is best to test this option to optimize the speed of BOP for your particular system configuration.

Only a single pair_coeff command is used with the *bop* style which specifies a BOP potential file, with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of BOP elements to atom types

As an example, imagine the CdTe.bop file has BOP values for Cd and Te. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Cd, and the 4th to be Te, you would use the following pair_coeff command:

```
pair_coeff * * CdTe Cd Cd Cd Te
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Cd arguments map LAMMPS atom types 1,2,3 to the Cd element in the BOP file. The final Te argument maps LAMMPS atom type 4 to the Te element in the BOP file.

BOP files in the *potentials* directory of the LAMMPS distribution have a ".bop" suffix. The potentials are in tabulated form containing pre-tabulated pair functions for phi_ij(r_ij), beta_(sigma,ij)(r_ij), and beta_pi,ij)(r_ij).

The parameters/coefficients format for the different kinds of BOP files are given below with variables matching the formulation of Ward (Ward) and Zhou (Zhou). Each header line containing a ":" is preceded by a blank

line.

No angular table file format:

The parameters/coefficients format for the BOP potentials input file containing pre-tabulated functions of g is given below with variables matching the formulation of Ward (Ward). This format also assumes the angular functions have the formulation of (Ward).

- Line 1: # elements N

The first line is followed by N lines containing the atomic number, mass, and element symbol of each element.

Following the definition of the elements several global variables for the tabulated functions are given.

- Line 1: nr, nBOt (nr is the number of divisions the radius is broken into for function tables and MUST be a factor of 5; nBOt is the number of divisions for the tabulated values of THETA_(S,ij)
- Line 2: delta_1-delta_7 (if all are not used in the particular
- formulation, set unused values to 0.0)

Following this N lines for e_1-e_N containing p_pi.

- Line 3: p_pi (for e_1)
- Line 4: p_pi (for e_2 and continues to e_N)

The next section contains several pair constants for the number of interaction types e_i-e_j, with i=1->N, j=i->N

- Line 1: r_cut (for e_1-e_1 interactions)
- Line 2: c_sigma, a_sigma, c_pi, a_pi
- Line 3: delta_sigma, delta_pi
- Line 4: f_sigma, k_sigma, delta_3 (This delta_3 is similar to that of the previous section but is interaction type dependent)

The next section contains a line for each three body interaction type e_j-e_i-e_k with i=0->N, j=0->N, k=j->N

- Line 1: g_(sigma0), g_(sigma1), g_(sigma2) (These are coefficients for g_(sigma,jik)(THETA_ijk) for e_1-e_1-e_1 interaction. Ward contains the full expressions for the constants as functions of b_(sigma,ijk), p_(sigma,ijk), u_(sigma,ijk))
- Line 2: g_(sigma0), g_(sigma1), g_(sigma2) (for e_1-e_1-e_2)

The next section contains a block for each interaction type for the phi_ij(r_ij). Each block has nr entries with 5 entries per line.

- Line 1: phi(r1), phi(r2), phi(r3), phi(r4), phi(r5) (for the e_1-e_1 interaction type)
- Line 2: phi(r6), phi(r7), phi(r8), phi(r9), phi(r10) (this continues until nr)
- ...
- Line nr/5_1: phi(r1), phi(r2), phi(r3), phi(r4), phi(r5), (for the e_1-e_1 interaction type)

The next section contains a block for each interaction type for the beta_(sigma,ij)(r_ij). Each block has nr entries with 5 entries per line.

- Line 1: beta_sigma(r1), beta_sigma(r2), beta_sigma(r3), beta_sigma(r4), beta_sigma(r5) (for the e_1-e_1 interaction type)
- Line 2: beta_sigma(r6), beta_sigma(r7), beta_sigma(r8), beta_sigma(r9), beta_sigma(r10) (this continues until nr)
- ...
- Line nr/5+1: beta_sigma(r1), beta_sigma(r2), beta_sigma(r3), beta_sigma(r4), beta_sigma(r5) (for the e_1-e_2 interaction type)

The next section contains a block for each interaction type for beta_(pi,ij)(r_ij). Each block has nr entries with 5 entries per line.

- Line 1: beta_pi(r1), beta_pi(r2), beta_pi(r3), beta_pi(r4), beta_pi(r5) (for the e_1-e_1 interaction type)
- Line 2: beta_pi(r6), beta_pi(r7), beta_pi(r8), beta_pi(r9), beta_pi(r10) (this continues until nr)
- ...
- Line nr/5+1: beta_pi(r1), beta_pi(r2), beta_pi(r3), beta_pi(r4), beta_pi(r5) (for the e_1-e_2 interaction type)

The next section contains a block for each interaction type for the THETA_(S,ij)((THETA_(sigma,ij))^(1/2), f_(sigma,ij)). Each block has nBOt entries with 5 entries per line.

- Line 1: THETA_(S,ij)(r1), THETA_(S,ij)(r2), THETA_(S,ij)(r3), THETA_(S,ij)(r4), THETA_(S,ij)(r5) (for the e_1-e_2 interaction type)
- Line 2: THETA_(S,ij)(r6), THETA_(S,ij)(r7), THETA_(S,ij)(r8), THETA_(S,ij)(r9), THETA_(S,ij)(r10) (this continues until nBOt)
- ...
- Line nBOt/5+1: THETA_(S,ij)(r1), THETA_(S,ij)(r2), THETA_(S,ij)(r3), THETA_(S,ij)(r4), THETA_(S,ij)(r5) (for the e_1-e_2 interaction type)

The next section contains a block of N lines for e_1-e_N

- Line 1: delta^mu (for e_1)
- Line 2: delta^mu (for e_2 and repeats to e_N)

The last section contains more constants for e_i-e_j interactions with i=0->N, j=i->N

- Line 1: (A_ij)^(mu*nu) (for e1-e1)
- Line 2: (A_ij)^(mu*nu) (for e1-e2 and repeats as above)

Angular spline table file format:

The parameters/coefficients format for the BOP potentials input file containing pre-tabulated functions of g is given below with variables matching the formulation of Ward (Ward). This format also assumes the angular functions have the formulation of (Zhou).

- Line 1: # elements N

The first line is followed by N lines containing the atomic number, mass, and element symbol of each element.

Following the definition of the elements several global variables for the tabulated functions are given.

- Line 1: nr, ntheta, nBOt (nr is the number of divisions the radius is broken into for function tables and MUST be a factor of 5; ntheta is the power of the power of the spline used to fit the angular function;

nBOt is the number of divisions for the tabulated values of THETA_(S,ij)

- Line 2: delta_1-delta_7 (if all are not used in the particular
- formulation, set unused values to 0.0)

Following this N lines for e_1-e_N containing p_pi.

- Line 3: p_pi (for e_1)
- Line 4: p_pi (for e_2 and continues to e_N)

The next section contains several pair constants for the number of interaction types e_i-e_j, with i=1->N, j=i->N

- Line 1: r_cut (for e_1-e_1 interactions)
- Line 2: c_sigma, a_sigma, c_pi, a_pi
- Line 3: delta_sigma, delta_pi
- Line 4: f_sigma, k_sigma, delta_3 (This delta_3 is similar to that of the previous section but is interaction type dependent)

The next section contains a line for each three body interaction type e_j-e_i-e_k with i=0->N, j=0->N, k=j->N

- Line 1: g0, g1, g2... (These are coefficients for the angular spline of the g_(sigma,jik)(THETA_ijk) for e_1-e_1-e_1 interaction. The function can contain up to 10 term thus 10 constants. The first line can contain up to five constants. If the spline has more than five terms the second line will contain the remaining constants The following lines will then contain the constants for the remainaing g0, g1, g2... (for e_1-e_1-e_2) and the other three body interactions

The rest of the table has the same structure as the previous section (see above).

Angular no-spline table file format:

The parameters/coefficients format for the BOP potentials input file containing pre-tabulated functions of g is given below with variables matching the formulation of Ward (Ward). This format also assumes the angular functions have the formulation of (Zhou).

- Line 1: # elements N

The first two lines are followed by N lines containing the atomic number, mass, and element symbol of each element.

Following the definition of the elements several global variables for the tabulated functions are given.

- Line 1: nr, ntheta, nBOt (nr is the number of divisions the radius is broken into for function tables and MUST be a factor of 5; ntheta is the number of divisions for the tabulated values of the g angular function; nBOt is the number of divisions for the tabulated values of THETA_(S,ij)
- Line 2: delta_1-delta_7 (if all are not used in the particular
- formulation, set unused values to 0.0)

Following this N lines for e_1-e_N containing p_pi.

- Line 3: p_pi (for e_1)
- Line 4: p_pi (for e_2 and continues to e_N)

The next section contains several pair constants for the number of interaction types e_i-e_j, with i=1->N, j=i->N

- Line 1: r_cut (for e_1-e_1 interactions)
- Line 2: c_sigma, a_sigma, c_pi, a_pi
- Line 3: delta_sigma, delta_pi
- Line 4: f_sigma, k_sigma, delta_3 (This delta_3 is similar to that of the previous section but is interaction type dependent)

The next section contains a line for each three body interaction type e_j-e_i-e_k with i=0->N, j=0->N, k=j->N

- Line 1: g(theta1), g(theta2), g(theta3), g(theta4), g(theta5) (for the e_1-e_1-e_1 interaction type)
- Line 2: g(theta6), g(theta7), g(theta8), g(theta9), g(theta10) (this continues until ntheta)
- ...
- Line ntheta/5+1: g(theta1), g(theta2), g(theta3), g(theta4), g(theta5), (for the e_1-e_1-e_2 interaction type)

The rest of the table has the same structure as the previous section (see above).

Mixing, shift, table tail correction, restart:

This pair style does not support the pair_modify mix, shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

These pair styles are part of the MANYBODY package. They are only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

These pair potentials require the newton setting to be "on" for pair interactions.

The CdTe.bop and GaAs.bop potential files provided with LAMMPS (see the potentials directory) are parameterized for metal units. You can use the BOP potential with any LAMMPS units, but you would need to create your own BOP potential file with coefficients listed in the appropriate units if your simulation does not use "metal" units.

Related commands:

pair_coeff

Default:

non-tabulated potential file, a_0 is non-zero.

(Pettifor_1) D.G. Pettifor and I.I. Oleinik, Phys. Rev. B, 59, 8487 (1999).

(Pettifor_2) D.G. Pettifor and I.I. Oleinik, Phys. Rev. Lett., 84, 4124 (2000).

(Pettifor_3) D.G. Pettifor and I.I. Oleinik, Phys. Rev. B, 65, 172103 (2002).

(Murdick) D.A. Murdick, X.W. Zhou, H.N.G. Wadley, D. Nguyen-Manh, R. Drautz, and D.G. Pettifor, Phys. Rev. B, 73, 45206 (2006).

(Ward) D.K. Ward, X.W. Zhou, B.M. Wong, F.P. Doty, and J.A. Zimmerman, Phys. Rev. B, 85,115206 (2012).

(Zhou) X.W. Zhou, D.K. Ward, M. Foster (TBP).

pair_style born command

pair_style born/omp command

pair_style born/gpu command

pair_style born/coul/long command

pair_style born/coul/long/cs command

pair_style born/coul/long/cuda command

pair_style born/coul/long/gpu command

pair_style born/coul/long/omp command

pair_style born/coul/msm command

pair_style born/coul/msm/omp command

pair_style born/coul/wolf command

pair_style born/coul/wolf/gpu command

pair_style born/coul/wolf/omp command

Syntax:

```
pair_style style args
```

- style = *born* or *born/coul/long* or *born/coul/long/cs* or *born/coul/msm* or *born/coul/wolf*
- args = list of arguments for a particular style

```
born args = cutoff
    cutoff = global cutoff for non-Coulombic interactions (distance units)
  born/coul/long or born/coul/long/cs args = cutoff (cutoff2)
    cutoff = global cutoff for non-Coulombic (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
  born/coul/msm args = cutoff (cutoff2)
    cutoff = global cutoff for non-Coulombic (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
  born/coul/wolf args = alpha cutoff (cutoff2)
    alpha = damping parameter (inverse distance units)
    cutoff = global cutoff for non-Coulombic (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

Examples:

```
pair_style born 10.0
pair_coeff * * 6.08 0.317 2.340 24.18 11.51
```

```
pair_coeff 1 1 6.08 0.317 2.340 24.18 11.51

pair_style born/coul/long 10.0
pair_style born/coul/long/cs 10.0
pair_style born/coul/long 10.0 8.0
pair_style born/coul/long/cs 10.0 8.0
pair_coeff * * 6.08 0.317 2.340 24.18 11.51
pair_coeff 1 1 6.08 0.317 2.340 24.18 11.51

pair_style born/coul/msm 10.0
pair_style born/coul/msm 10.0 8.0
pair_coeff * * 6.08 0.317 2.340 24.18 11.51
pair_coeff 1 1 6.08 0.317 2.340 24.18 11.51

pair_style born/coul/wolf 0.25 10.0
pair_style born/coul/wolf 0.25 10.0 9.0
pair_coeff * * 6.08 0.317 2.340 24.18 11.51
pair_coeff 1 1 6.08 0.317 2.340 24.18 11.51
```

Description:

The *born* style computes the Born-Mayer-Huggins or Tosi/Fumi potential described in (Fumi and Tosi), given by

$$E = A \exp\left(\frac{\sigma - r}{\rho}\right) - \frac{C}{r^6} + \frac{D}{r^8} \qquad r < r_c$$

where sigma is an interaction-dependent length parameter, rho is an ionic-pair dependent length parameter, and Rc is the cutoff.

The styles with *coul/long* or *coul/msm* add a Coulombic term as described for the lj/cut pair styles. An additional damping factor is applied to the Coulombic term so it can be used in conjunction with the kspace_style command and its *ewald* or *pppm* of *msm* option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

If one cutoff is specified for the *born/coul/long* and *born/coul/msm* style, it is used for both the A,C,D and Coulombic terms. If two cutoffs are specified, the first is used as the cutoff for the A,C,D terms, and the second is the cutoff for the Coulombic term.

The *born/coul/wolf* style adds a Coulombic term as described for the Wolf potential in the coul/wolf pair style.

Style *born/coul/long/cs* is identical to *born/coul/long* except that a term is added for the core/shell model to allow charges on core and shell particles to be separated by r = 0.0.

Note that these potentials are related to the Buckingham potential.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- A (energy units)

- rho (distance units)
- sigma (distance units)
- C (energy units * distance units^6)
- D (energy units * distance units^8)
- cutoff (distance units)

The second coefficient, rho, must be greater than zero.

The last coefficient is optional. If not specified, the global A,C,D cutoff specified in the pair_style command is used.

For *born/coul/long* and *born/coul/wolf* no Coulombic cutoff can be specified for an individual I,J type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

These styles support the pair_modify shift option for the energy of the exp(), 1/r^6, and 1/r^8 portion of the pair interaction.

The *born/coul/long* pair style supports the pair_modify table option ti tabulate the short-range portion of the long-range Coulombic interaction.

These styles support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

Thess styles writes thei information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These styles can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.

Restrictions:

The *born/coul/long* style is part of the KSPACE package. It is only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_style buck

Default: none

Fumi and Tosi, J Phys Chem Solids, 25, 31 (1964), Fumi and Tosi, J Phys Chem Solids, 25, 45 (1964).

pair_style brownian command

pair_style brownian/omp command

pair_style brownian/poly command

pair_style brownian/poly/omp command

Syntax:

```
pair_style style mu flaglog flagfld cutinner cutoff t_target seed flagHI flagVF
```

- style = *brownian* or *brownian/poly*
- mu = dynamic viscosity (dynamic viscosity units)
- flaglog = 0/1 log terms in the lubrication approximation on/off
- flagfld = 0/1 to include/exclude Fast Lubrication Dynamics effects
- cutinner = inner cutoff distance (distance units)
- cutoff = outer cutoff for interactions (distance units)
- t_target = target temp of the system (temperature units)
- seed = seed for the random number generator (positive integer)
- flagHI (optional) = 0/1 to include/exclude 1/r hydrodynamic interactions
- flagVF (optional) = 0/1 to include/exclude volume fraction corrections in the long-range isotropic terms

Examples:

```
pair_style brownian 1.5 1 1 2.01 2.5 2.0 5878567 (assuming radius = 1)
pair_coeff 1 1 2.05 2.8
pair_coeff * *
```

Description:

Styles *brownian* and *brownain/poly* compute Brownian forces and torques on finite-size particles. The former requires monodisperse spherical particles; the latter allows for polydisperse spherical particles.

These pair styles are designed to be used with either the pair_style lubricate or pair_style lubricateU commands to provide thermostatting when dissipative lubrication forces are acting. Thus the parameters *mu*, *flaglog*, *flagfld*, *cutinner*, and *cutoff* should be specified consistent with the settings in the lubrication pair styles. For details, refer to either of the lubrication pair styles.

The *t_target* setting is used to specify the target temperature of the system. The random number *seed* is used to generate random numbers for the thermostatting procedure.

The *flagHI* and *flagVF* settings are optional. Neither should be used, or both must be defined.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- cutinner (distance units)
- cutoff (distance units)

The two coefficients are optional. If neither is specified, the two cutoffs specified in the pair_style command are used. Otherwise both must be specified.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in this section of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See this section of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the two cutoff distances for this pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style does not support the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

These styles are part of the FLD package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Only spherical monodisperse particles are allowed for pair_style brownian.

Only spherical particles are allowed for pair_style brownian/poly.

Related commands:

pair_coeff, pair_style lubricate, pair_style lubricateU

Default:

The default settings for the optional args are flagHI = 1 and flagVF = 1.

pair_style buck command

pair_style buck/cuda command

pair_style buck/gpu command

pair_style buck/intel command

pair_style buck/kk command

pair_style buck/omp command

pair_style buck/coul/cut command

pair_style buck/coul/cut/cuda command

pair_style buck/coul/cut/gpu command

pair_style buck/coul/cut/intel command

pair_style buck/coul/cut/kk command

pair_style buck/coul/cut/omp command

pair_style buck/coul/long command

pair_style buck/coul/long/cs command

pair_style buck/coul/long/cuda command

pair_style buck/coul/long/gpu command

pair_style buck/coul/long/intel command

pair_style buck/coul/long/kk command

pair_style buck/coul/long/omp command

pair_style buck/coul/msm command

pair_style buck/coul/msm/omp command

Syntax:

```
pair_style style args
```

- style = *buck* or *buck/coul/cut* or *buck/coul/long* or *buck/coul/long/cs* or *buck/coul/msm*
- args = list of arguments for a particular style

```
buck args = cutoff
    cutoff = global cutoff for Buckingham interactions (distance units)
  buck/coul/cut args = cutoff (cutoff2)
    cutoff = global cutoff for Buckingham (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
  buck/coul/long or buck/coul/long/cs args = cutoff (cutoff2)
    cutoff = global cutoff for Buckingham (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
  buck/coul/msm args = cutoff (cutoff2)
    cutoff = global cutoff for Buckingham (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

Examples:

```
pair_style buck 2.5
pair_coeff * * 100.0 1.5 200.0
pair_coeff * * 100.0 1.5 200.0 3.0

pair_style buck/coul/cut 10.0
pair_style buck/coul/cut 10.0 8.0
pair_coeff * * 100.0 1.5 200.0
pair_coeff 1 1 100.0 1.5 200.0 9.0
pair_coeff 1 1 100.0 1.5 200.0 9.0 8.0

pair_style buck/coul/long 10.0
pair_style buck/coul/long/cs 10.0
pair_style buck/coul/long 10.0 8.0
pair_style buck/coul/long/cs 10.0 8.0
pair_coeff * * 100.0 1.5 200.0
pair_coeff 1 1 100.0 1.5 200.0 9.0

pair_style buck/coul/msm 10.0
pair_style buck/coul/msm 10.0 8.0
pair_coeff * * 100.0 1.5 200.0
pair_coeff 1 1 100.0 1.5 200.0 9.0
```

Description:

The *buck* style computes a Buckingham potential (exp/6 instead of Lennard-Jones 12/6) given by

$$E = Ae^{-r/\rho} - \frac{C}{r^6} \qquad r < r_c$$

where rho is an ionic-pair dependent length parameter, and Rc is the cutoff on both terms.

The styles with *coul/cut* or *coul/long* or *coul/msm* add a Coulombic term as described for the lj/cut pair styles. For *buck/coul/long* and *buc/coul/msm*, an additional damping factor is applied to the Coulombic term so it can be used in conjunction with the kspace_style command and its *ewald* or *pppm* or *msm* option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

If one cutoff is specified for the *born/coul/cut* and *born/coul/long* and *born/coul/msm* styles, it is used for both the A,C and Coulombic terms. If two cutoffs are specified, the first is used as the cutoff for the A,C terms, and the second is the cutoff for the Coulombic term.

Style *buck/coul/long/cs* is identical to *buck/coul/long* except that a term is added for the core/shell model to allow charges on core and shell particles to be separated by r = 0.0.

Note that these potentials are related to the Born-Mayer-Huggins potential.

NOTE: For all these pair styles, the terms with A and C are always cutoff. The additional Coulombic term can be cutoff or long-range (no cutoff) depending on whether the style name includes coul/cut or coul/long or coul/msm. If you wish the C/r^6 term to be long-range (no cutoff), then see the pair_style buck/long/coul/long command.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- A (energy units)
- rho (distance units)
- C (energy-distance^6 units)
- cutoff (distance units)
- cutoff2 (distance units)

The second coefficient, rho, must be greater than zero.

The latter 2 coefficients are optional. If not specified, the global A,C and Coulombic cutoffs are used. If only one cutoff is specified, it is used as the cutoff for both A,C and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the A,C and Coulombic cutoffs for this type pair. You cannot specify 2 cutoffs for style *buck*, since it has no Coulombic terms.

For *buck/coul/long* only the LJ cutoff can be specified since a Coulombic cutoff cannot be specified for an individual I,J type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

These styles support the pair_modify shift option for the energy of the exp() and 1/r^6 portion of the pair interaction.

The *buck/coul/long* pair style supports the pair_modify table option to tabulate the short-range portion of the long-range Coulombic interaction.

These styles support the pair_modify tail option for adding long-range tail corrections to energy and pressure for the A,C terms in the pair interaction.

These styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These styles can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.

Restrictions:

The *buck/coul/long* style is part of the KSPACE package. The *buck/coul/long/cs* style is part of the CORESHELL package. They are only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_style born

Default: none

pair_style buck/long/coul/long command

pair_style buck/long/coul/long/omp command

Syntax:

```
pair_style buck/long/coul/long flag_buck flag_coul cutoff (cutoff2)
```

- flag_buck = *long* or *cut*

```
  long = use Kspace long-range summation for the dispersion term 1/r^6
    cut = use a cutoff
```

- flag_coul = *long* or *off*

```
  long = use Kspace long-range summation for the Coulombic term 1/r
    off = omit the Coulombic term
```

- cutoff = global cutoff for Buckingham (and Coulombic if only 1 cutoff) (distance units)
- cutoff2 = global cutoff for Coulombic (optional) (distance units)

Examples:

```
pair_style buck/long/coul/long cut off 2.5
pair_style buck/long/coul/long cut long 2.5 4.0
pair_style buck/long/coul/long long long 4.0
pair_coeff * * 1 1
pair_coeff 1 1 1 3 4
```

Description:

The *buck/long/coul/long* style computes a Buckingham potential (exp/6 instead of Lennard-Jones 12/6) and Coulombic potential, given by

$$E = Ae^{-r/\rho} - \frac{C}{r^6} \qquad r < r_c$$

$$E = \frac{Cq_iq_j}{\epsilon r} \qquad r < r_c$$

Rc is the cutoff. If one cutoff is specified in the pair_style command, it is used for both the Buckingham and Coulombic terms. If two cutoffs are specified, they are used as cutoffs for the Buckingham and Coulombic terms respectively.

The purpose of this pair style is to capture long-range interactions resulting from both attractive 1/r^6 Buckingham and Coulombic 1/r interactions. This is done by use of the *flag_buck* and *flag_coul* settings. The "Ismail paper has more details on when it is appropriate to include long-range 1/r^6 interactions, using this

potential.

If *flag_buck* is set to *long*, no cutoff is used on the Buckingham 1/r^6 dispersion term. The long-range portion can be calculated by using the kspace_style ewald/disp or pppm/disp commands. The specified Buckingham cutoff then determines which portion of the Buckingham interactions are computed directly by the pair potential versus which part is computed in reciprocal space via the Kspace style. If *flag_buck* is set to *cut*, the Buckingham interactions are simply cutoff, as with pair_style buck.

If *flag_coul* is set to *long*, no cutoff is used on the Coulombic interactions. The long-range portion can calculated by using any of several kspace_style command options such as *pppm* or *ewald*. Note that if *flag_buck* is also set to long, then the *ewald/disp* or *pppm/disp* Kspace style needs to be used to perform the long-range calculations for both the Buckingham and Coulombic interactions. If *flag_coul* is set to *off*, Coulombic interactions are not computed.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- A (energy units)
- rho (distance units)
- C (energy-distance^6 units)
- cutoff (distance units)
- cutoff2 (distance units)

The second coefficient, rho, must be greater than zero.

The latter 2 coefficients are optional. If not specified, the global Buckingham and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both Buckingham and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the Buckingham and Coulombic cutoffs for this type pair. Note that if you are using *flag_buck* set to *long*, you cannot specify a Buckingham cutoff for an atom type pair, since only one global Buckingham cutoff is allowed. Similarly, if you are using *flag_coul* set to *long*, you cannot specify a Coulombic cutoff for an atom type pair, since only one global Coulombic cutoff is allowed.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair styles does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This pair style supports the pair_modify shift option for the energy of the exp() and 1/r^6 portion of the pair interaction, assuming *flag_buck* is *cut*.

This pair style does not support the pair_modify shift option for the energy of the Buckingham portion of the pair interaction.

This pair style supports the pair_modify table and table/disp options since they can tabulate the short-range portion of the long-range Coulombic and dispersion interactions.

This pair style write its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style supports the use of the *inner*, *middle*, and *outer* keywords of the run_style respa command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. See the run_style command for details.

Restrictions:

This style is part of the KSPACE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info. Note that the KSPACE package is installed by default.

Related commands:

pair_coeff

Default: none

(Ismail) Ismail, Tsige, In 't Veld, Grest, Molecular Physics (accepted) (2007).

pair_style lj/charmm/coul/charmm command

pair_style lj/charmm/coul/charmm/cuda command

pair_style lj/charmm/coul/charmm/omp command

pair_style lj/charmm/coul/charmm/implicit command

pair_style lj/charmm/coul/charmm/implicit/cuda command

pair_style lj/charmm/coul/charmm/implicit/omp command

pair_style lj/charmm/coul/long command

pair_style lj/charmm/coul/long/cuda command

pair_style lj/charmm/coul/long/gpu command

pair_style lj/charmm/coul/long/intel command

pair_style lj/charmm/coul/long/opt command

pair_style lj/charmm/coul/long/omp command

pair_style lj/charmm/coul/msm command

pair_style lj/charmm/coul/msm/omp command

Syntax:

```
pair_style style args
```

- style = *lj/charmm/coul/charmm* or *lj/charmm/coul/charmm/implicit* or *lj/charmm/coul/long* or *lj/charmm/coul/msm*
- args = list of arguments for a particular style

```
lj/charmm/coul/charmm args = inner outer (inner2) (outer2)
    inner, outer = global switching cutoffs for Lennard Jones (and Coulombic if only 2 args)
    inner2, outer2 = global switching cutoffs for Coulombic (optional)
  lj/charmm/coul/charmm/implicit args = inner outer (inner2) (outer2)
    inner, outer = global switching cutoffs for LJ (and Coulombic if only 2 args)
    inner2, outer2 = global switching cutoffs for Coulombic (optional)
  lj/charmm/coul/long args = inner outer (cutoff)
    inner, outer = global switching cutoffs for LJ (and Coulombic if only 2 args)
    cutoff = global cutoff for Coulombic (optional, outer is Coulombic cutoff if only 2 args)
  lj/charmm/coul/msm args = inner outer (cutoff)
    inner, outer = global switching cutoffs for LJ (and Coulombic if only 2 args)
    cutoff = global cutoff for Coulombic (optional, outer is Coulombic cutoff if only 2 args)
```

Examples:

```
pair_style lj/charmm/coul/charmm 8.0 10.0
pair_style lj/charmm/coul/charmm 8.0 10.0 7.0 9.0
pair_coeff * * 100.0 2.0
pair_coeff 1 1 100.0 2.0 150.0 3.5

pair_style lj/charmm/coul/charmm/implicit 8.0 10.0
pair_style lj/charmm/coul/charmm/implicit 8.0 10.0 7.0 9.0
pair_coeff * * 100.0 2.0
pair_coeff 1 1 100.0 2.0 150.0 3.5

pair_style lj/charmm/coul/long 8.0 10.0
pair_style lj/charmm/coul/long 8.0 10.0 9.0
pair_coeff * * 100.0 2.0
pair_coeff 1 1 100.0 2.0 150.0 3.5

pair_style lj/charmm/coul/msm 8.0 10.0
pair_style lj/charmm/coul/msm 8.0 10.0 9.0
pair_coeff * * 100.0 2.0
pair_coeff 1 1 100.0 2.0 150.0 3.5
```

Description:

The *lj/charmm* styles compute LJ and Coulombic interactions with an additional switching function S(r) that ramps the energy and force smoothly to zero between an inner and outer cutoff. It is a widely used potential in the CHARMM MD code. See (MacKerell) for a description of the CHARMM force field.

$$
\begin{aligned}
E &= LJ(r) && r < r_{\text{in}} \\
&= S(r) * LJ(r) && r_{\text{in}} < r < r_{\text{out}} \\
&= 0 && r > r_{\text{out}} \\
E &= C(r) && r < r_{\text{in}} \\
&= S(r) * C(r) && r_{\text{in}} < r < r_{\text{out}} \\
&= 0 && r > r_{\text{out}} \\
LJ(r) &= 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right] \\
C(r) &= \frac{C q_i q_j}{\epsilon r} \\
S(r) &= \frac{\left[r_{\text{out}}^2 - r^2 \right]^2 \left[r_{\text{out}}^2 + 2r^2 - 3r_{\text{in}}^2 \right]}{\left[r_{\text{out}}^2 - {r_{\text{in}}}^2 \right]^3}
\end{aligned}
$$

Both the LJ and Coulombic terms require an inner and outer cutoff. They can be the same for both formulas or

different depending on whether 2 or 4 arguments are used in the pair_style command. In each case, the inner cutoff distance must be less than the outer cutoff. It it typical to make the difference between the 2 cutoffs about 1.0 Angstrom.

Style *lj/charmm/coul/charmm/implicit* computes the same formulas as style *lj/charmm/coul/charmm* except that an additional 1/r term is included in the Coulombic formula. The Coulombic energy thus varies as 1/r^2. This is effectively a distance-dependent dielectric term which is a simple model for an implicit solvent with additional screening. It is designed for use in a simulation of an unsolvated biomolecule (no explicit water molecules).

Styles *lj/charmm/coul/long* and *lj/charmm/coul/msm* compute the same formulas as style *lj/charmm/coul/charmm* except that an additional damping factor is applied to the Coulombic term, as described for the lj/cut pair styles. Only one Coulombic cutoff is specified for *lj/charmm/coul/long* and *lj/charmm/coul/msm*; if only 2 arguments are used in the pair_style command, then the outer LJ cutoff is used as the single Coulombic cutoff.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- epsilon_14 (energy units)
- sigma_14 (distance units)

Note that sigma is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum at 2^(1/6) sigma.

The latter 2 coefficients are optional. If they are specified, they are used in the LJ formula between 2 atoms of these types which are also first and fourth atoms in any dihedral. No cutoffs are specified because this CHARMM force field does not allow varying cutoffs for individual atom pairs; all pairs use the global cutoff(s) specified in the pair_style command.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon, sigma, epsilon_14, and sigma_14 coefficients for all of the lj/charmm pair styles can be mixed. The default mix value is *arithmetic* to coincide with the usual settings for the CHARMM force field. See the "pair_modify" command for details.

None of the lj/charmm pair styles support the pair_modify shift option, since the Lennard-Jones portion of the pair interaction is smoothed to 0.0 at the cutoff.

The *lj/charmm/coul/long* style supports the pair_modify table option since it can tabulate the short-range portion of the long-range Coulombic interaction.

None of the lj/charmm pair styles support the pair_modify tail option for adding long-range tail corrections to energy and pressure, since the Lennard-Jones portion of the pair interaction is smoothed to 0.0 at the cutoff.

All of the lj/charmm pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

The lj/charmm/coul/long pair style supports the use of the *inner*, *middle*, and *outer* keywords of the run_style respa command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. The other styles only support the *pair* keyword of run_style respa. See the run_style command for details.

Restrictions:

The *lj/charmm/coul/charmm* and *lj/charmm/coul/charmm/implicit* styles are part of the MOLECULE package. The *lj/charmm/coul/long* style is part of the KSPACE package. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info. Note that the MOLECULE and KSPACE packages are installed by default.

Related commands:

pair_coeff

Default: none

(MacKerell) MacKerell, Bashford, Bellott, Dunbrack, Evanseck, Field, Fischer, Gao, Guo, Ha, et al, J Phys Chem, 102, 3586 (1998).

pair_style lj/class2 command

pair_style lj/class2/cuda command

pair_style lj/class2/gpu command

pair_style lj/class2/kk command

pair_style lj/class2/omp command

pair_style lj/class2/coul/cut command

pair_style lj/class2/coul/cut/cuda command

pair_style lj/class2/coul/cut/kk command

pair_style lj/class2/coul/cut/omp command

pair_style lj/class2/coul/long command

pair_style lj/class2/coul/long/cuda command

pair_style lj/class2/coul/long/gpu command

pair_style lj/class2/coul/long/kk command

pair_style lj/class2/coul/long/omp command

Syntax:

```
pair_style style args
```

- style = *lj/class2* or *lj/class2/coul/cut* or *lj/class2/coul/long*
- args = list of arguments for a particular style

```
lj/class2 args = cutoff
    cutoff = global cutoff for class 2 interactions (distance units)
  lj/class2/coul/cut args = cutoff (cutoff2)
    cutoff = global cutoff for class 2 (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
  lj/class2/coul/long args = cutoff (cutoff2)
    cutoff = global cutoff for class 2 (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

Examples:

```
pair_style lj/class2 10.0
pair_coeff * * 100.0 2.5
pair_coeff 1 2* 100.0 2.5 9.0
```

```
pair_style lj/class2/coul/cut 10.0
pair_style lj/class2/coul/cut 10.0 8.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0
pair_coeff 1 1 100.0 3.5 9.0 9.0

pair_style lj/class2/coul/long 10.0
pair_style lj/class2/coul/long 10.0 8.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0
```

Description:

The *lj/class2* styles compute a 6/9 Lennard-Jones potential given by

$$E = \epsilon \left[2 \left(\frac{\sigma}{r} \right)^9 - 3 \left(\frac{\sigma}{r} \right)^6 \right] \qquad r < r_c$$

Rc is the cutoff.

The *lj/class2/coul/cut* and *lj/class2/coul/long* styles add a Coulombic term as described for the lj/cut pair styles.

See (Sun) for a description of the COMPASS class2 force field.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- cutoff1 (distance units)
- cutoff2 (distance units)

The latter 2 coefficients are optional. If not specified, the global class 2 and Coulombic cutoffs are used. If only one cutoff is specified, it is used as the cutoff for both class 2 and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the class 2 and Coulombic cutoffs for this type pair. You cannot specify 2 cutoffs for style *lj/class2*, since it has no Coulombic terms.

For *lj/class2/coul/long* only the class 2 cutoff can be specified since a Coulombic cutoff cannot be specified for an individual I,J type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

If the pair_coeff command is not used to define coefficients for a particular I != J type pair, the mixing rule for epsilon and sigma for all class2 potentials is to use the *sixthpower* formulas documented by the pair_modify command. The pair_modify mix setting is thus ignored for class2 potentials for epsilon and sigma. However it is still followed for mixing the cutoff distance.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/class2 pair styles can be mixed. Epsilon and sigma are always mixed with the value *sixthpower*. The cutoff distance is mixed by whatever option is set by the pair_modify command (default = geometric). See the "pair_modify" command for details.

All of the lj/class2 pair styles support the pair_modify shift option for the energy of the Lennard-Jones portion of the pair interaction.

The *lj/class2/coul/long* pair style does not support the pair_modify table option since a tabulation capability has not yet been added to this potential.

All of the lj/class2 pair styles support the pair_modify tail option for adding a long-range tail correction to the energy and pressure of the Lennard-Jones portion of the pair interaction.

All of the lj/class2 pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

All of the lj/class2 pair styles can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.

Restrictions:

These styles are part of the CLASS2 package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff

Default: none

(Sun) Sun, J Phys Chem B 102, 7338-7364 (1998).

pair_coeff command

Syntax:

```
pair_coeff I J args
```

- I,J = atom types (see asterisk form below)
- args = coefficients for one or more pairs of atom types

Examples:

```
pair_coeff 1 2 1.0 1.0 2.5
pair_coeff 2 * 1.0 1.0
pair_coeff 3* 1*2 1.0 1.0 2.5
pair_coeff * * 1.0 1.0
pair_coeff * * nialhjea 1 1 2
pair_coeff * 3 morse.table ENTRY1
pair_coeff 1 2 lj/cut 1.0 1.0 2.5 (for pair_style hybrid)
```

Description:

Specify the pairwise force field coefficients for one or more pairs of atom types. The number and meaning of the coefficients depends on the pair style. Pair coefficients can also be set in the data file read by the read_data command or in a restart file.

I and J can be specified in one of two ways. Explicit numeric values can be used for each, as in the 1st example above. I <= J is required. LAMMPS sets the coefficients for the symmetric J,I interaction to the same values.

A wildcard asterisk can be used in place of or in conjunction with the I,J arguments to set the coefficients for multiple pairs of atom types. This takes the form "*" or "*n" or "n*" or "m*n". If N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). Note that only type pairs with I <= J are considered; if asterisks imply type pairs where J < I, they are ignored.

Note that a pair_coeff command can override a previous setting for the same I,J pair. For example, these commands set the coeffs for all I,J pairs, then overwrite the coeffs for just the I,J = 2,3 pair:

```
pair_coeff * * 1.0 1.0 2.5
pair_coeff 2 3 2.0 1.0 1.12
```

A line in a data file that specifies pair coefficients uses the exact same format as the arguments of the pair_coeff command in an input script, with the exception of the I,J type arguments. In each line of the "Pair Coeffs" section of a data file, only a single type I is specified, which sets the coefficients for type I interacting with type I. This is because the section has exactly N lines, where N = the number of atom types. For this reason, the wild-card asterisk should also not be used as part of the I argument. Thus in a data file, the line corresponding to the 1st example above would be listed as

```
2 1.0 1.0 2.5
```

For many potentials, if coefficients for type pairs with I != J are not set explicitly by a pair_coeff command, the values are inferred from the I,I and J,J settings by mixing rules; see the pair_modify command for a discussion.

Details on this option as it pertains to individual potentials are described on the doc page for the potential.

Many pair styles, typically for many-body potentials, use tabulated potential files as input, when specifying the pair_coeff command. Potential files provided with LAMMPS are in the potentials directory of the distribution. For some potentials, such as EAM, other archives of suitable files can be found on the Web. They can be used with LAMMPS so long as they are in the format LAMMPS expects, as discussed on the individual doc pages.

When a pair_coeff command using a potential file is specified, LAMMPS looks for the potential file in 2 places. First it looks in the location specified. E.g. if the file is specified as "niu3.eam", it is looked for in the current working directory. If it is specified as "../potentials/niu3.eam", then it is looked for in the potentials directory, assuming it is a sister directory of the current working directory. If the file is not found, it is then looked for in the directory specified by the LAMMPS_POTENTIALS environment variable. Thus if this is set to the potentials directory in the LAMMPS distro, then you can use those files from anywhere on your system, without copying them into your working directory. Environment variables are set in different ways for different shells. Here are example settings for

```
csh, tcsh:
% setenv LAMMPS_POTENTIALS /path/to/lammps/potentials

bash:
% export LAMMPS_POTENTIALS=/path/to/lammps/potentials

Windows:
% set LAMMPS_POTENTIALS="C:\Path to LAMMPS\Potentials
```

The alphabetic list of pair styles defined in LAMMPS is given on the pair_style doc page. They are also given in more compact form in the pair section of this page.

Click on the style to display the formula it computes, arguments specified in the pair_style command, and coefficients specified by the associated pair_coeff command.

Note that there are also additional pair styles (not listed on the pair_style doc page) submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the pair section of this page.

There are also additional accelerated pair styles (not listed on the pair_style doc page) included in the LAMMPS distribution for faster performance on CPUs and GPUs. The list of these with links to the individual styles are given in the pair section of this page.

Restrictions:

This command must come after the simulation box is defined by a read_data, read_restart, or create_box command.

Related commands:

pair_style, pair_modify, read_data, read_restart, pair_write

Default: none

pair_style colloid command

pair_style colloid/gpu command

pair_style colloid/omp command

Syntax:

```
pair_style colloid cutoff
```

- cutoff = global cutoff for colloidal interactions (distance units)

Examples:

```
pair_style colloid 10.0
pair_coeff * *  25 1.0 10.0 10.0
pair_coeff 1 1 144 1.0 0.0 0.0 3.0
pair_coeff 1 2  75.398 1.0 0.0 10.0 9.0
pair_coeff 2 2  39.478 1.0 10.0 10.0 25.0
```

Description:

Style *colloid* computes pairwise interactions between large colloidal particles and small solvent particles using 3 formulas. A colloidal particle has a size > sigma; a solvent particle is the usual Lennard-Jones particle of size sigma.

The colloid-colloid interaction energy is given by

$$U_A = -\frac{A_{cc}}{6}\left[\frac{2a_1a_2}{r^2-(a_1+a_2)^2}+\frac{2a_1a_2}{r^2-(a_1-a_2)^2}+\ln\left(\frac{r^2-(a_1+a_2)^2}{r^2-(a_1-a_2)^2}\right)\right]$$

$$\begin{aligned}U_R = \frac{A_{cc}}{37800}\frac{\sigma^6}{r}\Bigg[& \\ & \frac{r^2-7r\left(a_1+a_2\right)+6\left(a_1^2+7a_1a_2+a_2^2\right)}{\left(r-a_1-a_2\right)^7} \\ & +\frac{r^2+7r\left(a_1+a_2\right)+6\left(a_1^2+7a_1a_2+a_2^2\right)}{\left(r+a_1+a_2\right)^7} \\ & -\frac{r^2+7r\left(a_1-a_2\right)+6\left(a_1^2-7a_1a_2+a_2^2\right)}{\left(r+a_1-a_2\right)^7} \\ & -\frac{r^2-7r\left(a_1-a_2\right)+6\left(a_1^2-7a_1a_2+a_2^2\right)}{\left(r-a_1+a_2\right)^7}\Bigg]\end{aligned}$$

$$U = U_A + U_R, \qquad r < r_c$$

where A_cc is the Hamaker constant, a1 and a2 are the radii of the two colloidal particles, and Rc is the cutoff. This equation results from describing each colloidal particle as an integrated collection of Lennard-Jones particles of size sigma and is derived in (Everaers).

The colloid-solvent interaction energy is given by

$$U = \frac{2\,a^3\,\sigma^3\,A_{cs}}{9\left(a^2-r^2\right)^3}\left[1-\frac{\left(5\,a^6+45\,a^4\,r^2+63\,a^2\,r^4+15\,r^6\right)\sigma^6}{15\left(a-r\right)^6\left(a+r\right)^6}\right], \quad r < r_c$$

where A_cs is the Hamaker constant, a is the radius of the colloidal particle, and Rc is the cutoff. This formula is derived from the colloid-colloid interaction, letting one of the particle sizes go to zero.

The solvent-solvent interaction energy is given by the usual Lennard-Jones formula

$$U = \frac{A_{ss}}{36}\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \quad r < r_c$$

with A_ss set appropriately, which results from letting both particle sizes go to zero.

When used in combination with pair_style yukawa/colloid, the two terms become the so-called DLVO potential, which combines electrostatic repulsion and van der Waals attraction.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- A (energy units)
- sigma (distance units)
- d1 (distance units)
- d2 (distance units)
- cutoff (distance units)

A is the Hamaker energy prefactor and should typically be set as follows:

- A_cc = colloid/colloid = 4 pi^2 = 39.5
- A_cs = colloid/solvent = sqrt(A_cc*A_ss)
- A_ss = solvent/solvent = 144 (assuming epsilon = 1, so that 144/36 = 4)

Sigma is the size of the solvent particle or the constituent particles integrated over in the colloidal particle and should typically be set as follows:

- Sigma_cc = colloid/colloid = 1.0
- Sigma_cs = colloid/solvent = arithmetic mixing between colloid sigma and solvent sigma
- Sigma_ss = solvent/solvent = 1.0 or whatever size the solvent particle is

Thus typically Sigma_cs = 1.0, unless the solvent particle's size != 1.0.

D1 and d2 are particle diameters, so that d1 = 2*a1 and d2 = 2*a2 in the formulas above. Both d1 and d2 must be values >= 0. If d1 > 0 and d2 > 0, then the pair interacts via the colloid-colloid formula above. If d1 = 0 and d2 = 0, then the pair interacts via the solvent-solvent formula. I.e. a d value of 0 is a Lennard-Jones particle of size sigma. If either d1 = 0 or d2 = 0 and the other is larger, then the pair interacts via the colloid-solvent formula.

Note that the diameter of a particular particle type may appear in multiple pair_coeff commands, as it interacts with other particle types. You should insure the particle diameter is specified consistently each time it appears.

The last coefficient is optional. If not specified, the global cutoff specified in the pair_style command is used. However, you typically want different cutoffs for interactions between different particle sizes. E.g. if colloidal particles of diameter 10 are used with solvent particles of diameter 1, then a solvent-solvent cutoff of 2.5 would correspond to a colloid-colloid cutoff of 25. A good rule-of-thumb is to use a colloid-solvent cutoff that is half the big diameter + 4 times the small diameter. I.e. 9 = 5 + 4 for the colloid-solvent cutoff in this case.

NOTE: When using pair_style colloid for a mixture with 2 (or more) widely different particles sizes (e.g. sigma=10 colloids in a background sigam=1 LJ fluid), you will likely want to use these commands for efficiency:

neighbor multi and comm_modify multi.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the A, sigma, d1, and d2 coefficients and cutoff distance for this pair style can be mixed. A is an energy value mixed like a LJ epsilon. D1 and d2 are distance values and are mixed like sigma. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style supports the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This style is part of the COLLOID package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Normally, this pair style should be used with finite-size particles which have a diameter, e.g. see the atom_style sphere command. However, this is not a requirement, since the only definition of particle size is via the pair_coeff parameters for each type. In other words, the physical radius of the particle is ignored. Thus you should insure that the d1,d2 parameters you specify are consistent with the physical size of the particles of that type.

Per-particle polydispersity is not yet supported by this pair style; only per-type polydispersity is enabled via the pair_coeff parameters.

Related commands:

pair_coeff

Default: none

(Everaers) Everaers, Ejtehadi, Phys Rev E, 67, 041710 (2003).

pair_style comb command

pair_style comb/omp command

pair_style comb3 command

Syntax:

```
pair_style comb
pair_style comb3 keyword

keyword = polar
  polar value = polar_on or polar_off = whether or not to include atomic polarization
```

Examples:

```
pair_style comb
pair_coeff * * ../potentials/ffield.comb Si
pair_coeff * * ../potentials/ffield.comb Hf Si O

pair_style comb3 polar_off
pair_coeff * * ../potentials/ffield.comb3 O Cu N C O
```

Description:

Style *comb* computes the second-generation variable charge COMB (Charge-Optimized Many-Body) potential. Style *comb3* computes the third-generation COMB potential. These COMB potentials are described in (COMB) and (COMB3). Briefly, the total energy E_T of a system of atoms is given by

$$E_T = \sum_i [E_i^{self}(q_i) + \sum_{j>i} [E_{ij}^{short}(r_{ij}, q_i, q_j) + E_{ij}^{Coul}(r_{ij}, q_i, q_j)] + E^{polar}(q_i, r_{ij}) + E^{vdW}(r_{ij}) + E^{barr}(q_i) + E^{corr}(r_{ij}, \theta_{jik})]$$

where E_i^{self} is the self-energy of atom i (including atomic ionization energies and electron affinities), E_{ij}^{short} is the bond-order potential between atoms i and j, E_{ij}^{Coul} is the Coulomb interactions, E^{polar} is the polarization term for organic systems (style *comb3* only), E^{vdW} is the van der Waals energy (style *comb3* only), E^{barr} is a charge barrier function, and E^{corr} are angular correction terms.

The COMB potentials (styles *comb* and *comb3*) are variable charge potentials. The equilibrium charge on each atom is calculated by the electronegativity equalization (QEq) method. See Rick for further details. This is implemented by the fix qeq/comb command, which should normally be specified in the input script when running a model with the COMB potential. The fix qeq/comb command has options that determine how often charge equilibration is performed, its convergence criterion, and which atoms are included in the calculation.

Only a single pair_coeff command is used with the *comb* and *comb3* styles which specifies the COMB potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the potential file in the pair_coeff command, where N is the number of LAMMPS atom types.

For example, if your LAMMPS simulation of a $Si/SiO_2/ HfO_2$ interface has 4 atom types, and you want the 1st and last to be Si, the 2nd to be Hf, and the 3rd to be O, and you would use the following pair_coeff command:

```
pair_coeff * * ../potentials/ffield.comb Si Hf O Si
```

The first two arguments must be * * so as to span all LAMMPS atom types. The first and last Si arguments map LAMMPS atom types 1 and 4 to the Si element in the *ffield.comb* file. The second Hf argument maps LAMMPS atom type 2 to the Hf element, and the third O argument maps LAMMPS atom type 3 to the O element in the potential file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *comb* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

For style *comb*, the provided potential file *ffield.comb* contains all currently-available 2nd generation COMB parameterizations: for Si, Cu, Hf, Ti, O, their oxides and Zr, Zn and U metals. For style *comb3*, the potential file *ffield.comb3* contains all currently-available 3rd generation COMB paramterizations: O, Cu, N, C, H, Ti, Zn and Zr. The status of the optimization of the compounds, for example Cu_2O, TiN and hydrocarbons, are given in the following table:

	O	Cu	N	C	H	Ti	Zn	Zr
O	F	F	F	F	F	F	F	F
Cu	F	F	P	F	F	P	F	P
N	F	P	F	M	F	P	P	P
C	F	F	M	F	F	M	M	M
H	F	F	F	F	F	M	M	F
Ti	F	P	P	M	M	F	P	P
Zn	F	F	P	M	M	P	F	P
Zr	F	P	P	M	F	P	P	F

F: Fully optimized
M: Only optimized for dimer molecule
P: in Progress but have it from mixing rule

For style *comb3*, in addition to ffield.comb3, a special parameter file, *lib.comb3*, that is exclusively used for C/O/H systems, will be automatically loaded if carbon atom is detected in LAMMPS input structure. This file must be in your working directory or in the directory pointed to by the environment variable LAMMPS_POTENTIALS, as described on the pair_coeff command doc page.

Keyword *polar* indicates whether the force field includes the atomic polarization. Since the equilibration of the polarization has not yet been implemented, it can only set polar_off at present.

NOTE: You can not use potential file *ffield.comb* with style *comb3*, nor file *ffield.comb3* with style *comb*.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above from values in the potential file.

These pair styles does not support the pair_modify shift, table, and tail options.

These pair styles do not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style, pair_coeff, and fix qeq/comb commands in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

These pair styles are part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

These pair styles requires the newton setting to be "on" for pair interactions.

The COMB potentials in the *ffield.comb* and *ffield.comb3* files provided with LAMMPS (see the potentials directory) are parameterized for metal units. You can use the COMB potential with any LAMMPS units, but you would need to create your own COMB potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

Related commands:

pair_style, pair_coeff, fix_qeq/comb

Default: none

(COMB) T.-R. Shan, B. D. Devine, T. W. Kemper, S. B. Sinnott, and S. R. Phillpot, Phys. Rev. B 81, 125328 (2010)

(COMB3) T. Liang, T.-R. Shan, Y.-T. Cheng, B. D. Devine, M. Noordhoek, Y. Li, Z. Lu, S. R. Phillpot, and S. B. Sinnott, Mat. Sci. & Eng: R 74, 255-279 (2013).

(Rick) S. W. Rick, S. J. Stuart, B. J. Berne, J Chem Phys 101, 6141 (1994).

pair_style coul/cut command

pair_style coul/cut/gpu command

pair_style coul/cut/kk command

pair_style coul/cut/omp command

pair_style coul/debye command

pair_style coul/debye/gpu command

pair_style coul/debye/kk command

pair_style coul/debye/omp command

pair_style coul/dsf command

pair_style coul/dsf/gpu command

pair_style coul/dsf/kk command

pair_style coul/dsf/omp command

pair_style coul/long command

pair_style coul/long/cs command

pair_style coul/long/omp command

pair_style coul/long/gpu command

pair_style coul/long/kk command

pair_style coul/msm command

pair_style coul/msm/omp command

pair_style coul/streitz command

pair_style coul/wolf command

pair_style coul/wolf/kk command

pair_style coul/wolf/omp command

pair_style tip4p/cut command

pair_style tip4p/long command

pair_style tip4p/cut/omp command

pair_style tip4p/long/omp command

Syntax:

```
pair_style coul/cut cutoff
pair_style coul/debye kappa cutoff
pair_style coul/dsf alpha cutoff
pair_style coul/long cutoff
pair_style coul/long/cs cutoff
pair_style coul/long/gpu cutoff
pair_style coul/wolf alpha cutoff
pair_style coul/streitz cutoff keyword alpha
pair_style tip4p/cut otype htype btype atype qdist cutoff
pair_style tip4p/long otype htype btype atype qdist cutoff
```

- cutoff = global cutoff for Coulombic interactions
- kappa = Debye length (inverse distance units)
- alpha = damping parameter (inverse distance units)

Examples:

```
pair_style coul/cut 2.5
pair_coeff * *
pair_coeff 2 2 3.5

pair_style coul/debye 1.4 3.0
pair_coeff * *
pair_coeff 2 2 3.5

pair_style coul/dsf 0.05 10.0
pair_coeff * *

pair_style coul/long 10.0
pair_style coul/long/cs 10.0
pair_coeff * *

pair_style coul/msm 10.0
pair_coeff * *

pair_style coul/wolf 0.2 9.0
pair_coeff * *

pair_style coul/streitz 12.0 ewald
pair_style coul/streitz 12.0 wolf 0.30
pair_coeff * * AlO.streitz Al O
```

```
pair_style tip4p/cut 1 2 7 8 0.15 12.0
pair_coeff * *

pair_style tip4p/long 1 2 7 8 0.15 10.0
pair_coeff * *
```

Description:

The *coul/cut* style computes the standard Coulombic interaction potential given by

$$E = \frac{Cq_iq_j}{\epsilon r} \qquad r < r_c$$

where C is an energy-conversion constant, Qi and Qj are the charges on the 2 atoms, and epsilon is the dielectric constant which can be set by the dielectric command. The cutoff Rc truncates the interaction distance.

Style *coul/debye* adds an additional exp() damping factor to the Coulombic term, given by

$$E = \frac{Cq_iq_j}{\epsilon r}\exp(-\kappa r) \qquad r < r_c$$

where kappa is the Debye length. This potential is another way to mimic the screening effect of a polar solvent.

Style *coul/dsf* computes Coulombic interactions via the damped shifted force model described in Fennell, given by:

$$E = q_iq_j \left[\frac{\mathrm{erfc}(\alpha r)}{r} - \frac{\mathrm{erfc}(\alpha r_c)}{r_c} + \left(\frac{\mathrm{erfc}(\alpha r_c)}{r_c^2} + \frac{2\alpha}{\sqrt{\pi}} \frac{\exp(-\alpha^2 r_c^2)}{r_c} \right) (r - r_c) \right] \qquad r$$

where *alpha* is the damping parameter and erfc() is the complementary error-function. The potential corrects issues in the Wolf model (described below) to provide consistent forces and energies (the Wolf potential is not differentiable at the cutoff) and smooth decay to zero.

Style *coul/wolf* computes Coulombic interactions via the Wolf summation method, described in Wolf, given by:

$$E_i = \frac{1}{2}\sum_{j \neq i} \frac{q_iq_j\mathrm{erfc}(\alpha r_{ij})}{r_{ij}} + \frac{1}{2}\sum_{j \neq i} \frac{q_iq_j\mathrm{erf}(\alpha r_{ij})}{r_{ij}} \qquad r < r_c$$

where *alpha* is the damping parameter, and erc() and erfc() are error-fuction and complementary error-function terms. This potential is essentially a short-range, spherically-truncated, charge-neutralized, shifted, pairwise *1/r* summation. With a manipulation of adding and substracting a self term (for i = j) to the first and second term on the right-hand-side, respectively, and a small enough *alpha* damping parameter, the second term shrinks and the potential becomes a rapidly-converging real-space summation. With a long enough cutoff and small enough alpha parameter, the energy and forces calcluated by the Wolf summation method approach those of the Ewald sum. So it is a means of getting effective long-range interactions with a short-range potential.

Style *coul/streitz* is the Coulomb pair interaction defined as part of the Streitz-Mintmire potential, as described in this paper, in which charge distribution about an atom is modeled as a Slater 1*s* orbital. More details can be found in the referenced paper. To fully reproduce the published Streitz-Mintmire potential, which is a variable charge potential, style *coul/streitz* must be used with pair_style eam/alloy (or some other short-range potential that has been parameterized appropriately) via the pair_style hybrid/overlay command. Likewise, charge equilibration must be performed via the fix qeq/slater command. For example:

```
pair_style hybrid/overlay coul/streitz 12.0 wolf 0.31 eam/alloy
pair_coeff * * coul/streitz AlO.streitz Al O
pair_coeff * * eam/alloy AlO.eam.alloy Al O
fix 1 all qeq/slater 1 12.0 1.0e-6 100 coul/streitz
```

The keyword *wolf* in the coul/streitz command denotes computing Coulombic interactions via Wolf summation. An additional damping parameter is required for the Wolf summation, as described for the coul/wolf potential above. Alternatively, Coulombic interactions can be computed via an Ewald summation. For example:

```
pair_style hybrid/overlay coul/streitz 12.0 ewald eam/alloy
kspace_style ewald 1e-6
```

Keyword *ewald* does not need a damping parameter, but a kspace_style must be defined, which can be style *ewald* or *pppm*. The Ewald method was used in Streitz and Mintmire's original paper, but a Wolf summation offers a speed-up in some cases.

For the fix qeq/slater command, the *qfile* can be a filename that contains QEq parameters as discussed on the fix qeq command doc page. Alternatively *qfile* can be replaced by "coul/streitz", in which case the fix will extract QEq parameters from the coul/streitz pair style itself.

See the examples/strietz directory for an example input script that uses the Streitz-Mintmire potential. The potentials directory has the AlO.eam.alloy and AlO.streitz potential files used by the example.

Note that the Streiz-Mintmire potential is generally used for oxides, but there is no conceptual problem with extending it to nitrides and carbides (such as SiC, TiN). Pair coul/strietz used by itself or with any other pair style such as EAM, MEAM, Tersoff, or LJ in hybrid/overlay mode. To do this, you would need to provide a Streitz-Mintmire parameterizaion for the material being modeled.

Styles *coul/long* and *coul/msm* compute the same Coulombic interactions as style *coul/cut* except that an additional damping factor is applied so it can be used in conjunction with the kspace_style command and its *ewald* or *pppm* option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

Style *coul/long/cs* is identical to *coul/long* except that a term is added for the core/shell model to allow charges on core and shell particles to be separated by r = 0.0.

Styles *tip4p/cut* and *tip4p/long* implement the coulomb part of the TIP4P water model of (Jorgensen), which introduces a massless site located a short distance away from the oxygen atom along the bisector of the HOH

angle. The atomic types of the oxygen and hydrogen atoms, the bond and angle types for OH and HOH interactions, and the distance to the massless charge site are specified as pair_style arguments. Style *tip4p/cut* uses a global cutoff for Coulomb interactions; style *tip4p/long* is for use with a long-range Coulombic solver (Ewald or PPPM).

NOTE: For each TIP4P water molecule in your system, the atom IDs for the O and 2 H atoms must be consecutive, with the O atom first. This is to enable LAMMPS to "find" the 2 H atoms associated with each O atom. For example, if the atom ID of an O atom in a TIP4P water molecule is 500, then its 2 H atoms must have IDs 501 and 502.

See the howto section for more information on how to use the TIP4P pair styles and lists of parameters to set. Note that the neighobr list cutoff for Coulomb interactions is effectively extended by a distance 2*qdist when using the TIP4P pair style, to account for the offset distance of the fictitious charges on O atoms in water molecules. Thus it is typically best in an efficiency sense to use a LJ cutoff >= Coulomb cutoff + 2*qdist, to shrink the size of the neighbor list. This leads to slightly larger cost for the long-range calculation, so you can test the trade-off for your model.

Note that these potentials are designed to be combined with other pair potentials via the pair_style hybrid/overlay command. This is because they have no repulsive core. Hence if they are used by themselves, there will be no repulsion to keep two oppositely charged particles from moving arbitrarily close to each other.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- cutoff (distance units)

For *coul/cut* and *coul/debye*, the cutoff coefficient is optional. If it is not used (as in some of the examples above), the default global value specified in the pair_style command is used.

For *coul/long* and *coul/msm* no cutoff can be specified for an individual I,J type pair via the pair_coeff command. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the cutoff distance for the *coul/cut* style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

The pair_modify shift option is not relevant for these pair styles.

The *coul/long* style supports the pair_modify table option for tabulation of the short-range portion of the long-range Coulombic interaction.

These pair styles do not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

These pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

The *coul/long*, *coul/msm* and *tip4p/long* styles are part of the KSPACE package. The *coul/long/cs* style is part of the CORESHELL package. They are only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_style, hybrid/overlay, kspace_style

Default: none

(Wolf) D. Wolf, P. Keblinski, S. R. Phillpot, J. Eggebrecht, J Chem Phys, 110, 8254 (1999).

(Fennell) C. J. Fennell, J. D. Gezelter, J Chem Phys, 124, 234104 (2006).

(Streitz) F. H. Streitz, J. W. Mintmire, Phys Rev B, 50, 11996-12003 (1994).

pair_style coul/diel command

pair_style coul/diel/omp command

Syntax:

```
pair_style coul/diel cutoff
```

cutoff = global cutoff (distance units)

Examples:

```
pair_style coul/diel 3.5
pair_coeff 1 4 78. 1.375 0.112
```

Description:

Style *coul/diel* computes a Coulomb correction for implict solvent ion interactions in which the dielectric perimittivity is distance dependent. The dielectric permittivity epsilon_D(r) connects to limiting regimes: One limit is defined by a small dielectric permittivity (close to vacuum) at or close to contact seperation between the ions. At larger separations the dielectric permittivity reaches a bulk value used in the regular Coulomb interaction coul/long or coul/cut. The transition is modeled by a hyperbolic function which is incorporated in the Coulomb correction term for small ion separations as follows

$$E = \frac{C q_i q_j}{\epsilon r}\left(\frac{\epsilon}{\epsilon_D(r)} - 1\right) \qquad r < r_c$$

$$\epsilon_D(r) = \frac{5.2+\epsilon}{2} + \frac{\epsilon - 5.2}{2}\tanh\left(\frac{r - r_{me}}{\sigma_e}\right)$$

where r_me is the inflection point of epsilon_D(r) and sigma_e is a slope defining length scale. C is the same Coulomb conversion factor as in the pair_styles coul/cut, coul/long, and coul/debye. In this way the Coulomb interaction between ions is corrected at small distances r. The lower limit of epsilon_D(r->0)=5.2 due to dielectric saturation (Stiles) while the Coulomb interaction reaches its bulk limit by setting epsilon_D(r->\infty)=epsilon, the bulk value of the solvent which is 78 for water at 298K.

Examples of the use of this type of Coulomb interaction include implicit solvent simulations of salt ions (Lenart) and of ionic surfactants (Jusufi). Note that this potential is only reasonable for implicit solvent simulations and in combiantion with coul/cut or coul/long. It is also usually combined with gauss/cut, see (Lenart) or (Jusufi).

The following coefficients must be defined for each pair of atom types via the pair_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- epsilon (no units)
- r_me (distance units)
- sigma_e (distance units)

The global cutoff (r_c) specified in the pair_style command is used.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support parameter mixing. Coefficients must be given explicitly for each type of particle pairs.

This pair style supports the pair_modify shift option for the energy of the Gauss-potential portion of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This style is part of the "user-misc" package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff pair_style gauss/cut

Default: none

(Stiles) Stiles , Hubbard, and Kayser, J Chem Phys, 77, 6189 (1982).

(Lenart) Lenart , Jusufi, and Panagiotopoulos, J Chem Phys, 126, 044509 (2007).

(Jusufi) Jusufi, Hynninen, and Panagiotopoulos, J Phys Chem B, 112, 13783 (2008).

pair_style born/coul/long/cs command

pair_style buck/coul/long/cs command

Syntax:

```
pair_style style args
```

- style = *born/coul/long/cs* or *buck/coul/long/cs*
- args = list of arguments for a particular style

```
born/coul/long/cs args = cutoff (cutoff2)
    cutoff = global cutoff for non-Coulombic (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
  buck/coul/long/cs args = cutoff (cutoff2)
    cutoff = global cutoff for Buckingham (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

Examples:

```
pair_style born/coul/long/cs 10.0 8.0
pair_coeff 1 1 6.08 0.317 2.340 24.18 11.51

pair_style buck/coul/long/cs 10.0
pair_style buck/coul/long/cs 10.0 8.0
pair_coeff * * 100.0 1.5 200.0
pair_coeff 1 1 100.0 1.5 200.0 9.0
```

Description:

These pair styles are designed to be used with the adiabatic core/shell model of (Mitchell and Finchham). See Section_howto 25 of the manual for an overview of the model as implemented in LAMMPS.

These pair styles are identical to the pair_style born/coul/long and pair_style buck/coul/long styles, except they correctly treat the special case where the distance between two charged core and shell atoms in the same core/shell pair approach r = 0.0. This needs special treatment when a long-range solver for Coulombic interactions is also used, i.e. via the kspace_style command.

More specifically, the short-range Coulomb interaction between a core and its shell should be turned off using the special_bonds command by setting the 1-2 weight to 0.0, which works because the core and shell atoms are bonded to each other. This induces a long-range correction approximation which fails at small distances (~< 10e-8). Therefore, the Coulomb term which is used to calculate the correction factor is extended by a minimal distance (r_min = 1.0-6) when the interaction between a core/shell pair is treated, as follows

$$E = \frac{C q_i q_j}{\epsilon(r + r_{min})} \qquad r \to 0$$

where C is an energy-conversion constant, Qi and Qj are the charges on the core and shell, epsilon is the dielectric constant and r_min is the minimal distance.

Restrictions:

These pair styles are part of the CORESHELL package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_style born, pair_style buck

Default: none

(Mitchell and Finchham) Mitchell, Finchham, J Phys Condensed Matter, 5, 1031-1038 (1993).

pair_style lj/cut/dipole/cut command

pair_style lj/cut/dipole/cut/gpu command

pair_style lj/cut/dipole/cut/omp command

pair_style lj/sf/dipole/sf command

pair_style lj/sf/dipole/sf/gpu command

pair_style lj/sf/dipole/sf/omp command

pair_style lj/cut/dipole/long command

pair_style lj/long/dipole/long command

Syntax:

```
pair_style lj/cut/dipole/cut cutoff (cutoff2)
pair_style lj/sf/dipole/sf cutoff (cutoff2)
pair_style lj/cut/dipole/long cutoff (cutoff2)
pair_style lj/long/dipole/long flag_lj flag_coul cutoff (cutoff2)
```

- cutoff = global cutoff LJ (and Coulombic if only 1 arg) (distance units)
- cutoff2 = global cutoff for Coulombic and dipole (optional) (distance units)
- flag_lj = *long* or *cut* or *off*

```
  long = use long-range damping on dispersion 1/r^6 term
    cut = use a cutoff on dispersion 1/r^6 term
    off = omit disperion 1/r^6 term entirely
```

- flag_coul = *long* or *off*

```
  long = use long-range damping on Coulombic 1/r and point-dipole terms
    off = omit Coulombic and point-dipole terms entirely
```

Examples:

```
pair_style lj/cut/dipole/cut 10.0
pair_coeff * * 1.0 1.0
pair_coeff 2 3 1.0 1.0 2.5 4.0

pair_style lj/sf/dipole/sf 9.0
pair_coeff * * 1.0 1.0
pair_coeff 2 3 1.0 1.0 2.5 4.0

pair_style lj/cut/dipole/long 10.0
pair_coeff * * 1.0 1.0
pair_coeff 2 3 1.0 1.0 2.5 4.0

pair_style lj/long/dipole/long long long 3.5 10.0
pair_coeff * * 1.0 1.0
pair_coeff 2 3 1.0 1.0 2.5 4.0
```

Description:

Style *lj/cut/dipole/cut* computes interactions between pairs of particles that each have a charge and/or a point dipole moment. In addition to the usual Lennard-Jones interaction between the particles (Elj) the charge-charge (Eqq), charge-dipole (Eqp), and dipole-dipole (Epp) interactions are computed by these formulas for the energy (E), force (F), and torque (T) between particles I and J.

$$
\begin{aligned}
E_{LJ} &= 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right] \\
E_{qq} &= \frac{q_i q_j}{r} \\
E_{qp} &= \frac{q}{r^3} (p \bullet \vec{r}) \\
E_{pp} &= \frac{1}{r^3} (\vec{p_i} \bullet \vec{p_j}) - \frac{3}{r^5} (\vec{p_i} \bullet \vec{r}) (\vec{p_j} \bullet \vec{r})
\end{aligned}
$$

$$
\begin{aligned}
F_{qq} &= \frac{q_i q_j}{r^3} \vec{r} \\
F_{qp} &= -\frac{q}{r^3} \vec{p} + \frac{3q}{r^5} (\vec{p} \bullet \vec{r}) \vec{r} \\
F_{pp} &= \frac{3}{r^5} (\vec{p_i} \bullet \vec{p_j}) \vec{r} - \frac{15}{r^7} (\vec{p_i} \bullet \vec{r}) (\vec{p_j} \bullet \vec{r}) \vec{r} + \frac{3}{r^5} \left[(\vec{p_j} \bullet \vec{r}) \vec{p_i} + (\vec{p_i} \bullet \vec{r}) \vec{p_j} \right]
\end{aligned}
$$

$$
\begin{aligned}
T_{pq} = T_{ij} &= \frac{q_j}{r^3} (\vec{p_i} \times \vec{r}) \\
T_{qp} = T_{ji} &= -\frac{q_i}{r^3} (\vec{p_j} \times \vec{r}) \\
T_{pp} = T_{ij} &= -\frac{1}{r^3} (\vec{p_i} \times \vec{p_j}) + \frac{3}{r^5} (\vec{p_j} \bullet \vec{r}) (\vec{p_i} \times \vec{r}) \\
T_{pp} = T_{ji} &= -\frac{1}{r^3} (\vec{p_j} \times \vec{p_i}) + \frac{3}{r^5} (\vec{p_i} \bullet \vec{r}) (\vec{p_j} \times \vec{r})
\end{aligned}
$$

where qi and qj are the charges on the two particles, pi and pj are the dipole moment vectors of the two particles, r is their separation distance, and the vector r = Ri - Rj is the separation vector between the two particles. Note that Eqq and Fqq are simply Coulombic energy and force, Fij = -Fji as symmetric forces, and Tij != -Tji since the torques do not act symmetrically. These formulas are discussed in (Allen) and in (Toukmaji).

Style *lj/sf/dipole/sf* computes "shifted-force" interactions between pairs of particles that each have a charge and/or a point dipole moment. In general, a shifted-force potential is a (sligthly) modified potential containing extra terms that make both the energy and its derivative go to zero at the cutoff distance; this removes (cutoff-related) problems in energy conservation and any numerical instability in the equations of motion (Allen). Shifted-force interactions for the Lennard-Jones (E_LJ), charge-charge (Eqq), charge-dipole (Eqp), dipole-charge (Epq) and dipole-dipole (Epp) potentials are computed by these formulas for the energy (E), force (F), and torque (T) between particles I and J:

$$
\begin{aligned}
E_{LJ} &= 4\epsilon\left\{\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right]+\left[6\left(\frac{\sigma}{r_c}\right)^{12}-3\left(\frac{\sigma}{r_c}\right)^{6}\right]\left(\frac{r}{r_c}\right)^{2}-7\left(\frac{\sigma}{r_c}\right)^{12}+4\left(\right.\right. \\
E_{qq} &= \frac{q_i q_j}{r}\left(1-\frac{r}{r_c}\right)^{2} \\
E_{pq} &= E_{ji}=-\frac{q}{r^3}\left[1-3\left(\frac{r}{r_c}\right)^{2}+2\left(\frac{r}{r_c}\right)^{3}\right](\vec{p}\bullet\vec{r}) \\
E_{qp} &= E_{ij}=\frac{q}{r^3}\left[1-3\left(\frac{r}{r_c}\right)^{2}+2\left(\frac{r}{r_c}\right)^{3}\right](\vec{p}\bullet\vec{r}) \\
E_{pp} &= \left[1-4\left(\frac{r}{r_c}\right)^{3}+3\left(\frac{r}{r_c}\right)^{4}\right]\left[\frac{1}{r^3}(\vec{p_i}\bullet\vec{p_j})-\frac{3}{r^5}(\vec{p_i}\bullet\vec{r})(\vec{p_j}\bullet\vec{r})\right]
\end{aligned}
$$

$$
\begin{aligned}
F_{LJ} &= \left\{\left[48\epsilon\left(\frac{\sigma}{r}\right)^{12}-24\epsilon\left(\frac{\sigma}{r}\right)^{6}\right]\frac{1}{r^2}-\left[48\epsilon\left(\frac{\sigma}{r_c}\right)^{12}-24\epsilon\left(\frac{\sigma}{r_c}\right)^{6}\right]\frac{1}{r_c^2}\right\}\vec{r} \\
F_{qq} &= \frac{q_i q_j}{r}\left(\frac{1}{r^2}-\frac{1}{r_c^2}\right)\vec{r} \\
F_{pq} &= F_{ij}=-\frac{3q}{r^5}\left[1-\left(\frac{r}{r_c}\right)^{2}\right](\vec{p}\bullet\vec{r})\vec{r}+\frac{q}{r^3}\left[1-3\left(\frac{r}{r_c}\right)^{2}+2\left(\frac{r}{r_c}\right)^{3}\right]\vec{p} \\
F_{qp} &= F_{ij}=\frac{3q}{r^5}\left[1-\left(\frac{r}{r_c}\right)^{2}\right](\vec{p}\bullet\vec{r})\vec{r}-\frac{q}{r^3}\left[1-3\left(\frac{r}{r_c}\right)^{2}+2\left(\frac{r}{r_c}\right)^{3}\right]\vec{p} \\
F_{pp} &= \frac{3}{r^5}\left\{\left[1-\left(\frac{r}{r_c}\right)^{4}\right]\left[(\vec{p_i}\bullet\vec{p_j})-\frac{3}{r^2}(\vec{p_i}\bullet\vec{r})(\vec{p_j}\bullet\vec{r})\right]\vec{r}+\right. \\
&\quad \left[1-4\left(\frac{r}{r_c}\right)^{3}+3\left(\frac{r}{r_c}\right)^{4}\right]\left[(\vec{p_j}\bullet\vec{r})\vec{p_i}+(\vec{p_i}\bullet\vec{r})\vec{p_j}-\frac{2}{r^2}(\vec{p_i}\bullet\vec{r})(\vec{p_j}\bullet\vec{r})\vec{r}\right]
\end{aligned}
$$

$$
\begin{aligned}
T_{pq} = T_{ij} &= \frac{q_j}{r^3}\left[1 - 3\left(\frac{r}{r_c}\right)^2 + 2\left(\frac{r}{r_c}\right)^3\right](\vec{p_i} \times \vec{r}) \\
T_{qp} = T_{ji} &= -\frac{q_i}{r^3}\left[1 - 3\left(\frac{r}{r_c}\right)^2 + 2\left(\frac{r}{r_c}\right)^3\right](\vec{p_j} \times \vec{r}) \\
T_{pp} = T_{ij} &= -\frac{1}{r^3}\left[1 - 4\left(\frac{r}{r_c}\right)^3 + e3\left(\frac{r}{r_c}\right)^4\right](\vec{p_i} \times \vec{p_j}) + \\
&\quad \frac{3}{r^5}\left[1 - 4\left(\frac{r}{r_c}\right)^3 + 3\left(\frac{r}{r_c}\right)^4\right](\vec{p_j} \bullet \vec{r})(\vec{p_i} \times \vec{r}) \\
T_{pp} = T_{ji} &= -\frac{1}{r^3}\left[1 - 4\left(\frac{r}{r_c}\right)^3 + 3\left(\frac{r}{r_c}\right)^4\right](\vec{p_j} \times \vec{p_i}) + \\
&\quad \frac{3}{r^5}\left[1 - 4\left(\frac{r}{r_c}\right)^3 + 3\left(\frac{r}{r_c}\right)^4\right](\vec{p_i} \bullet \vec{r})(\vec{p_j} \times \vec{r})
\end{aligned}
$$

where epsilon and sigma are the standard LJ parameters, r_c is the cutoff, qi and qj are the charges on the two particles, pi and pj are the dipole moment vectors of the two particles, r is their separation distance, and the vector r = Ri - Rj is the separation vector between the two particles. Note that Eqq and Fqq are simply Coulombic energy and force, Fij = -Fji as symmetric forces, and Tij != -Tji since the torques do not act symmetrically. The shifted-force formula for the Lennard-Jones potential is reported in (Stoddard). The original (unshifted) formulas for the electrostatic potentials, forces and torques can be found in (Price). The shifted-force electrostatic potentials have been obtained by applying equation 5.13 of (Allen). The formulas for the corresponding forces and torques have been obtained by applying the 'chain rule' as in appendix C.3 of (Allen).

If one cutoff is specified in the pair_style command, it is used for both the LJ and Coulombic (q,p) terms. If two cutoffs are specified, they are used as cutoffs for the LJ and Coulombic (q,p) terms respectively.

Style *lj/cut/dipole/long* computes long-range point-dipole interactions as discussed in (Toukmaji). Dipole-dipole, dipole-charge, and charge-charge interactions are all supported, along with the standard 12/6 Lennard-Jones interactions, which are computed with a cutoff. A kspace_style must be defined to use this pair style. Currently, only kspace_style ewald/disp support long-range point-dipole interactions.

Style *lj/long/dipole/long* also computes point-dipole interactions as discussed in (Toukmaji). Long-range dipole-dipole, dipole-charge, and charge-charge interactions are all supported, along with the standard 12/6 Lennard-Jones interactions. LJ interactions can be cutoff or long-ranged.

For style *lj/long/dipole/long*, if *flag_lj* is set to *long*, no cutoff is used on the LJ 1/r^6 dispersion term. The long-range portion is calculated by using the kspace_style ewald_disp command. The specified LJ cutoff then determines which portion of the LJ interactions are computed directly by the pair potential versus which part is computed in reciprocal space via the Kspace style. If *flag_lj* is set to *cut*, the LJ interactions are simply cutoff, as with pair_style lj/cut. If *flag_lj* is set to *off*, LJ interactions are not computed at all.

If *flag_coul* is set to *long*, no cutoff is used on the Coulombic or dipole interactions. The long-range portion is calculated by using *ewald_disp* of the kspace_style command. If *flag_coul* is set to *off*, Coulombic and dipole interactions are not computed at all.

Atoms with dipole moments should be integrated using the fix nve/sphere update dipole command to rotate the dipole moments. The *omega* option on the fix langevin command can be used to thermostat the rotational motion. The compute temp/sphere command can be used to monitor the temperature, since it includes rotational degrees of freedom. The atom_style dipole command should be used since it defines the point dipoles and their rotational state. The magnitude of the dipole moment for each type of particle can be defined by the dipole command or in the "Dipoles" section of the data file read in by the read_data command. Their initial orientation can be defined by the set dipole command or in the "Atoms" section of the data file.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- cutoff1 (distance units)
- cutoff2 (distance units)

The latter 2 coefficients are optional. If not specified, the global LJ and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both LJ and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the LJ and Coulombic cutoffs for this type pair.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distances for this pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

For atom type pairs I,J and I != J, the A, sigma, d1, and d2 coefficients and cutoff distance for this pair style can be mixed. A is an energy value mixed like a LJ epsilon. D1 and d2 are distance values and are mixed like sigma. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style does not support the pair_modify shift option for the energy of the Lennard-Jones portion of the pair interaction; such energy goes to zero at the cutoff by construction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

The *lj/cut/dipole/cut*, *lj/cut/dipole/long*, and *lj/long/dipole/long* styles are part of the DIPOLE package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The *lj/sf/dipole/sf* style is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Using dipole pair styles with *electron* units is not currently supported.

Related commands:

pair_coeff

Default: none

(Allen) Allen and Tildesley, Computer Simulation of Liquids, Clarendon Press, Oxford, 1987.

(Toukmaji) Toukmaji, Sagui, Board, and Darden, J Chem Phys, 113, 10913 (2000).

(Stoddard) Stoddard and Ford, Phys Rev A, 8, 1504 (1973).

(Price) Price, Stone and Alderton, Mol Phys, 52, 987 (1984).

pair_style dpd command

pair_style dpd/gpu command

pair_style dpd/omp command

pair_style dpd/tstat command

pair_style dpd/tstat/gpu command

pair_style dpd/tstat/omp command

Syntax:

```
pair_style dpd T cutoff seed
pair_style dpd/tstat Tstart Tstop cutoff seed
```

- T = temperature (temperature units)
- Tstart,Tstop = desired temperature at start/end of run (temperature units)
- cutoff = global cutoff for DPD interactions (distance units)
- seed = random # seed (positive integer)

Examples:

```
pair_style dpd 1.0 2.5 34387
pair_coeff * * 3.0 1.0
pair_coeff 1 1 3.0 1.0 1.0

pair_style dpd/tstat 1.0 1.0 2.5 34387
pair_coeff * * 1.0
pair_coeff 1 1 1.0 1.0
```

Description:

Style *dpd* computes a force field for dissipative particle dynamics (DPD) following the exposition in (Groot).

Style *dpd/tstat* invokes a DPD thermostat on pairwise interactions, which is equivalent to the non-conservative portion of the DPD force field. This pair-wise thermostat can be used in conjunction with any pair style, and in leiu of per-particle thermostats like fix langevin or ensemble thermostats like Nose Hoover as implemented by fix nvt. To use *dpd/stat* as a thermostat for another pair style, use the pair_style hybrid/overlay command to compute both the desired pair interaction and the thermostat for each pair of particles.

For style *dpd*, the force on atom I due to atom J is given as a sum of 3 terms

$$
\begin{aligned}
\vec{f} &= (F^C + F^D + F^R)\hat{r_{ij}} \qquad r < r_c \\
F^C &= Aw(r) \\
F^D &= -\gamma w^2(r)(\hat{r_{ij}} \bullet \vec{v_{ij}}) \\
F^R &= \sigma w(r)\alpha(\Delta t)^{-1/2} \\
w(r) &= 1 - r/r_c
\end{aligned}
$$

where Fc is a conservative force, Fd is a dissipative force, and Fr is a random force. Rij is a unit vector in the direction Ri - Rj, Vij is the vector difference in velocities of the two atoms = Vi - Vj, alpha is a Gaussian random number with zero mean and unit variance, dt is the timestep size, and w(r) is a weighting factor that varies between 0 and 1. Rc is the cutoff. Sigma is set equal to sqrt(2 Kb T gamma), where Kb is the Boltzmann constant and T is the temperature parameter in the pair_style command.

For style *dpd/tstat*, the force on atom I due to atom J is the same as the above equation, except that the conservative Fc term is dropped. Also, during the run, T is set each timestep to a ramped value from Tstart to Tstop.

For style *dpd*, the pairwise energy associated with style *dpd* is only due to the conservative force term Fc, and is shifted to be zero at the cutoff distance Rc. The pairwise virial is calculated using all 3 terms. For style *dpd/tstat* there is no pairwise energy, but the last two terms of the formula make a contribution to the virial.

For style *dpd*, the following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- A (force units)
- gamma (force/velocity units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global DPD cutoff is used. Note that sigma is set equal to sqrt(2 T gamma), where T is the temperature set by the pair_style command so it does not need to be specified.

For style *dpd/tstat*, the coefficiencts defined for each pair of atoms types via the pair_coeff command is the same, except that A is not included.

The GPU-accelerated versions of these styles are implemented based on the work of (Afshar) and (Phillips).

NOTE: If you are modeling DPD polymer chains, you may want to use the pair_style srp command in conjuction with these pair styles. It is a soft segmental repulsive potential (SRP) that can prevent DPD polymer chains from crossing each other.

NOTE: The virial calculation for pressure when using this pair style includes all the components of force listed above, including the random force.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

These pair styles do not support the pair_modify shift option for the energy of the pair interaction. Note that as discussed above, the energy due to the conservative Fc term is already shifted to be 0.0 at the cutoff distance Rc.

The pair_modify table option is not relevant for these pair styles.

These pair style do not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

These pair styles writes their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file. Note that the user-specified random number seed is stored in the restart file, so when a simulation is restarted, each processor will re-initialize its random number generator the same way it did initially. This means the random forces will be random, but will not be the same as they would have been if the original simulation had continued past the restart time.

These pair styles can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.

The *dpd/tstat* style can ramp its target temperature over multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

Restrictions:

The default frequency for rebuilding neighbor lists is every 10 steps (see the neigh_modify command). This may be too infrequent for style *dpd* simulations since particles move rapidly and can overlap by large amounts. If this setting yields a non-zero number of "dangerous" reneighborings (printed at the end of a simulation), you should experiment with forcing reneighboring more often and see if system energies/trajectories change.

These pair styles requires you to use the comm_modify vel yes command so that velocites are stored by ghost atoms.

These pair styles will not restart exactly when using the read_restart command, though they should provide statistically similar results. This is because the forces they compute depend on atom velocities. See the read_restart command for more details.

Related commands:

pair_coeff, fix nvt, fix langevin, pair_style srp

Default: none

(Groot) Groot and Warren, J Chem Phys, 107, 4423-35 (1997).

(Afshar) Afshar, F. Schmid, A. Pishevar, S. Worley, Comput Phys Comm, 184, 1119-1128 (2013).

(Phillips) C. L. Phillips, J. A. Anderson, S. C. Glotzer, Comput Phys Comm, 230, 7191-7201 (2011).

pair_style dpd/conservative command

Syntax:

```
pair_style dpd/conservative cutoff
```

- cutoff = global cutoff for DPD interactions (distance units)

Examples:

```
pair_style dpd/conservative 2.5
pair_coeff * * 3.0 2.5
pair_coeff 1 1 3.0
```

Description:

Style *dpd/conservative* computes the conservative force for dissipative particle dynamics (DPD). The conservative force on atom I due to atom J is given by

$$F^C = A\omega_{ij}$$ 

where the weighting factor, omega_ij, varies between 0 and 1, and is chosen to have the following functional form:

$$\omega_{ij} = 1 - \frac{r_{ij}}{r_c}$$

where Rij is a unit vector in the direction Ri - Rj, and Rc is the cutoff. Note that alternative definitions of the weighting function exist, but would have to be implemented as a separate pair style command.

Style *dpd/conservative* differs from the other dpd styles in that the dissipative and random forces are not computed within the pair style.

For style *dpd/conservative*, the pairwise energy is due only to the conservative force term Fc, and is shifted to be zero at the cutoff distance Rc. The pairwise virial is calculated using only the conservative term.

Style *dpd/conservative* requires the following coefficients to be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- A (force units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global DPD cutoff is used.

Restrictions:

The pair style *dpd/conservative* is only available if LAMMPS is built with the USER-DPD package.

Related commands:

pair_coeff, pair_dpd

Default: none

pair_style dpd/fdt command

pair_style dpd/fdt/energy command

Syntax:

```
pair_style style args
```

- style = *dpd/fdt* or *dpd/fdt/energy*
- args = list of arguments for a particular style

```
dpd/fdt args = T cutoff seed
    T = temperature (temperature units)
    cutoff = global cutoff for DPD interactions (distance units)
    seed = random # seed (positive integer)
  dpd/fdt/energy args = cutoff seed
    cutoff = global cutoff for DPD interactions (distance units)
    seed = random # seed (positive integer)
```

Examples:

```
pair_style dpd/fdt 300.0 2.5 34387
pair_coeff * * 3.0 1.0 2.5

pair_style dpd/fdt/energy 2.5 34387
pair_coeff * * 3.0 1.0 0.1 2.5
```

Description:

Styles *dpd/fdt* and *dpd/fdt/energy* set the fluctuation-dissipation theorem parameters and compute the conservative force for dissipative particle dynamics (DPD). The conservative force on atom I due to atom J is given by

$$F^C = A\omega_{ij}$$ 

where the weighting factor, omega_ij, varies between 0 and 1, and is chosen to have the following functional form:

$$\omega_{ij} = 1 - \frac{r_{ij}}{r_c}$$

where Rij is a unit vector in the direction Ri - Rj, and Rc is the cutoff. Note that alternative definitions of the weighting function exist, but would have to be implemented as a separate pair style command.

These pair style differ from the other dpd styles in that the dissipative and random forces are not computed within the pair style. This style can be combined with the fix shardlow to perform the stochastic integration of the dissipative and random forces through the Shardlow splitting algorithm approach.

The pairwise energy associated with styles *dpd/fdt* and *dpd/fdt/energy* is only due to the conservative force term Fc, and is shifted to be zero at the cutoff distance Rc. The pairwise virial is calculated using only the conservative term.

For style *dpd/fdt*, the fluctuation-dissipation theorem defines gamma to be set equal to sigma*sigma/(2 T), where T is the set point temperature specified as a pair style parameter in the above examples. This style can be combined with fix shardlow to perform DPD simulations under isothermal and isobaric conditions (see (Lisal)). The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- A (force units)
- sigma (force*time^(1/2) units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global DPD cutoff is used.

For style *dpd/fdt/energy*, the fluctuation-dissipation theorem defines gamma to be set equal to sigma*sigma/(2 dpdTheta), where dpdTheta is the average internal temperature for the pair. Furthermore, the fluctuation-dissipation defines alpha*alpha to be set equal to 2*kB*kappa, where kappa is the mesoparticle thermal conductivity parameter. This style can be combined with fix shardlow to perform DPD simulations under isoenergetic and isoenthalpic conditions (see (Lisal)). The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- A (force units)
- sigma (force*time^(1/2) units)
- kappa (1/time units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global DPD cutoff is used.

For style *dpd/fdt/energy*, the particle internal temperature is related to the particle internal energy through a mesoparticle equation of state. Thus, an an additional fix eos must be specified.

Restrictions:

Pair styles *dpd/fdt* and *dpd/fdt/energy* are only available if LAMMPS is built with the USER-DPD package.

Pair styles *dpd/fdt* and *dpd/fdt/energy* require use of the communicate vel yes option so that velocites are stored by ghost atoms.

Pair style *dpd/fdt/energy* requires atom_style dpd to be used in order to properly account for the particle internal energies and temperatures.

Related commands:

pair_coeff, fix shardlow

Default: none

(Lisal) M. Lisal, J.K. Brennan, J. Bonet Avalos, "Dissipative particle dynamics as isothermal, isobaric, isoenergetic, and isoenthalpic conditions using Shardlow-like splitting algorithms.", J. Chem. Phys., 135, 204105 (2011).

pair_style dsmc command

Syntax:

```
pair_style dsmc max_cell_size seed weighting Tref Nrecompute Nsample
```

- max_cell_size = global maximum cell size for DSMC interactions (distance units)
- seed = random # seed (positive integer)
- weighting = macroparticle weighting
- Tref = reference temperature (temperature units)
- Nrecompute = recompute v*sigma_max every this many timesteps (timesteps)
- Nsample = sample this many times in recomputing v*sigma_max

Examples:

```
pair_style dsmc 2.5 34387 10 1.0 100 20
pair_coeff * * 1.0
pair_coeff 1 1 1.0
```

Description:

Style *dsmc* computes collisions between pairs of particles for a direct simulation Monte Carlo (DSMC) model following the exposition in (Bird). Each collision resets the velocities of the two particles involved. The number of pairwise collisions for each pair or particle types and the length scale within which they occur are determined by the parameters of the pair_style and pair_coeff commands.

Stochastic collisions are performed using the variable hard sphere (VHS) approach, with the user-defined *max_cell_size* value used as the maximum DSMC cell size, and reference cross-sections for collisions given using the pair_coeff command.

There is no pairwise energy or virial contributions associated with this pair style.

The following coefficient must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- sigma (area units, i.e. distance-squared)

The global DSMC *max_cell_size* determines the maximum cell length used in the DSMC calculation. A structured mesh is overlayed on the simulation box such that an integer number of cells are created in each direction for each processor's sub-domain. Cell lengths are adjusted up to the user-specified maximum cell size.

To perform a DSMC simulation with LAMMPS, several additional options should be set in your input script, though LAMMPS does not check for these settings.

Since this pair style does not compute particle forces, you should use the "fix nve/noforce" time integration fix for the DSMC particles, e.g.

```
fix 1 all nve/noforce
```

This pair style assumes that all particles will communicated to neighboring processors every timestep as they move. This makes it possible to perform all collisions between pairs of particles that are on the same processor.

To ensure this occurs, you should use these commands:

```
neighbor 0.0 bin
neigh_modify every 1 delay 0 check no
atom_modify sort 0 0.0
communicate single cutoff 0.0
```

These commands ensure that LAMMPS communicates particles to neighboring processors every timestep and that no ghost atoms are created. The output statistics for a simulation run should indicate there are no ghost particles or neighbors.

In order to get correct DSMC collision statistics, users should specify a Gaussian velocity distribution when populating the simulation domain. Note that the default velocity distribution is uniform, which will not give good DSMC collision rates. Specify "dist gaussian" when using the velocity command as in the following:

```
velocity all create 594.6 87287 loop geom dist gaussian
```

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This pair style does not support the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file. Note that the user-specified random number seed is stored in the restart file, so when a simulation is restarted, each processor will re-initialize its random number generator the same way it did initially. This means the random forces will be random, but will not be the same as they would have been if the original simulation had continued past the restart time.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This style is part of the MC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, fix nve/noforce, neigh_modify, neighbor, comm_modify

Default: none

(Bird) G. A. Bird, "Molecular Gas Dynamics and the Direct Simulation of Gas Flows" (1994).

pair_style eam command

pair_style eam/cuda command

pair_style eam/gpu command

pair_style eam/kk command

pair_style eam/omp command

pair_style eam/opt command

pair_style eam/alloy command

pair_style eam/alloy/cuda command

pair_style eam/alloy/gpu command

pair_style eam/alloy/kk command

pair_style eam/alloy/omp command

pair_style eam/alloy/opt command

pair_style eam/cd command

pair_style eam/cd/omp command

pair_style eam/fs command

pair_style eam/fs/cuda command

pair_style eam/fs/gpu command

pair_style eam/fs/kk command

pair_style eam/fs/omp command

pair_style eam/fs/opt command

Syntax:

```
pair_style style
```

- style = *eam* or *eam/alloy* or *eam/cd* or *eam/fs*

Examples:

```
pair_style eam
pair_coeff * * cuu3
pair_coeff 1*3 1*3 niu3.eam

pair_style eam/alloy
pair_coeff * * ../potentials/NiAlH_jea.eam.alloy Ni Al Ni Ni

pair_style eam/cd
pair_coeff * * ../potentials/FeCr.cdeam Fe Cr

pair_style eam/fs
pair_coeff * * NiAlH_jea.eam.fs Ni Al Ni Ni
```

Description:

Style *eam* computes pairwise interactions for metals and metal alloys using embedded-atom method (EAM) potentials (Daw). The total energy Ei of an atom I is given by

$$E_i = F_\alpha \left(\sum_{j \neq i} \rho_\beta(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij})$$

where F is the embedding energy which is a function of the atomic electron density rho, phi is a pair potential interaction, and alpha and beta are the element types of atoms I and J. The multi-body nature of the EAM potential is a result of the embedding energy term. Both summations in the formula are over all neighbors J of atom I within the cutoff distance.

The cutoff distance and the tabulated values of the functionals F, rho, and phi are listed in one or more files which are specified by the pair_coeff command. These are ASCII text files in a DYNAMO-style format which is described below. DYNAMO was the original serial EAM MD code, written by the EAM originators. Several DYNAMO potential files for different metals are included in the "potentials" directory of the LAMMPS distribution. All of these files are parameterized in terms of LAMMPS metal units.

NOTE: The *eam* style reads single-element EAM potentials in the DYNAMO *funcfl* format. Either single element or alloy systems can be modeled using multiple *funcfl* files and style *eam*. For the alloy case LAMMPS mixes the single-element potentials to produce alloy potentials, the same way that DYNAMO does. Alternatively, a single DYNAMO *setfl* file or Finnis/Sinclair EAM file can be used by LAMMPS to model alloy systems by invoking the *eam/alloy* or *eam/cd* or *eam/fs* styles as described below. These files require no mixing since they specify alloy interactions explicitly.

NOTE: Note that unlike for other potentials, cutoffs for EAM potentials are not set in the pair_style or pair_coeff command; they are specified in the EAM potential files themselves. Likewise, the EAM potential files list atomic masses; thus you do not need to use the mass command to specify them.

There are several WWW sites that distribute and document EAM potentials stored in DYNAMO or other formats:

```
http://www.ctcms.nist.gov/potentials
http://cst-www.nrl.navy.mil/ccm6/ap
http://enpub.fulton.asu.edu/cms/potentials/main/main.htm
```

These potentials should be usable with LAMMPS, though the alternate formats would need to be converted to the DYNAMO format used by LAMMPS and described on this page. The NIST site is maintained by Chandler Becker (cbecker at nist.gov) who is good resource for info on interatomic potentials and file formats.

For style *eam*, potential values are read from a file that is in the DYNAMO single-element *funcfl* format. If the DYNAMO file was created by a Fortran program, it cannot have "D" values in it for exponents. C only recognizes "e" or "E" for scientific notation.

Note that unlike for other potentials, cutoffs for EAM potentials are not set in the pair_style or pair_coeff command; they are specified in the EAM potential files themselves.

For style *eam* a potential file must be assigned to each I,I pair of atom types by using one or more pair_coeff commands, each with a single argument:

- filename

Thus the following command

```
pair_coeff *2 1*2 cuu3.eam
```

will read the cuu3 potential file and use the tabulated Cu values for F, phi, rho that it contains for type pairs 1,1 and 2,2 (type pairs 1,2 and 2,1 are ignored). See the pair_coeff doc page for alternate ways to specify the path for the potential file. In effect, this makes atom types 1 and 2 in LAMMPS be Cu atoms. Different single-element files can be assigned to different atom types to model an alloy system. The mixing to create alloy potentials for type pairs with I != J is done automatically the same way that the serial DYNAMO code originally did it; you do not need to specify coefficients for these type pairs.

Funcfl files in the *potentials* directory of the LAMMPS distribution have an ".eam" suffix. A DYNAMO single-element *funcfl* file is formatted as follows:

- line 1: comment (ignored)
- line 2: atomic number, mass, lattice constant, lattice type (e.g. FCC)
- line 3: Nrho, drho, Nr, dr, cutoff

On line 2, all values but the mass are ignored by LAMMPS. The mass is in mass units, e.g. mass number or grams/mole for metal units. The cubic lattice constant is in Angstroms. On line 3, Nrho and Nr are the number of tabulated values in the subsequent arrays, drho and dr are the spacing in density and distance space for the values in those arrays, and the specified cutoff becomes the pairwise cutoff used by LAMMPS for the potential. The units of dr are Angstroms; I'm not sure of the units for drho - some measure of electron density.

Following the three header lines are three arrays of tabulated values:

- embedding function F(rho) (Nrho values)
- effective charge function Z(r) (Nr values)
- density function rho(r) (Nr values)

The values for each array can be listed as multiple values per line, so long as each array starts on a new line. For example, the individual Z(r) values are for r = 0,dr,2*dr, ... (Nr-1)*dr.

The units for the embedding function F are eV. The units for the density function rho are the same as for drho (see above, electron density). The units for the effective charge Z are "atomic charge" or sqrt(Hartree * Bohr-radii). For two interacting atoms i,j this is used by LAMMPS to compute the pair potential term in the EAM energy

expression as r*phi, in units of eV-Angstroms, via the formula

```
r*phi = 27.2 * 0.529 * Zi * Zj
```

where 1 Hartree = 27.2 eV and 1 Bohr = 0.529 Angstroms.

Style *eam/alloy* computes pairwise interactions using the same formula as style *eam*. However the associated pair_coeff command reads a DYNAMO *setfl* file instead of a *funcfl* file. *Setfl* files can be used to model a single-element or alloy system. In the alloy case, as explained above, *setfl* files contain explicit tabulated values for alloy interactions. Thus they allow more generality than *funcfl* files for modeling alloys.

For style *eam/alloy*, potential values are read from a file that is in the DYNAMO multi-element *setfl* format, except that element names (Ni, Cu, etc) are added to one of the lines in the file. If the DYNAMO file was created by a Fortran program, it cannot have "D" values in it for exponents. C only recognizes "e" or "E" for scientific notation.

Only a single pair_coeff command is used with the *eam/alloy* style which specifies a DYNAMO *setfl* file, which contains information for M elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of *setfl* elements to atom types

As an example, the potentials/NiAlH_jea.eam.alloy file is a *setfl* file which has tabulated EAM values for 3 elements and their alloy interactions: Ni, Al, and H. See the pair_coeff doc page for alternate ways to specify the path for the potential file. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Ni, and the 4th to be Al, you would use the following pair_coeff command:

```
pair_coeff * * NiAlH_jea.eam.alloy Ni Ni Ni Al
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Ni arguments map LAMMPS atom types 1,2,3 to the Ni element in the *setfl* file. The final Al argument maps LAMMPS atom type 4 to the Al element in the *setfl* file. Note that there is no requirement that your simulation use all the elements specified by the *setfl* file.

If a mapping value is specified as NULL, the mapping is not performed. This can be used when an *eam/alloy* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Setfl files in the *potentials* directory of the LAMMPS distribution have an ".eam.alloy" suffix. A DYNAMO multi-element *setfl* file is formatted as follows:

- lines 1,2,3 = comments (ignored)
- line 4: Nelements Element1 Element2 ... ElementN
- line 5: Nrho, drho, Nr, dr, cutoff

In a DYNAMO *setfl* file, line 4 only lists Nelements = the # of elements in the *setfl* file. For LAMMPS, the element name (Ni, Cu, etc) of each element must be added to the line, in the order the elements appear in the file.

The meaning and units of the values in line 5 is the same as for the *funcfl* file described above. Note that the cutoff (in Angstroms) is a global value, valid for all pairwise interactions for all element pairings.

Following the 5 header lines are Nelements sections, one for each element, each with the following format:

- line 1 = atomic number, mass, lattice constant, lattice type (e.g. FCC)
- embedding function F(rho) (Nrho values)
- density function rho(r) (Nr values)

As with the *funcfl* files, only the mass (in mass units, e.g. mass number or grams/mole for metal units) is used by LAMMPS from the 1st line. The cubic lattice constant is in Angstroms. The F and rho arrays are unique to a single element and have the same format and units as in a *funcfl* file.

Following the Nelements sections, Nr values for each pair potential phi(r) array are listed for all i,j element pairs in the same format as other arrays. Since these interactions are symmetric (i,j = j,i) only phi arrays with i >= j are listed, in the following order: i,j = (1,1), (2,1), (2,2), (3,1), (3,2), (3,3), (4,1), ..., (Nelements, Nelements). Unlike the effective charge array Z(r) in *funcfl* files, the tabulated values for each phi function are listed in *setfl* files directly as r*phi (in units of eV-Angstroms), since they are for atom pairs.

Style *eam/cd* is similar to the *eam/alloy* style, except that it computes alloy pairwise interactions using the concentration-dependent embedded-atom method (CD-EAM). This model can reproduce the enthalpy of mixing of alloys over the full composition range, as described in (Stukowski).

The pair_coeff command is specified the same as for the *eam/alloy* style. However the DYNAMO *setfl* file must has two lines added to it, at the end of the file:

- line 1: Comment line (ignored)
- line 2: N Coefficient0 Coefficient1 ... CoeffincientN

The last line begins with the degree *N* of the polynomial function *h(x)* that modifies the cross interaction between A and B elements. Then *N+1* coefficients for the terms of the polynomial are then listed.

Modified EAM *setfl* files used with the *eam/cd* style must contain exactly two elements, i.e. in the current implementation the *eam/cd* style only supports binary alloys. The first and second elements in the input EAM file are always taken as the *A* and *B* species.

CD-EAM files in the *potentials* directory of the LAMMPS distribution have a ".cdeam" suffix.

Style *eam/fs* computes pairwise interactions for metals and metal alloys using a generalized form of EAM potentials due to Finnis and Sinclair (Finnis). The total energy Ei of an atom I is given by

$$E_i = F_\alpha \left(\sum_{j \neq i} \rho_{\alpha\beta}(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij})$$

This has the same form as the EAM formula above, except that rho is now a functional specific to the atomic types of both atoms I and J, so that different elements can contribute differently to the total electron density at an atomic site depending on the identity of the element at that atomic site.

The associated pair_coeff command for style *eam/fs* reads a DYNAMO *setfl* file that has been extended to include additional rho_alpha_beta arrays of tabulated values. A discussion of how FS EAM differs from conventional EAM alloy potentials is given in (Ackland1). An example of such a potential is the same author's Fe-P FS potential (Ackland2). Note that while FS potentials always specify the embedding energy with a square root dependence on the total density, the implementation in LAMMPS does not require that; the user can tabulate any

functional form desired in the FS potential files.

For style *eam/fs*, the form of the pair_coeff command is exactly the same as for style *eam/alloy*, e.g.

```
pair_coeff * * NiAlH_jea.eam.fs Ni Ni Ni Al
```

where there are N additional arguments after the filename, where N is the number of LAMMPS atom types. See the pair_coeff doc page for alternate ways to specify the path for the potential file. The N values determine the mapping of LAMMPS atom types to EAM elements in the file, as described above for style *eam/alloy*. As with *eam/alloy*, if a mapping value is NULL, the mapping is not performed. This can be used when an *eam/fs* potential is used as part of the *hybrid* pair style. The NULL values are used as placeholders for atom types that will be used with other potentials.

FS EAM files include more information than the DYNAMO *setfl* format files read by *eam/alloy*, in that i,j density functionals for all pairs of elements are included as needed by the Finnis/Sinclair formulation of the EAM.

FS EAM files in the *potentials* directory of the LAMMPS distribution have an ".eam.fs" suffix. They are formatted as follows:

- lines 1,2,3 = comments (ignored)
- line 4: Nelements Element1 Element2 ... ElementN
- line 5: Nrho, drho, Nr, dr, cutoff

The 5-line header section is identical to an EAM *setfl* file.

Following the header are Nelements sections, one for each element I, each with the following format:

- line 1 = atomic number, mass, lattice constant, lattice type (e.g. FCC)
- embedding function F(rho) (Nrho values)
- density function rho(r) for element I at element 1 (Nr values)
- density function rho(r) for element I at element 2
- ...
- density function rho(r) for element I at element Nelement

The units of these quantities in line 1 are the same as for *setfl* files. Note that the rho(r) arrays in Finnis/Sinclair can be asymmetric (i,j != j,i) so there are Nelements^2 of them listed in the file.

Following the Nelements sections, Nr values for each pair potential phi(r) array are listed in the same manner (r*phi, units of eV-Angstroms) as in EAM *setfl* files. Note that in Finnis/Sinclair, the phi(r) arrays are still symmetric, so only phi arrays for i >= j are listed.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input

script.

See Section_accerlate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above with the individual styles. You never need to specify a pair_coeff command with I != J arguments for the eam styles.

This pair style does not support the pair_modify shift, table, and tail options.

The eam pair styles do not write their information to binary restart files, since it is stored in tabulated potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

The eam pair styles can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.

Restrictions:

All of these styles except the *eam/cd* style are part of the MANYBODY package. They are only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

The *eam/cd* style is part of the USER-MISC package and also requires the MANYBODY package. It is only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

Related commands:

pair_coeff

Default: none

(Ackland1) Ackland, Condensed Matter (2005).

(Ackland2) Ackland, Mendelev, Srolovitz, Han and Barashev, Journal of Physics: Condensed Matter, 16, S2629 (2004).

(Daw) Daw, Baskes, Phys Rev Lett, 50, 1285 (1983). Daw, Baskes, Phys Rev B, 29, 6443 (1984).

(Finnis) Finnis, Sinclair, Philosophical Magazine A, 50, 45 (1984).

(Stukowski) Stukowski, Sadigh, Erhart, Caro; Modeling Simulation Materials Science & Engineering, 7, 075005 (2009).

pair_style edip command

Syntax:

```
pair_style edip
```

```
pair_style edip/omp
```

Examples:

pair_style edip pair_coeff * * Si.edip Si

Description:

The *edip* style computes a 3-body EDIP potential which is popular for modeling silicon materials where it can have advantages over other models such as the Stillinger-Weber or Tersoff potentials. In EDIP, the energy E of a system of atoms is

$$
\begin{aligned}
E &= \sum_{j \neq i} \phi_2(R_{ij}, Z_i) + \sum_{j \neq i} \sum_{k \neq i, k > j} \phi_3(R_{ij}, R_{ik}, Z_i) \\
\phi_2(r, Z) &= A \left[\left(\frac{B}{r} \right)^{\rho} - e^{-\beta Z^2} \right] exp\left(\frac{\sigma}{r - a} \right) \\
\phi_3(R_{ij}, R_{ik}, Z_i) &= exp\left(\frac{\gamma}{R_{ij} - a} \right) exp\left(\frac{\gamma}{R_{ik} - a} \right) h(cos\theta_{ijk}, Z_i) \\
Z_i &= \sum_{m \neq i} f(R_{im}) \qquad f(r) = \begin{cases} 1 & r < c \\ \exp\left(\frac{\alpha}{1 - x^{-3}} \right) & c < r < a \\ 0 & r > a \end{cases} \\
h(l, Z) &= \lambda [(1 - e^{-Q(Z)(l + \tau(Z))^2}) + \eta Q(Z) (l + \tau(Z))^2] \\
Q(Z) &= Q_0 e^{-\mu Z} \qquad \tau(Z) = u_1 + u_2 (u_3 e^{-u_4 Z} - e^{-2 u_4 Z})
\end{aligned}
$$

where phi2 is a two-body term and phi3 is a three-body term. The summations in the formula are over all neighbors J and K of atom I within a cutoff distance = a. Both terms depend on the local environment of atom I through its effective coordination number defined by Z, which is unity for a cutoff distance < c and gently goes to 0 at distance = a.

Only a single pair_coeff command is used with the *edip* style which specifies a EDIP potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional

arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of EDIP elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file.

As an example, imagine a file Si.edip has EDIP values for Si.

EDIP files in the *potentials* directory of the LAMMPS distribution have a ".edip" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to the two-body and three-body coefficients in the formula above:

- element 1 (the center atom in a 3-body interaction)
- element 2
- element 3
- A (energy units)
- B (distance units)
- cutoffA (distance units)
- cutoffC (distance units)
- alpha
- beta
- eta
- gamma (distance units)
- lambda (energy units)
- mu
- tho
- sigma (distance units)
- Q0
- u1
- u2
- u3
- u4

The A, B, beta, sigma parameters are used only for two-body interactions. The eta, gamma, lambda, mu, Q0 and all u1 to u4 parameters are used only for three-body interactions. The alpha and cutoffC parameters are used for the coordination environment function only.

The EDIP potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries.

For a single-element simulation, only a single entry is required (e.g. SiSiSi). For a two-element simulation, the file must contain 8 entries (for SiSiSi, SiSiC, SiCSi, SiCC, CSiSi, CSiC, CCSi, CCC), that specify EDIP parameters for all permutations of the two elements interacting in three-body configurations. Thus for 3 elements, 27 entries would be required, etc.

At the moment, only a single element parametrization is implemented. However, the author is not aware of other multi-element EDIP parametrizations. If you know any and you are interest in that, please contact the author of the EDIP package.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in

Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the pair_modify shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This angle style can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

This pair style requires the newton setting to be "on" for pair interactions.

The EDIP potential files provided with LAMMPS (see the potentials directory) are parameterized for metal units. You can use the SW potential with any LAMMPS units, but you would need to create your own EDIP potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

Related commands:

pair_coeff

Default: none

(EDIP) J. F. Justo et al., Phys. Rev. B 58, 2539 (1998).

pair_style eff/cut command

Syntax:

```
pair_style eff/cut cutoff keyword args ...
```

- cutoff = global cutoff for Coulombic interactions
- zero or more keyword/value pairs may be appended

```
keyword = limit/eradius or pressure/evirials or ecp
  limit/eradius args = none
  pressure/evirials args = none
  ecp args = type element type element ...
    type = LAMMPS atom type (1 to Ntypes)
    element = element symbol (e.g. H, Si)
```

Examples:

```
pair_style eff/cut 39.7
pair_style eff/cut 40.0 limit/eradius
pair_style eff/cut 40.0 limit/eradius pressure/evirials
pair_style eff/cut 40.0 ecp 1 Si 3 C
pair_coeff * *
pair_coeff 2 2 20.0
pair_coeff 1 s 0.320852 2.283269 0.814857
pair_coeff 3 p 22.721015 0.728733 1.103199 17.695345 6.693621
```

Description:

This pair style contains a LAMMPS implementation of the electron Force Field (eFF) potential currently under development at Caltech, as described in (Jaramillo-Botero). The eFF for Z(Su) in 2007. It has been extended to higher Zs by using effective core potentials (ECPs) that now cover up to 2nd and 3rd row p-block elements of the periodic table.

eFF can be viewed as an approximation to QM wave packet dynamics and Fermionic molecular dynamics, combining the ability of electronic structure methods to describe atomic structure, bonding, and chemistry in materials, and of plasma methods to describe nonequilibrium dynamics of large systems with a large number of highly excited electrons. Yet, eFF relies on a simplification of the electronic wavefunction in which electrons are described as floating Gaussian wave packets whose position and size respond to the various dynamic forces between interacting classical nuclear particles and spherical Gaussian electron wavepackets. The wavefunction is taken to be a Hartree product of the wave packets. To compensate for the lack of explicit antisymmetry in the resulting wavefunction, a spin-dependent Pauli potential is included in the Hamiltonian. Substituting this wavefunction into the time-dependent Schrodinger equation produces equations of motion that correspond - to second order - to classical Hamiltonian relations between electron position and size, and their conjugate momenta. The N-electron wavefunction is described as a product of one-electron Gaussian functions, whose size is a dynamical variable and whose position is not constrained to a nuclear center. This form allows for straightforward propagation of the wavefunction, with time, using a simple formulation from which the equations of motion are then integrated with conventional MD algorithms. In addition to this spin-dependent Pauli repulsion potential term between Gaussians, eFF includes the electron kinetic energy from the Gaussians. These two terms are based on first-principles quantum mechanics. On the other hand, nuclei are described as point charges, which interact with other nuclei and electrons through standard electrostatic potential forms.

The full Hamiltonian (shown below), contains then a standard description for electrostatic interactions between a set of delocalized point and Gaussian charges which include, nuclei-nuclei (NN), electron-electron (ee), and nuclei-electron (Ne). Thus, eFF is a mixed QM-classical mechanics method rather than a conventional force field method (in which electron motions are averaged out into ground state nuclear motions, i.e a single electronic state, and particle interactions are described via empirically parameterized interatomic potential functions). This makes eFF uniquely suited to simulate materials over a wide range of temperatures and pressures where electronically excited and ionized states of matter can occur and coexist. Furthermore, the interactions between particles -nuclei and electrons- reduce to the sum of a set of effective pairwise potentials in the eFF formulation. The *eff/cut* style computes the pairwise Coulomb interactions between nuclei and electrons (E_NN,E_Ne,E_ee), and the quantum-derived Pauli (E_PR) and Kinetic energy interactions potentials between electrons (E_KE) for a total energy expression given as,

$$U\left(R,r,s\right)=E_{NN}\left(R\right)+E_{Ne}\left(R,r,s\right)+E_{ee}\left(r,s\right)+E_{KE}\left(r,s\right)+E_{PR}\left(\uparrow\downarrow,S\right.$$

The individual terms are defined as follows:

$$E_{KE}=\frac{\hbar^{2}}{m_{e}}\sum_{i}\frac{3}{2s_{i}^{2}}$$

$$E_{NN}=\frac{1}{4\pi\varepsilon_{0}}\sum_{i<j}\frac{Z_{i}Z_{j}}{R_{ij}}$$

$$E_{Ne}=-\frac{1}{4\pi\varepsilon_{0}}\sum_{i,j}\frac{Z_{i}}{R_{ij}}Erf\left(\frac{\sqrt{2}R_{ij}}{s_{j}}\right)$$

$$E_{ee}=\frac{1}{4\pi\varepsilon_{0}}\sum_{i<j}\frac{1}{r_{ij}}Erf\left(\frac{\sqrt{2}r_{ij}}{\sqrt{s_{i}^{2}+s_{j}^{2}}}\right)$$

$$E_{Pauli}=\sum_{\sigma_{i}=\sigma_{j}}E\left(\uparrow\uparrow\right)_{ij}+\sum_{\sigma_{i}\neq\sigma_{j}}E\left(\uparrow\downarrow\right)_{ij}$$

where, s_i correspond to the electron sizes, the sigmas i's to the fixed spins of the electrons, Z_i to the charges on the nuclei, R_ij to the distances between the nuclei or the nuclei and electrons, and r_ij to the distances between electrons. For additional details see (Jaramillo-Botero).

The overall electrostatics energy is given in Hartree units of energy by default and can be modified by an energy-conversion constant, according to the units chosen (see electron_units). The cutoff Rc, given in Bohrs (by default), truncates the interaction distance. The recommended cutoff for this pair style should follow the minimum image criterion, i.e. half of the minimum unit cell length.

Style *eff/long* (not yet available) computes the same interactions as style *eff/cut* except that an additional damping factor is applied so it can be used in conjunction with the kspace_style command and its *ewald* or *pppm* option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

This potential is designed to be used with atom_style electron definitions, in order to handle the description of systems with interacting nuclei and explicit electrons.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- cutoff (distance units)

For *eff/cut*, the cutoff coefficient is optional. If it is not used (as in some of the examples above), the default global value specified in the pair_style command is used.

For *eff/long* (not yet available) no cutoff will be specified for an individual I,J type pair via the pair_coeff command. All type pairs use the same global cutoff specified in the pair_style command.

The *limit/eradius* and *pressure/evirials* keywrods are optional. Neither or both must be specified. If not specified they are unset.

The *limit/eradius* keyword is used to restrain electron size from becoming excessively diffuse at very high temperatures were the Gaussian wave packet representation breaks down, and from expanding as free particles to infinite size. If unset, electron radius is free to increase without bounds. If set, a restraining harmonic potential of the form E = 1/2k_ss^2 for s > L_box/2, where k_s = 1 Hartrees/Bohr^2, is applied on the electron radius.

The *pressure/evirials* keyword is used to control between two types of pressure computation: if unset, the computed pressure does not include the electronic radial virials contributions to the total pressure (scalar or tensor). If set, the computed pressure will include the electronic radial virial contributions to the total pressure (scalar and tensor).

The *ecp* keyword is used to associate an ECP representation for a particular atom type. The ECP captures the orbital overlap between a core pseudo particle and valence electrons within the Pauli repulsion. A list of type:element-symbol pairs may be provided for all ECP representations, after the "ecp" keyword.

NOTE: Default ECP parameters are provided for C, N, O, Al, and Si. Users can modify these using the pair_coeff command as exemplified above. For this, the User must distinguish between two different functional forms supported, one that captures the orbital overlap assuming the s-type core interacts with an s-like valence electron (s-s) and another that assumes the interaction is s-p. For systems that exhibit significant p-character (e.g. C, N, O) the s-p form is recommended. The "s" ECP form requires 3 parameters and the "p" 5 parameters.

NOTE: there are two different pressures that can be reported for eFF when defining this pair_style, one (default) that considers electrons do not contribute radial virial components (i.e. electrons treated as incompressible 'rigid' spheres) and one that does. The radial electronic contributions to the virials are only tallied if the flexible pressure option is set, and this will affect both global and per-atom quantities. In principle, the true pressure of a system is somewhere in between the rigid and the flexible eFF pressures, but, for most cases, the difference between these two pressures will not be significant over long-term averaged runs (i.e. even though the energy partitioning changes, the total energy remains similar).

NOTE: This implemention of eFF gives a reasonably accurate description for systems containing nuclei from Z = 1-6 in "all electron" representations. For systems with increasingly non-spherical electrons, Users should use the ECP representations. ECPs are now supported and validated for most of the 2nd and 3rd row elements of the p-block. Predefined parameters are provided for C, N, O, Al, and Si. The ECP captures the orbital overlap between the core and valence electrons (i.e. Pauli repulsion) with one of the functional forms:

$$E_{Pauli(ECP_s)} = p_1 \exp\left(-\frac{p_2 r^2}{p_3 + s^2}\right)$$

$$E_{Pauli(ECP_p)} = p_1 \left(\frac{2}{p_2/s + s/p_2}\right) (r - p_3 s)^2 \exp\left[-\frac{p_4 (r - p_3 s)^2}{p_5 + s^2}\right]$$

Where the 1st form correspond to core interactions with s-type valence electrons and the 2nd to core interactions with p-type valence electrons.

The current version adds full support for models with fixed-core and ECP definitions. to enable larger timesteps (i.e. by avoiding the high frequency vibrational modes -translational and radial- of the 2 s electrons), and in the ECP case to reduce the increased orbital complexity in higher Z elements (up to Z

In general, eFF excels at computing the properties of materials in extreme conditions and tracing the system dynamics over multi-picosend timescales; this is particularly relevant where electron excitations can change significantly the nature of bonding in the system. It can capture with surprising accuracy the behavior of such systems because it describes consistently and in an unbiased manner many different kinds of bonds, including covalent, ionic, multicenter, ionic, and plasma, and how they interconvert and/or change when they become excited. eFF also excels in computing the relative thermochemistry of isodemic reactions and conformational changes, where the bonds of the reactants are of the same type as the bonds of the products. eFF assumes that kinetic energy differences dominate the overall exchange energy, which is true when the electrons present are nearly spherical and nodeless and valid for covalent compounds such as dense hydrogen, hydrocarbons, and diamond; alkali metals (e.g. lithium), alkali earth metals (e.g. beryllium) and semimetals such as boron; and various compounds containing ionic and/or multicenter bonds, such as boron dihydride.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the cutoff distance for the *eff/cut* style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

The pair_modify shift option is not relevant for these pair styles.

The *eff/long* (not yet available) style supports the pair_modify table option for tabulation of the short-range portion of the long-range Coulombic interaction.

These pair styles do not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

These pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.

Restrictions:

These pair styles will only be enabled if LAMMPS is built with the USER-EFF package. It will only be enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

These pair styles require that particles store electron attributes such as radius, radial velocity, and radital force, as defined by the atom_style. The *electron* atom style does all of this.

Thes pair styles require you to use the comm_modify vel yes command so that velocites are stored by ghost atoms.

Related commands:

pair_coeff

Default:

If not specified, limit_eradius = 0 and pressure_with_evirials = 0.

(Su) Su and Goddard, Excited Electron Dynamics Modeling of Warm Dense Matter, Phys Rev Lett, 99:185003 (2007).

(Jaramillo-Botero) Jaramillo-Botero, Su, Qi, Goddard, Large-scale, Long-term Non-adiabatic Electron Molecular Dynamics for Describing Material Properties and Phenomena in Extreme Environments, J Comp Chem, 32, 497-512 (2011).

pair_style eim command

pair_style eim/omp command

Syntax:

```
pair_style style
```

- style = *eim*

Examples:

```
pair_style eim
pair_coeff * * Na Cl ../potentials/ffield.eim Na Cl
pair_coeff * * Na Cl ffield.eim  Na Na Na Cl
pair_coeff * * Na Cl ../potentials/ffield.eim Cl NULL Na
```

Description:

Style *eim* computes pairwise interactions for ionic compounds using embedded-ion method (EIM) potentials (Zhou). The energy of the system E is given by

$$E = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=i_1}^{i_N} \phi_{ij}\left(r_{ij}\right) + \sum_{i=1}^{N} E_i\left(q_i, \sigma_i\right)$$

The first term is a double pairwise sum over the J neighbors of all I atoms, where phi_ij is a pair potential. The second term sums over the embedding energy E_i of atom I, which is a function of its charge q_i and the electrical potential sigma_i at its location. E_i, q_i, and sigma_i are calculated as

$$\begin{aligned} q_i &= \sum_{j=i_1}^{i_N} \eta_{ji}\left(r_{ij}\right) \\ \sigma_i &= \sum_{j=i_1}^{i_N} q_j \cdot \psi_{ij}\left(r_{ij}\right) \\ E_i\left(q_i, \sigma_i\right) &= \frac{1}{2} \cdot q_i \cdot \sigma_i \end{aligned}$$

where eta_ji is a pairwise function describing electron flow from atom I to atom J, and psi_ij is another pairwise function. The multi-body nature of the EIM potential is a result of the embedding energy term. A complete list of all the pair functions used in EIM is summarized below

$$(r) = \begin{cases} \left[\frac{E_{b,ij}\beta_{ij}}{\beta_{ij}-\alpha_{ij}} \exp\left(-\alpha_{ij}\frac{r-r_{e,ij}}{r_{e,ij}}\right) - \frac{E_{b,ij}\alpha_{ij}}{\beta_{ij}-\alpha_{ij}} \exp\left(-\beta_{ij}\frac{r-r_{e,ij}}{r_{e,ij}}\right)\right] f_c\left(r, r_{e,ij}, r_{c,\phi,ij}\right), \\ \left[\frac{E_{b,ij}\beta_{ij}}{\beta_{ij}-\alpha_{ij}} \left(\frac{r_{e,ij}}{r}\right)^{\alpha_{ij}} - \frac{E_{b,ij}\alpha_{ij}}{\beta_{ij}-\alpha_{ij}} \left(\frac{r_{e,ij}}{r}\right)^{\beta_{ij}}\right] f_c\left(r, r_{e,ij}, r_{c,\phi,ij}\right), \end{cases}$$

$$\eta_{ji} = A_{\eta,ij}\left(\chi_j - \chi_i\right) f_c\left(r, r_{s,\eta,ij}, r_{c,\eta,ij}\right)$$

$$\psi_{ij}\left(r\right) = A_{\psi,ij} \exp\left(-\zeta_{ij} r\right) f_c\left(r, r_{s,\psi,ij}, r_{c,\psi,ij}\right)$$

$$f_c\left(r, r_p, r_c\right) = 0.510204 erfc\left[\frac{1.64498\left(2r - r_p - r_c\right)}{r_c - r_p}\right] - 0.010204$$

Here E_b, r_e, r_(c,phi), alpha, beta, A_(psi), zeta, r_(s,psi), r_(c,psi), A_(eta), r_(s,eta), r_(c,eta), chi, and pair function type p are parameters, with subscripts ij indicating the two species of atoms in the atomic pair.

NOTE: Even though the EIM potential is treating atoms as charged ions, you should not use a LAMMPS atom_style that stores a charge on each atom and thus requires you to assign a charge to each atom, e.g. the *charge* or *full* atom styles. This is because the EIM potential infers the charge on an atom from the equation above for q_i; you do not assign charges explicitly.

All the EIM parameters are listed in a potential file which is specified by the pair_coeff command. This is an ASCII text file in a format described below. The "ffield.eim" file included in the "potentials" directory of the LAMMPS distribution currently includes nine elements Li, Na, K, Rb, Cs, F, Cl, Br, and I. A system with any combination of these elements can be modeled. This file is parameterized in terms of LAMMPS metal units.

Note that unlike other potentials, cutoffs for EIM potentials are not set in the pair_style or pair_coeff command; they are specified in the EIM potential file itself. Likewise, the EIM potential file lists atomic masses; thus you do not need to use the mass command to specify them.

Only a single pair_coeff command is used with the *eim* style which specifies an EIM potential file and the element(s) to extract information for. The EIM elements are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- Elem1, Elem2, ...
- EIM potential file
- N element names = mapping of EIM elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file.

As an example like one of those above, suppose you want to model a system with Na and Cl atoms. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Na, and the 4th to be Cl, you would use the following pair_coeff command:

```
pair_coeff * * Na Cl ffield.eim Na Na Na Cl
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The filename is the EIM potential file. The Na and Cl arguments (before the file name) are the two elements for which info will be extracted from the potentail file. The first three trailing Na arguments map LAMMPS atom types 1,2,3 to the EIM Na element. The final Cl argument maps LAMMPS atom type 4 to the EIM Cl element.

If a mapping value is specified as NULL, the mapping is not performed. This can be used when an *eim* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

The ffield.eim file in the *potentials* directory of the LAMMPS distribution is formated as follows:

Lines starting with # are comments and are ignored by LAMMPS. Lines starting with "global:" include three global values. The first value divides the cations from anions, i.e., any elements with electronegativity above this value are viewed as anions, and any elements with electronegativity below this value are viewed as cations. The second and third values are related to the cutoff function - i.e. the 0.510204, 1.64498, and 0.010204 shown in the above equation can be derived from these values.

Lines starting with "element:" are formatted as follows: name of element, atomic number, atomic mass, electronic negativity, atomic radius (LAMMPS ignores it), ionic radius (LAMMPS ignores it), cohesive energy (LAMMPS ignores it), and q0 (must be 0).

Lines starting with "pair:" are entered as: element 1, element 2, r_(c,phi), r_(c,phi) (redundant for historical reasons), E_b, r_e, alpha, beta, r_(c,eta), A_(eta), r_(s,eta), r_(c,psi), A_(psi), zeta, r_(s,psi), and p.

The lines in the file can be in any order; LAMMPS extracts the info it needs.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default).

Related commands:

pair_coeff

Default: none

(Zhou) Zhou, submitted for publication (2010). Please contact Xiaowang Zhou (Sandia) for details via email at xzhou at sandia.gov.

pair_style gauss command

pair_style gauss/gpu command

pair_style gauss/omp command

pair_style gauss/cut command

pair_style gauss/cut/omp command

Syntax:

```
pair_style gauss cutoff
pair_style gauss/cut cutoff
```

- cutoff = global cutoff for Gauss interactions (distance units)

Examples:

```
pair_style gauss 12.0
pair_coeff * * 1.0 0.9
pair_coeff 1 4 1.0 0.9 10.0

pair_style gauss/cut 3.5
pair_coeff 1 4 0.2805 1.45 0.112
```

Description:

Style *gauss* computes a tethering potential of the form

$$E = -A \exp(-Br^2) \qquad r < r_c$$

between an atom and its corresponding tether site which will typically be a frozen atom in the simulation. Rc is the cutoff.

The following coefficients must be defined for each pair of atom types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- A (energy units)
- B (1/distance^2 units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global cutoff is used.

Style *gauss/cut* computes a generalized Gaussian interaction potential between pairs of particles:

$$E = \frac{H}{\sigma_h \sqrt{2\pi}} \exp\left[-\frac{(r-r_{mh})^2}{2\sigma_h^2}\right]$$

where H determines together with the standard deviation sigma_h the peak height of the Gaussian function, and r_mh the peak position. Examples of the use of the Gaussian potentials include implicit solvent simulations of salt ions (Lenart) and of surfactants (Jusufi). In these instances the Gaussian potential mimics the hydration barrier between a pair of particles. The hydration barrier is located at r_mh and has a width of sigma_h. The prefactor determines the hight of the potential barrier.

The following coefficients must be defined for each pair of atom types via the pair_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- H (energy * distance units)
- r_mh (distance units)
- sigma_h (distance units)

The global cutoff (r_c) specified in the pair_style command is used.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the "-suffix command-line switch7_Section_start.html#start_6 when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

The *gauss* style does not support the pair_modify shift option. There is no effect due to the Gaussian well beyond the cutoff; hence reasonable cutoffs need to be specified.

The *gauss/cut* style supports the pair_modify shift option for the energy of the Gauss-potential portion of the pair interaction.

The pair_modify table and tail options are not relevant for these pair styles.

These pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.

The *gauss* pair style tallies an "occupancy" count of how many Gaussian-well sites have an atom within the distance at which the force is a maximum = sqrt(0.5/b). This quantity can be accessed via the compute pair command as a vector of values of length 1.

To print this quantity to the log file (with a descriptive column heading) the following commands could be included in an input script:

```
compute gauss all pair gauss
variable occ equal c_gauss[1]
thermo_style custom step temp epair v_occ
```

Restrictions:

The *gauss/cut* style is part of the "user-misc" package. It is only enabled if LAMMPS is build with that package. See the Making of LAMMPS section for more info.

Related commands:

pair_coeff, pair_style coul/diel

Default: none

(Lenart) Lenart , Jusufi, and Panagiotopoulos, J Chem Phys, 126, 044509 (2007).

(Jusufi) Jusufi, Hynninen, and Panagiotopoulos, J Phys Chem B, 112, 13783 (2008).

pair_style gayberne command

pair_style gayberne/gpu command

pair_style gayberne/intel command

pair_style gayberne/omp command

Syntax:

```
pair_style gayberne gamma upsilon mu cutoff
```

- gamma = shift for potential minimum (typically 1)
- upsilon = exponent for eta orientation-dependent energy function
- mu = exponent for chi orientation-dependent energy function
- cutoff = global cutoff for interactions (distance units)

Examples:

```
pair_style gayberne 1.0 1.0 1.0 10.0
pair_coeff * * 1.0 1.7 1.7 3.4 3.4 1.0 1.0 1.0
```

Description:

The *gayberne* styles compute a Gay-Berne anisotropic LJ interaction (Berardi) between pairs of ellipsoidal particles or an ellipsoidal and spherical particle via the formulas

$$U(\mathbf{A_1}, \mathbf{A_2}, \mathbf{r_{12}}) = \mathbf{U_r}(\mathbf{A_1}, \mathbf{A_2}, \mathbf{r_{12}}, \gamma) \cdot \eta_{12}(\mathbf{A_1}, \mathbf{A_2}, \upsilon) \cdot \chi_{12}(\mathbf{A_1}, \mathbf{A_2}, \mathbf{r_{12}}, \mu)$$

$$U_r = 4\epsilon(\varrho^{12} - \varrho^6)$$

$$\varrho = \frac{\sigma}{h_{12} + \gamma\sigma}$$

where A1 and A2 are the transformation matrices from the simulation box frame to the body frame and r12 is the center to center vector between the particles. Ur controls the shifted distance dependent interaction based on the distance of closest approach of the two particles (h12) and the user-specified shift parameter gamma. When both particles are spherical, the formula reduces to the usual Lennard-Jones interaction (see details below for when Gay-Berne treats a particle as "spherical").

For large uniform molecules it has been shown that the energy parameters are approximately representable in terms of local contact curvatures (Everaers):

$$\epsilon_a = \sigma \cdot \frac{a}{b \cdot c}; \epsilon_b = \sigma \cdot \frac{b}{a \cdot c}; \epsilon_c = \sigma \cdot \frac{c}{a \cdot b}$$

The variable names utilized as potential parameters are for the most part taken from (Everaers) in order to be consistent with the RE-squared pair potential. Details on the upsilon and mu parameters are given here.

More details of the Gay-Berne formulation are given in the references listed below and in this supplementary document.

Use of this pair style requires the NVE, NVT, or NPT fixes with the *asphere* extension (e.g. fix nve/asphere) in order to integrate particle rotation. Additionally, atom_style ellipsoid should be used since it defines the rotational state and the size and shape of each ellipsoidal particle.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon = well depth (energy units)
- sigma = minimum effective particle radii (distance units)
- epsilon_i_a = relative well depth of type I for side-to-side interactions
- epsilon_i_b = relative well depth of type I for face-to-face interactions
- epsilon_i_c = relative well depth of type I for end-to-end interactions
- epsilon_j_a = relative well depth of type J for side-to-side interactions
- epsilon_j_b = relative well depth of type J for face-to-face interactions
- epsilon_j_c = relative well depth of type J for end-to-end interactions
- cutoff (distance units)

The last coefficient is optional. If not specified, the global cutoff specified in the pair_style command is used.

It is typical with the Gay-Berne potential to define *sigma* as the minimum of the 3 shape diameters of the particles involved in an I,I interaction, though this is not required. Note that this is a different meaning for *sigma* than the pair_style resquared potential uses.

The epsilon_i and epsilon_j coefficients are actually defined for atom types, not for pairs of atom types. Thus, in a series of pair_coeff commands, they only need to be specified once for each atom type.

Specifically, if any of epsilon_i_a, epsilon_i_b, epsilon_i_c are non-zero, the three values are assigned to atom type I. If all the epsilon_i values are zero, they are ignored. If any of epsilon_j_a, epsilon_j_b, epsilon_j_c are non-zero, the three values are assigned to atom type J. If all three epsilon_j values are zero, they are ignored. Thus the typical way to define the epsilon_i and epsilon_j coefficients is to list their values in "pair_coeff I J" commands when I = J, but set them to 0.0 when I != J. If you do list them when I != J, you should insure they are consistent with their values in other pair_coeff commands, since only the last setting will be in effect.

Note that if this potential is being used as a sub-style of pair_style hybrid, and there is no "pair_coeff I I" setting made for Gay-Berne for a particular type I (because I-I interactions are computed by another hybrid pair potential), then you still need to insure the epsilon a,b,c coefficients are assigned to that type. e.g. in a "pair_coeff I J" command.

NOTE: If the epsilon a = b = c for an atom type, and if the shape of the particle itself is spherical, meaning its 3 shape parameters are all the same, then the particle is treated as an LJ sphere by the Gay-Berne potential. This is significant because if two LJ spheres interact, then the simple Lennard-Jones formula is used to compute their interaction energy/force using the specified epsilon and sigma as the standard LJ parameters. This is much cheaper to compute than the full Gay-Berne formula. To treat the particle as a LJ sphere with sigma = D, you should normally set epsilon a = b = c = 1.0, set the pair_coeff sigma = D, and also set the 3 shape parameters for the particle to D. The one exception is that if the 3 shape parameters are set to 0.0, which is a valid way in LAMMPS to specify a point particle, then the Gay-Berne potential will treat that as shape parameters of 1.0 (i.e. a LJ particle with sigma = 1), since it requires finite-size particles. In this case you should still set the pair_coeff sigma to 1.0 as well.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for this pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair styles supports the pair_modify shift option for the energy of the Lennard-Jones portion of the pair interaction, but only for sphere-sphere interactions. There is no shifting performed for ellipsoidal interactions due to the anisotropic dependence of the interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

The *gayberne* style is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

These pair style require that atoms store torque and a quaternion to represent their orientation, as defined by the atom_style. It also require they store a per-type shape. The particles cannot store a per-particle diameter.

This pair style requires that atoms be ellipsoids as defined by the atom_style ellipsoid command.

Particles acted on by the potential can be finite-size aspherical or spherical particles, or point particles. Spherical particles have all 3 of their shape parameters equal to each other. Point particles have all 3 of their shape parameters equal to 0.0.

The Gay-Berne potential does not become isotropic as r increases (Everaers). The distance-of-closest-approach approximation used by LAMMPS becomes less accurate when high-aspect ratio ellipsoids are used.

Related commands:

pair_coeff, fix nve/asphere, compute temp/asphere, pair_style resquared

Default: none

(Everaers) Everaers and Ejtehadi, Phys Rev E, 67, 041710 (2003).

(Berardi) Berardi, Fava, Zannoni, Chem Phys Lett, 297, 8-14 (1998). Berardi, Muccioli, Zannoni, J Chem Phys, 128, 024905 (2008).

(Perram) Perram and Rasmussen, Phys Rev E, 54, 6565-6572 (1996).

(Allen) Allen and Germano, Mol Phys 104, 3225-3235 (2006).

pair_style gran/hooke command

pair_style gran/cuda command

pair_style gran/omp command

pair_style gran/hooke/history command

pair_style gran/hooke/history/omp command

pair_style gran/hertz/history command

pair_style gran/hertz/history/omp command

Syntax:

```
pair_style style Kn Kt gamma_n gamma_t xmu dampflag
```

- style = *gran/hooke* or *gran/hooke/history* or *gran/hertz/history*
- Kn = elastic constant for normal particle repulsion (force/distance units or pressure units - see discussion below)
- Kt = elastic constant for tangential contact (force/distance units or pressure units - see discussion below)
- gamma_n = damping coefficient for collisions in normal direction (1/time units or 1/time-distance units - see discussion below)
- gamma_t = damping coefficient for collisions in tangential direction (1/time units or 1/time-distance units - see discussion below)
- xmu = static yield criterion (unitless value between 0.0 and 1.0e4)
- dampflag = 0 or 1 if tangential damping force is excluded or included

NOTE: Versions of LAMMPS before 9Jan09 had different style names for granular force fields. This is to emphasize the fact that the Hertzian equation has changed to model polydispersity more accurately. A side effect of the change is that the Kn, Kt, gamma_n, and gamma_t coefficients in the pair_style command must be specified with different values in order to reproduce calculations made with earlier versions of LAMMPS, even for monodisperse systems. See the NOTE below for details.

Examples:

```
pair_style gran/hooke/history 200000.0 NULL 50.0 NULL 0.5 1
pair_style gran/hooke 200000.0 70000.0 50.0 30.0 0.5 0
```

Description:

The *gran* styles use the following formulas for the frictional force between two granular particles, as described in (Brilliantov), (Silbert), and (Zhang), when the distance r between two particles of radii Ri and Rj is less than their contact distance d = Ri + Rj. There is no force between the particles when r > d.

The two Hookean styles use this formula:

$$F_{hk} = (k_n \delta \mathbf{n}_{ij} - m_{\text{eff}} \gamma_n \mathbf{v}_n) - (k_t \mathbf{\Delta s}_t + m_{\text{eff}} \gamma_t \mathbf{v}_t)$$

The Hertzian style uses this formula:

$$F_{hz} = \sqrt{\delta} \sqrt{\frac{R_i R_j}{R_i + R_j}} F_{hk} = \sqrt{\delta} \sqrt{\frac{R_i R_j}{R_i + R_j}} \left[(k_n \delta \mathbf{n}_{ij} - m_{\text{eff}} \gamma_n \mathbf{v}_n) - (k_t \mathbf{\Delta s}_t + m_{\text{eff}} \gamma_t \mathbf{v}_t \right.$$

In both equations the first parenthesized term is the normal force between the two particles and the second parenthesized term is the tangential force. The normal force has 2 terms, a contact force and a damping force. The tangential force also has 2 terms: a shear force and a damping force. The shear force is a "history" effect that accounts for the tangential displacement between the particles for the duration of the time they are in contact. This term is included in pair styles *hooke/history* and *hertz/history*, but is not included in pair style *hooke*. The tangential damping force term is included in all three pair styles if *dampflag* is set to 1; it is not included if *dampflag* is set to 0.

The other quantities in the equations are as follows:

- delta = d - r = overlap distance of 2 particles
- Kn = elastic constant for normal contact
- Kt = elastic constant for tangential contact
- gamma_n = viscoelastic damping constant for normal contact
- gamma_t = viscoelastic damping constant for tangential contact
- m_eff = Mi Mj / (Mi + Mj) = effective mass of 2 particles of mass Mi and Mj
- Delta St = tangential displacement vector between 2 spherical particles which is truncated to satisfy a frictional yield criterion
- n_ij = unit vector along the line connecting the centers of the 2 particles
- Vn = normal component of the relative velocity of the 2 particles
- Vt = tangential component of the relative velocity of the 2 particles

The Kn, Kt, gamma_n, and gamma_t coefficients are specified as parameters to the pair_style command. If a NULL is used for Kt, then a default value is used where Kt = 2/7 Kn. If a NULL is used for gamma_t, then a default value is used where gamma_t = 1/2 gamma_n.

The interpretation and units for these 4 coefficients are different in the Hookean versus Hertzian equations.

The Hookean model is one where the normal push-back force for two overlapping particles is a linear function of the overlap distance. Thus the specified Kn is in units of (force/distance). Note that this push-back force is independent of absolute particle size (in the monodisperse case) and of the relative sizes of the two particles (in the polydisperse case). This model also applies to the other terms in the force equation so that the specified gamma_n is in units of (1/time), Kt is in units of (force/distance), and gamma_t is in units of (1/time).

The Hertzian model is one where the normal push-back force for two overlapping particles is proportional to the area of overlap of the two particles, and is thus a non-linear function of overlap distance. Thus Kn has units of force per area and is thus specified in units of (pressure). The effects of absolute particle size (monodispersity) and relative size (polydispersity) are captured in the radii-dependent pre-factors. When these pre-factors are

carried through to the other terms in the force equation it means that the specified gamma_n is in units of (1/(time*distance)), Kt is in units of (pressure), and gamma_t is in units of (1/(time*distance)).

Note that in the Hookean case, Kn can be thought of as a linear spring constant with units of force/distance. In the Hertzian case, Kn is like a non-linear spring constant with units of force/area or pressure, and as shown in the (Zhang) paper, Kn = 4G / (3(1-nu)) where nu = the Poisson ratio, G = shear modulus = E / (2(1+nu)), and E = Young's modulus. Similarly, Kt = 4G / (2-nu). (NOTE: in an earlier version of the manual, we incorrectly stated that Kt = 8G / (2-nu).)

Thus in the Hertzian case Kn and Kt can be set to values that corresponds to properties of the material being modeled. This is also true in the Hookean case, except that a spring constant must be chosen that is appropriate for the absolute size of particles in the model. Since relative particle sizes are not accounted for, the Hookean styles may not be a suitable model for polydisperse systems.

NOTE: In versions of LAMMPS before 9Jan09, the equation for Hertzian interactions did not include the sqrt(RiRj/Ri+Rj) term and thus was not as accurate for polydisperse systems. For monodisperse systems, sqrt(RiRj/Ri+Rj) is a constant factor that effectively scales all 4 coefficients: Kn, Kt, gamma_n, gamma_t. Thus you can set the values of these 4 coefficients appropriately in the current code to reproduce the results of a previous Hertzian monodisperse calculation. For example, for the common case of a monodisperse system with particles of diameter 1, all 4 of these coefficients should now be set 2x larger than they were previously.

Xmu is also specified in the pair_style command and is the upper limit of the tangential force through the Coulomb criterion Ft = xmu*Fn, where Ft and Fn are the total tangential and normal force components in the formulas above. Thus in the Hookean case, the tangential force between 2 particles grows according to a tangential spring and dash-pot model until Ft/Fn = xmu and is then held at Ft = Fn*xmu until the particles lose contact. In the Hertzian case, a similar analogy holds, though the spring is no longer linear.

NOTE: Normally, xmu should be specified as a fractional value between 0.0 and 1.0, however LAMMPS allows large values (up to 1.0e4) to allow for modeling of systems which can sustain very large tangential forces.

For granular styles there are no additional coefficients to set for each pair of atom types via the pair_coeff command. All settings are global and are made via the pair_style command. However you must still use the pair_coeff for all pairs of granular atom types. For example the command

```
pair_coeff * *
```

should be used if all atoms in the simulation interact via a granular potential (i.e. one of the pair styles above is used). If a granular potential is used as a sub-style of pair_style hybrid, then specific atom types can be used in the pair_coeff command to determine which atoms interact via a granular potential.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

The pair_modify mix, shift, table, and tail options are not relevant for granular pair styles.

These pair styles write their information to binary restart files, so a pair_style command does not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.

The single() function of these pair styles returns 0.0 for the energy of a pairwise interaction, since energy is not conserved in these dissipative potentials. It also returns only the normal component of the pairwise interaction force. However, the single() function also calculates 4 extra pairwise quantities. The first 3 are the components of the tangential force between particles I and J, acting on particle I. *P4* is the magnitude of this tangential force. These extra quantites can be accessed by the compute pair/local command, as *p1*, *p2*, *p3*, *p4*.

Restrictions: none

All the granular pair styles are part of the GRANULAR package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

These pair styles require that atoms store torque and angular velocity (omega) as defined by the atom_style. They also require a per-particle radius is stored. The *sphere* atom style does all of this.

This pair style requires you to use the comm_modify vel yes command so that velocites are stored by ghost atoms.

These pair styles will not restart exactly when using the read_restart command, though they should provide statistically similar results. This is because the forces they compute depend on atom velocities. See the read_restart command for more details.

Related commands:

pair_coeff

Default: none

(Brilliantov) Brilliantov, Spahn, Hertzsch, Poschel, Phys Rev E, 53, p 5382-5392 (1996).

(Silbert) Silbert, Ertas, Grest, Halsey, Levine, Plimpton, Phys Rev E, 64, p 051302 (2001).

(Zhang) Zhang and Makse, Phys Rev E, 72, p 011301 (2005).

pair_style lj/gromacs command

pair_style lj/gromacs/cuda command

pair_style lj/gromacs/gpu command

pair_style lj/gromacs/omp command

pair_style lj/gromacs/coul/gromacs command

pair_style lj/gromacs/coul/gromacs/cuda command

pair_style lj/gromacs/coul/gromacs/omp command

Syntax:

```
pair_style style args
```

- style = *lj/gromacs* or *lj/gromacs/coul/gromacs*
- args = list of arguments for a particular style

```
lj/gromacs args = inner outer
    inner, outer = global switching cutoffs for Lennard Jones
  lj/gromacs/coul/gromacs args = inner outer (inner2) (outer2)
    inner, outer = global switching cutoffs for Lennard Jones (and Coulombic if only 2 args)
    inner2, outer2 = global switching cutoffs for Coulombic (optional)
```

Examples:

```
pair_style lj/gromacs 9.0 12.0
pair_coeff * * 100.0 2.0
pair_coeff 2 2 100.0 2.0 8.0 10.0

pair_style lj/gromacs/coul/gromacs 9.0 12.0
pair_style lj/gromacs/coul/gromacs 8.0 10.0 7.0 9.0
pair_coeff * * 100.0 2.0
```

Description:

The *lj/gromacs* styles compute shifted LJ and Coulombic interactions with an additional switching function S(r) that ramps the energy and force smoothly to zero between an inner and outer cutoff. It is a commonly used potential in the GROMACS MD code and for the coarse-grained models of (Marrink).

$$
\begin{aligned}
E_{LJ} &= 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] + S_{LJ}(r) \qquad r < r_c \\
E_C &= \frac{Cq_iq_j}{\epsilon r} + S_C(r) \qquad r < r_c \\
S(r) &= C \qquad r < r_1 \\
S(r) &= \frac{A}{3}(r-r_1)^3 + \frac{B}{4}(r-r_1)^4 + C \qquad r_1 < r < r_c \\
A &= (-3E'(r_c) + (r_c - r_1)E''(r_c))/(r_c - r_1)^2 \\
B &= (2E'(r_c) - (r_c - r_1)E''(r_c))/(r_c - r_1)^3 \\
C &= -E(r_c) + \frac{1}{2}(r_c - r_1)E'(r_c) - \frac{1}{12}(r_c - r_1)^2E''(r_c))
\end{aligned}
$$

r1 is the inner cutoff; rc is the outer cutoff. The coefficients A, B, and C are computed by LAMMPS to perform the shifting and smoothing. The function S(r) is actually applied once to each term of the LJ formula and once to the Coulombic formula, so there are 2 or 3 sets of A,B,C coefficients depending on which pair_style is used. The boundary conditions applied to the smoothing function are as follows: S'(r1) = S''(r1) = 0, S(rc) = -E(rc), S'(rc) = -E'(rc), and S''(rc) = -E''(rc), where E(r) is the corresponding term in the LJ or Coulombic potential energy function. Single and double primes denote first and second derivatives with respect to r, respectively.

The inner and outer cutoff for the LJ and Coulombic terms can be the same or different depending on whether 2 or 4 arguments are used in the pair_style command. The inner LJ cutoff must be > 0, but the inner Coulombic cutoff can be >= 0.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- inner (distance units)
- outer (distance units)

Note that sigma is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum at 2^(1/6) sigma.

The last 2 coefficients are optional inner and outer cutoffs for style *lj/gromacs*. If not specified, the global *inner* and *outer* values are used.

The last 2 coefficients cannot be used with style *lj/gromacs/coul/gromacs* because this force field does not allow varying cutoffs for individual atom pairs; all pairs use the global cutoff(s) specified in the pair_style command.

Styles *intel*, *kk*, with a *cuda*, *gpu*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/cut pair styles can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

None of the GROMACS pair styles support the pair_modify shift option, since the Lennard-Jones portion of the pair interaction is already smoothed to 0.0 at the cutoff.

The pair_modify table option is not relevant for this pair style.

None of the GROMACS pair styles support the pair_modify tail option for adding long-range tail corrections to energy and pressure, since there are no corrections for a potential that goes to 0.0 at the cutoff.

All of the GROMACS pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

All of the GROMACS pair styles can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.

Restrictions: none

Related commands:

pair_coeff

Default: none

(Marrink) Marrink, de Vries, Mark, J Phys Chem B, 108, 750-760 (2004).

pair_style hbond/dreiding/lj command

pair_style hbond/dreiding/lj/omp command

pair_style hbond/dreiding/morse command

pair_style hbond/dreiding/morse/omp command

Syntax:

```
pair_style style N inner_distance_cutoff outer_distance_cutoff angle_cutof
```

- style = *hbond/dreiding/lj* or *hbond/dreiding/morse*
- n = cosine angle periodicity
- inner_distance_cutoff = global inner cutoff for Donor-Acceptor interactions (distance units)
- outer_distance_cutoff = global cutoff for Donor-Acceptor interactions (distance units)
- angle_cutoff = global angle cutoff for Acceptor-Hydrogen-Donor
- interactions (degrees)

Examples:

```
pair_style hybrid/overlay lj/cut 10.0 hbond/dreiding/lj 4 9.0 11.0 90
pair_coeff 1 2 hbond/dreiding/lj 3 i 9.5 2.75 4 9.0 11.0 90.0

pair_style hybrid/overlay lj/cut 10.0 hbond/dreiding/morse 2 9.0 11.0 90
pair_coeff 1 2 hbond/dreiding/morse 3 i 3.88 1.7241379 2.9 2 9 11 90
```

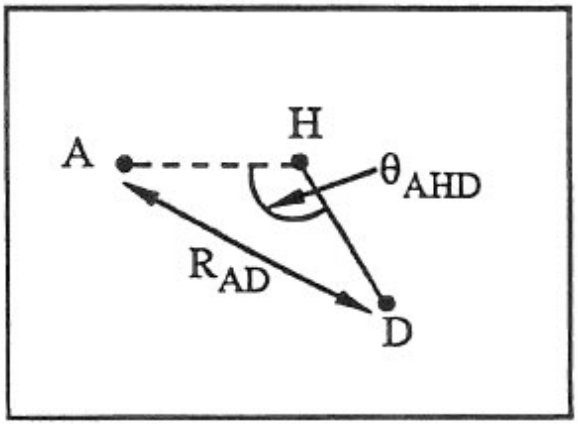
Description:

The *hbond/dreiding* styles compute the Acceptor-Hydrogen-Donor (AHD) 3-body hydrogen bond interaction for the DREIDING force field, given by:

$$
\begin{aligned}
E &= [LJ(r)|Morse(r)] && r < r_{\text{in}} \\
&= S(r) * [LJ(r)|Morse(r)] && r_{\text{in}} < r < r_{\text{out}} \\
&= 0 && r > r_{\text{out}} \\
LJ(r) &= AR^{-12} - BR^{-10} cos^n\theta = \epsilon \left\{ 5 \left[\frac{\sigma}{r}\right]^{12} - 6 \left[\frac{\sigma}{r}\right]^{10} \right\} cos^n\theta \\
Morse(r) &= D_0 \left\{ \chi^2 - 2\chi \right\} cos^n\theta = D_0 \left\{ e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)} \right\} cos^n\theta \\
S(r) &= \frac{\left[r_{\text{out}}^2 - r^2\right]^2 \left[r_{\text{out}}^2 + 2r^2 - 3r_{\text{in}}^2\right]}{\left[r_{\text{out}}^2 - {r_{\text{in}}}^2\right]^3}
\end{aligned}
$$

where Rin is the inner spline distance cutoff, Rout is the outer distance cutoff, theta_c is the angle cutoff, and n is the cosine periodicity.

Here, *r* is the radial distance between the donor (D) and acceptor (A) atoms and *theta* is the bond angle between the acceptor, the hydrogen (H) and the donor atoms:



These 3-body interactions can be defined for pairs of acceptor and donor atoms, based on atom types. For each donor/acceptor atom pair, the 3rd atom in the interaction is a hydrogen permanently bonded to the donor atom, e.g. in a bond list read in from a data file via the read_data command. The atom types of possible hydrogen atoms for each donor/acceptor type pair are specified by the pair_coeff command (see below).

Style *hbond/dreiding/lj* is the original DREIDING potential of (Mayo). It uses a LJ 12/10 functional for the Donor-Acceptor interactions. To match the results in the original paper, use n = 4.

Style *hbond/dreiding/morse* is an improved version using a Morse potential for the Donor-Acceptor interactions. (Liu) showed that the Morse form gives improved results for Dendrimer simulations, when n = 2.

See this howto section of the manual for more information on the DREIDING forcefield.

NOTE: Because the Dreiding hydrogen bond potential is only one portion of an overall force field which typically includes other pairwise interactions, it is common to use it as a sub-style in a pair_style hybrid/overlay command, where another pair style provides the repulsive core interaction between pairs of atoms, e.g. a 1/r^12 Lennard-Jones repulsion.

NOTE: When using the hbond/dreiding pair styles with pair_style hybrid/overlay, you should explicitly define pair interactions between the donor atom and acceptor atoms, (as well as between these atoms and ALL other atoms in your system). Whenever pair_style hybrid/overlay is used, ordinary mixing rules are not applied to atoms like the donor and acceptor atoms because they are typically referenced in multiple pair styles. Neglecting to do this can cause difficult-to-detect physics problems.

NOTE: In the original Dreiding force field paper 1-4 non-bonded interactions ARE allowed. If this is desired for your model, use the special_bonds command (e.g. "special_bonds lj 0.0 0.0 1.0") to turn these interactions on.

The following coefficients must be defined for pairs of eligible donor/acceptor types via the pair_coeff command as in the examples above.

NOTE: Unlike other pair styles and their associated pair_coeff commands, you do not need to specify pair_coeff settings for all possible I,J type pairs. Only I,J type pairs for atoms which act as joint donors/acceptors need to be specified; all other type pairs are assumed to be inactive.

NOTE: A pair_coeff command can be speficied multiple times for the same donor/acceptor type pair. This enables multiple hydrogen types to be assigned to the same donor/acceptor type pair. For other pair_styles, if the pair_coeff command is re-used for the same I.J type pair, the settings for that type pair are overwritten. For the hydrogen bond potentials this is not the case; the settings are cummulative. This means the only way to turn off a previous setting, is to re-use the pair_style command and start over.

For the *hbond/dreiding/lj* style the list of coefficients is as follows:

- K = hydrogen atom type = 1 to Ntypes
- donor flag = *i* or *j*
- epsilon (energy units)
- sigma (distance units)
- n = exponent in formula above
- distance cutoff Rin (distance units)
- distance cutoff Rout (distance units)
- angle cutoff (degrees)

For the *hbond/dreiding/morse* style the list of coefficients is as follows:

- K = hydrogen atom type = 1 to Ntypes
- donor flag = *i* or *j*
- D0 (energy units)
- alpha (1/distance units)
- r0 (distance units)
- n = exponent in formula above
- distance cutoff Rin (distance units)
- distance cutoff Rout (distance units)
- angle cutoff (degrees)

A single hydrogen atom type K can be specified, or a wild-card asterisk can be used in place of or in conjunction with the K arguments to select multiple types as hydrogens. This takes the form "*" or "*n" or "n*" or "m*n". See

the pair_coeff command doc page for details.

If the donor flag is *i*, then the atom of type I in the pair_coeff command is treated as the donor, and J is the acceptor. If the donor flag is *j*, then the atom of type J in the pair_coeff command is treated as the donor and I is the donor. This option is required because the pair_coeff command requires that I <= J.

Epsilon and sigma are settings for the hydrogen bond potential based on a Lennard-Jones functional form. Note that sigma is defined as the zero-crossing distance for the potential, not as the energy minimum at 2^(1/6) sigma.

D0 and alpha and r0 are settings for the hydrogen bond potential based on a Morse functional form.

The last 3 coefficients for both styles are optional. If not specified, the global n, distance cutoff, and angle cutoff specified in the pair_style command are used. If you wish to only override the 2nd or 3rd optional parameter, you must also specify the preceding optional parameters.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. You must explicitly identify each donor/acceptor type pair.

These styles do not support the pair_modify shift option for the energy of the interactions.

The pair_modify table option is not relevant for these pair styles.

These pair styles do not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

These pair styles do not write their information to binary restart files, so pair_style and pair_coeff commands need to be re-specified in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.

These pair styles tally a count of how many hydrogen bonding interactions they calculate each timestep and the hbond energy. These quantities can be accessed via the compute pair command as a vector of values of length 2.

To print these quantities to the log file (with a descriptive column heading) the following commands could be included in an input script:

```
compute hb all pair hbond/dreiding/lj
variable n_hbond equal c_hb[1] #number hbonds
variable E_hbond equal c_hb[2] #hbond energy
thermo_style custom step temp epair v_E_hbond
```

Restrictions: none

Related commands:

pair_coeff

Default: none

(Mayo) Mayo, Olfason, Goddard III, J Phys Chem, 94, 8897-8909 (1990).

(Liu) Liu, Bryantsev, Diallo, Goddard III, J. Am. Chem. Soc 131 (8) 2798 (2009)

pair_style hybrid command

pair_style hybrid/omp command

pair_style hybrid/overlay command

pair_style hybrid/overlay/omp command

Syntax:

```
pair_style hybrid style1 args style2 args ...
pair_style hybrid/overlay style1 args style2 args ...
```

- style1,style2 = list of one or more pair styles and their arguments

Examples:

```
pair_style hybrid lj/cut/coul/cut 10.0 eam lj/cut 5.0
pair_coeff 1*2 1*2 eam niu3
pair_coeff 3 3 lj/cut/coul/cut 1.0 1.0
pair_coeff 1*2 3 lj/cut 0.5 1.2

pair_style hybrid/overlay lj/cut 2.5 coul/long 2.0
pair_coeff * * lj/cut 1.0 1.0
pair_coeff * * coul/long
```

Description:

The *hybrid* and *hybrid/overlay* styles enable the use of multiple pair styles in one simulation. With the *hybrid* style, exactly one pair style is assigned to each pair of atom types. With the *hybrid/overlay* style, one or more pair styles can be assigned to each pair of atom types. The assignment of pair styles to type pairs is made via the pair_coeff command.

Here are two examples of hybrid simulations. The *hybrid* style could be used for a simulation of a metal droplet on a LJ surface. The metal atoms interact with each other via an *eam* potential, the surface atoms interact with each other via a *lj/cut* potential, and the metal/surface interaction is also computed via a *lj/cut* potential. The *hybrid/overlay* style could be used as in the 2nd example above, where multiple potentials are superposed in an additive fashion to compute the interaction between atoms. In this example, using *lj/cut* and *coul/long* together gives the same result as if the *lj/cut/coul/long* potential were used by itself. In this case, it would be more efficient to use the single combined potential, but in general any combination of pair potentials can be used together in to produce an interaction that is not encoded in any single pair_style file, e.g. adding Coulombic forces between granular particles.

All pair styles that will be used are listed as "sub-styles" following the *hybrid* or *hybrid/overlay* keyword, in any order. Each sub-style's name is followed by its usual arguments, as illustrated in the example above. See the doc pages of individual pair styles for a listing and explanation of the appropriate arguments.

Note that an individual pair style can be used multiple times as a sub-style. For efficiency this should only be done if your model requires it. E.g. if you have different regions of Si and C atoms and wish to use a Tersoff potential for pure Si for one set of atoms, and a Tersoff potetnial for pure C for the other set (presumably with some 3rd potential for Si-C interactions), then the sub-style *tersoff* could be listed twice. But if you just want to

use a Lennard-Jones or other pairwise potential for several different atom type pairs in your model, then you should just list the sub-style once and use the pair_coeff command to assign parameters for the different type pairs.

NOTE: There are two exceptions to this option to list an individual pair style multiple times. The first is for pair styles implemented as Fortran libraries: pair_style meam and pair_style reax (pair_style reax/c is OK). This is because unlike a C++ class, they can not be instantiated multiple times, due to the manner in which they were coded in Fortran. The second is for GPU-enabled pair styles in the GPU package. This is b/c the GPU package also currently assumes that only one instance of a pair style is being used.

In the pair_coeff commands, the name of a pair style must be added after the I,J type specification, with the remaining coefficients being those appropriate to that style. If the pair style is used multiple times in the pair_style command, then an additional numeric argument must also be specified which is a number from 1 to M where M is the number of times the sub-style was listed in the pair style command. The extra number indicates which instance of the sub-style these coefficients apply to.

For example, consider a simulation with 3 atom types: types 1 and 2 are Ni atoms, type 3 are LJ atoms with charges. The following commands would set up a hybrid simulation:

```
pair_style hybrid eam/alloy lj/cut/coul/cut 10.0 lj/cut 8.0
pair_coeff * * eam/alloy nialhjea Ni Ni NULL
pair_coeff 3 3 lj/cut/coul/cut 1.0 1.0
pair_coeff 1*2 3 lj/cut 0.8 1.3
```

As an example of using the same pair style multiple times, consider a simulation with 2 atom types. Type 1 is Si, type 2 is C. The following commands would model the Si atoms with Tersoff, the C atoms with Tersoff, and the cross-interactions with Lennard-Jones:

```
pair_style hybrid lj/cut 2.5 tersoff tersoff
pair_coeff * * tersoff 1 Si.tersoff Si NULL
pair_coeff * * tersoff 2 C.tersoff NULL C
pair_coeff 1 2 lj/cut 1.0 1.5
```

If pair coefficients are specified in the data file read via the read_data command, then the same rule applies. E.g. "eam/alloy" or "lj/cut" must be added after the atom type, for each line in the "Pair Coeffs" section, e.g.

```
Pair Coeffs

1 lj/cut/coul/cut 1.0 1.0
...
```

Note that the pair_coeff command for some potentials such as pair_style eam/alloy includes a mapping specification of elements to all atom types, which in the hybrid case, can include atom types not assigned to the *eam/alloy* potential. The NULL keyword is used by many such potentials (eam/alloy, Tersoff, AIREBO, etc), to denote an atom type that will be assigned to a different sub-style.

For the *hybrid* style, each atom type pair I,J is assigned to exactly one sub-style. Just as with a simulation using a single pair style, if you specify the same atom type pair in a second pair_coeff command, the previous assignment will be overwritten.

For the *hybrid/overlay* style, each atom type pair I,J can be assigned to one or more sub-styles. If you specify the same atom type pair in a second pair_coeff command with a new sub-style, then the second sub-style is added to the list of potentials that will be calculated for two interacting atoms of those types. If you specify the same atom type pair in a second pair_coeff command with a sub-style that has already been defined for that pair of atoms,

then the new pair coefficients simply override the previous ones, as in the normal usage of the pair_coeff command. E.g. these two sets of commands are the same:

```
pair_style lj/cut 2.5
pair_coeff * * 1.0 1.0
pair_coeff 2 2 1.5 0.8

pair_style hybrid/overlay lj/cut 2.5
pair_coeff * * lj/cut 1.0 1.0
pair_coeff 2 2 lj/cut 1.5 0.8
```

Coefficients must be defined for each pair of atoms types via the pair_coeff command as described above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below.

For both the *hybrid* and *hybrid/overlay* styles, every atom type pair I,J (where I <= J) must be assigned to at least one sub-style via the pair_coeff command as in the examples above, or in the data file read by the read_data, or by mixing as described below.

If you want there to be no interactions between a particular pair of atom types, you have 3 choices. You can assign the type pair to some sub-style and use the neigh_modify exclude type command. You can assign it to some sub-style and set the coefficients so that there is effectively no interaction (e.g. epsilon = 0.0 in a LJ potential). Or, for *hybrid* and *hybrid/overlay* simulations, you can use this form of the pair_coeff command in your input script:

```
pair_coeff      2 3 none
```

or this form in the "Pair Coeffs" section of the data file:

```
3 none
```

If an assignment to *none* is made in a simulation with the *hybrid/overlay* pair style, it wipes out all previous assignments of that atom type pair to sub-styles.

Note that you may need to use an atom_style hybrid command in your input script, if atoms in the simulation will need attributes from several atom styles, due to using multiple pair potentials.

Different force fields (e.g. CHARMM vs AMBER) may have different rules for applying weightings that change the strength of pairwise interactions bewteen pairs of atoms that are also 1-2, 1-3, and 1-4 neighbors in the molecular bond topology, as normally set by the special_bonds command. Different weights can be assigned to different pair hybrid sub-styles via the pair_modify special command. This allows multiple force fields to be used in a model of a hybrid system, however, there is no consistent approach to determine parameters automatically for the interactions between the two force fields, this is only recommended when particles described by the different force fields do not mix.

Here is an example for mixing CHARMM and AMBER: The global *amber* setting sets the 1-4 interactions to non-zero scaling factors and then overrides them with 0.0 only for CHARMM:

```
special_bonds amber
pair_hybrid lj/charmm/coul/long 8.0 10.0 lj/cut/coul/long 10.0
pair_modify pair lj/charmm/coul/long special lj/coul 0.0 0.0 0.0
```

The this input achieves the same effect:

```
special_bonds 0.0 0.0 0.1
pair_hybrid lj/charmm/coul/long 8.0 10.0 lj/cut/coul/long 10.0
```

```
pair_modify pair lj/cut/coul/long special lj 0.0 0.0 0.5
pair_modify pair lj/cut/coul/long special coul 0.0 0.0 0.83333333
pair_modify pair lj/charmm/coul/long special lj/coul 0.0 0.0 0.0
```

Here is an example for mixing Tersoff with OPLS/AA based on a data file that defines bonds for all atoms where for the Tersoff part of the system the force constants for the bonded interactions have been set to 0. Note the global settings are effectively *lj/coul 0.0 0.0 0.5* as required for OPLS/AA:

```
special_bonds lj/coul 1e-20 1e-20 0.5
pair_hybrid tersoff lj/cut/coul/long 12.0
pair_modify pair tersoff special lj/coul 1.0 1.0 1.0
```

See the pair_modify doc page for details on the specific syntax, requirements and restrictions.

The potential energy contribution to the overall system due to an individual sub-style can be accessed and output via the compute pair command.

NOTE: Several of the potentials defined via the pair_style command in LAMMPS are really many-body potentials, such as Tersoff, AIREBO, MEAM, ReaxFF, etc. The way to think about using these potentials in a hybrid setting is as follows.

A subset of atom types is assigned to the many-body potential with a single pair_coeff command, using "* *" to include all types and the NULL keywords described above to exclude specific types not assigned to that potential. If types 1,3,4 were assigned in that way (but not type 2), this means that all many-body interactions between all atoms of types 1,3,4 will be computed by that potential. Pair_style hybrid allows interactions between type pairs 2-2, 1-2, 2-3, 2-4 to be specified for computation by other pair styles. You could even add a second interaction for 1-1 to be computed by another pair style, assuming pair_style hybrid/overlay is used.

But you should not, as a general rule, attempt to exclude the many-body interactions for some subset of the type pairs within the set of 1,3,4 interactions, e.g. exclude 1-1 or 1-3 interactions. That is not conceptually well-defined for many-body interactions, since the potential will typically calculate energies and foces for small groups of atoms, e.g. 3 or 4 atoms, using the neighbor lists of the atoms to find the additional atoms in the group. It is typically non-physical to think of excluding an interaction between a particular pair of atoms when the potential computes 3-body or 4-body interactions.

However, you can still use the pair_coeff none setting or the neigh_modify exclude command to exclude certain type pairs from the neighbor list that will be passed to a manybody sub-style. This will alter the calculations made by a many-body potential, since it builds its list of 3-body, 4-body, etc interactions from the pair list. You will need to think carefully as to whether it produces a physically meaningful result for your model.

For example, imagine you have two atom types in your model, type 1 for atoms in one surface, and type 2 for atoms in the other, and you wish to use a Tersoff potential to compute interactions within each surface, but not between surfaces. Then either of these two command sequences would implement that model:

```
pair_style hybrid tersoff
pair_coeff * * tersoff SiC.tersoff C C
pair_coeff 1 2 none

pair_style tersoff
pair_coeff * * SiC.tersoff C C
neigh_modify exclude type 1 2
```

Either way, only neighbor lists with 1-1 or 2-2 interactions would be passed to the Tersoff potential, which means it would compute no 3-body interactions containing both type 1 and 2 atoms.

Here is another example, using hybrid/overlay, to use 2 many-body potentials together, in an overlapping manner. Imagine you have CNT (C atoms) on a Si surface. You want to use Tersoff for Si/Si and Si/C interactions, and AIREBO for C/C interactions. Si atoms are type 1; C atoms are type 2. Something like this will work:

```
pair_style hybrid/overlay tersoff airebo 3.0
pair_coeff * * tersoff SiC.tersoff.custom Si C
pair_coeff * * airebo CH.airebo NULL C
```

Note that to prevent the Tersoff potential from computing C/C interactions, you would need to modify the SiC.tersoff file to turn off C/C interaction, i.e. by setting the appropriate coefficients to 0.0.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual.

Since the *hybrid* and *hybrid/overlay* styles delegate computation to the individual sub-styles, the suffix versions of the *hybrid* and *hybrid/overlay* styles are used to propagate the corresponding suffix to all sub-styles, if those versions exist. Otherwise the non-accelerated version will be used.

The individual accelerated sub-styles are part of the USER-CUDA, GPU, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

Any pair potential settings made via the pair_modify command are passed along to all sub-styles of the hybrid potential.

For atom type pairs I,J and I != J, if the sub-style assigned to I,I and J,J is the same, and if the sub-style allows for mixing, then the coefficients for I,J can be mixed. This means you do not have to specify a pair_coeff command for I,J since the I,J type pair will be assigned automatically to the sub-style defined for both I,I and J,J and its coefficients generated by the mixing rule used by that sub-style. For the *hybrid/overlay* style, there is an additional requirement that both the I,I and J,J pairs are assigned to a single sub-style. See the "pair_modify" command for details of mixing rules. See the See the doc page for the sub-style to see if allows for mixing.

The hybrid pair styles supports the pair_modify shift, table, and tail options for an I,J pair interaction, if the associated sub-style supports it.

For the hybrid pair styles, the list of sub-styles and their respective settings are written to binary restart files, so a pair_style command does not need to specified in an input script that reads a restart file. However, the coefficient information is not stored in the restart file. Thus, pair_coeff commands need to be re-specified in the restart input script.

These pair styles support the use of the *inner*, *middle*, and *outer* keywords of the run_style respa command, if their sub-styles do.

Restrictions:

When using a long-range Coulombic solver (via the kspace_style command) with a hybrid pair_style, one or more sub-styles will be of the "long" variety, e.g. *lj/cut/coul/long* or *buck/coul/long*. You must insure that the short-range Coulombic cutoff used by each of these long pair styles is the same or else LAMMPS will generate an error.

Related commands:

pair_coeff

Default: none

pair_style kim command

Syntax:

```
pair_style kim virialmode model printflag
```

- virialmode = KIMvirial or LAMMPSvirial
- model = name of KIM model (potential)
- printflag = 1/0 do or do not print KIM descriptor file, optional

Examples:

```
pair_style kim KIMvirial model_Ar_P_Morse
pair_coeff * * Ar Ar

pair_style kim KIMvirial model_Ar_P_Morse 1
pair_coeff * * Ar Ar
```

Description:

This pair style is a wrapper on the Knowledge Base for Interatomic Models (KIM) repository of interatomic potentials, so that they can be used by LAMMPS scripts.

In KIM lingo, a potential is a "model" and a model contains both the analytic formulas that define the potential as well as the parameters needed to run it for one or more materials, including coefficients and cutoffs.

The argument *virialmode* determines how the global virial is calculated. If *KIMvirial* is specified, the KIM model performs the global virial calculation (if it knows how). If *LAMMPSvirial* is specified, LAMMPS computes the global virial using its fdotr mechanism.

The argument *model* is the name of the KIM model for a specific potential as KIM defines it. In principle, LAMMPS can invoke any KIM model. You should get an error or warning message from either LAMMPS or KIM if there is an incompatibility.

The argument *printflag* is optional. If it is set to a non-zero value then a KIM dsecriptor file is printed when KIM is invoked. This can be useful for debugging. The default is to not print this file.

Only a single pair_coeff command is used with the *kim* style which specifies the mapping of LAMMPS atom types to KIM elements. This is done by specifying N additional arguments after the * * in the pair_coeff command, where N is the number of LAMMPS atom types:

- N element names = mapping of KIM elements to atom types

As an example, imagine the KIM model supports Si and C atoms. If your LAMMPS simulation has 4 atom types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to Si as defined within KIM. The final C argument maps LAMMPS atom type 4 to C as defined within KIM. If a mapping value is specified as NULL, the mapping is not performed. This can only be

used when a *kim* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

In addition to the usual LAMMPS error messages, the KIM library itself may generate errors, which should be printed to the screen. In this case it is also useful to check the kim.log file for additional error information. This file kim.log should be generated in the same directory where LAMMPS is running.

To download, build, and install the KIM library on your system, see the lib/kim/README file. Once you have done this and built LAMMPS with the KIM package installed you can run the example input scripts in examples/kim.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the pair_modify mix, shift, table, and tail options.

This pair style does not write its information to binary restart files, since KIM stores the potential parameters. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the KIM package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This current version of pair_style kim is compatible with the kim-api package version 1.6.0 and higher.

Related commands:

pair_coeff

Default: none

pair_style lcbop command

Syntax:

```
pair_style lcbop
```

Examples:

```
pair_style lcbop
pair_coeff * * ../potentials/C.lcbop C
```

Description:

The *lcbop* pair style computes the long-range bond-order potential for carbon (LCBOP) of (Los and Fasolino). See section II in that paper for the analytic equations associated with the potential.

Only a single pair_coeff command is used with the *lcbop* style which specifies an LCBOP potential file with parameters for specific elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of LCBOP elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file.

As an example, if your LAMMPS simulation has 4 atom types and you want the 1st 3 to be C you would use the following pair_coeff command:

```
pair_coeff * * C.lcbop C C C NULL
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first C argument maps LAMMPS atom type 1 to the C element in the LCBOP file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *lcbop* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

The parameters/coefficients for the LCBOP potential as applied to C are listed in the C.lcbop file to agree with the original (Los and Fasolino) paper. Thus the parameters are specific to this potential and the way it was fit, so modifying the file should be done carefully.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the pair_modify mix, shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair styles is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

This pair potential requires the newton setting to be "on" for pair interactions.

The C.lcbop potential file provided with LAMMPS (see the potentials directory) is parameterized for metal units. You can use the LCBOP potential with any LAMMPS units, but you would need to create your own LCBOP potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

Related commands:

pair_airebo, pair_coeff

Default: none

(Los and Fasolino) J. H. Los and A. Fasolino, Phys. Rev. B 68, 024107 (2003).

pair_style line/lj command

Syntax:

```
pair_style line/lj cutoff
```

cutoff = global cutoff for interactions (distance units)

Examples:

```
pair_style line/lj 3.0
pair_coeff * * 1.0 1.0 1.0 0.8 1.12
pair_coeff 1 2 1.0 2.0 1.0 1.5 1.12 5.0
pair_coeff 1 2 1.0 0.0 1.0 1.0 2.5
```

Description:

Style *line/lj* treats particles which are line segments as a set of small spherical particles that tile the line segment length as explained below. Interactions between two line segments, each with N1 and N2 spherical particles, are calculated as the pairwise sum of N1*N2 Lennard-Jones interactions. Interactions between a line segment with N spherical particles and a point particle are treated as the pairwise sum of N Lennard-Jones interactions. See the pair_style lj/cut doc page for the definition of Lennard-Jones interactions.

The set of non-overlapping spherical sub-particles that represent a line segment are generated in the following manner. Their size is a function of the line segment length and the specified sub-particle size for that particle type. If a line segment has a length L and is of type I, then the number of spheres N that represent the segment is calculated as N = L/sizeI, rounded up to an integer value. Thus if L is not evenly divisibly by sizeI, N is incremented to include one extra sphere. The centers of the spheres are spaced equally along the line segment. Imagine N+1 equally-space points, which include the 2 end points of the segment. The sphere centers are halfway between each pair of points.

The LJ interaction between 2 spheres on different line segments (or a sphere on a line segment and a point particles) is computed with sub-particle epsilon, sigma, and cutoff values that are set by the pair_coeff command, as described below. If the distance bewteen the 2 spheres is greater than the sub-particle cutoff, there is no interaction. This means that some pairs of sub-particles on 2 line segments may interact, but others may not.

For purposes of creating the neighbor list for pairs of interacting line segments or lines/point particles, a regular particle-particle cutoff is used, as defined by the *cutoff* setting above in the pair_style command or overridden with an optional argument in the pair_coeff command for a type pair as discussed below. The distance between the centers of 2 line segments, or the center of a line segment and a point particle, must be less than this distance (plus the neighbor skin; see the neighbor command), for the pair of particles to be included in the neighbor list.

NOTE: This means that a too-short value for the *cutoff* setting can exclude a pair of particles from the neighbor list even if pairs of their sub-particle spheres would interact, based on the sub-particle cutoff specified in the pair_coeff command. E.g. sub-particles at the ends of the line segments that are close to each other. Which may not be what you want, since it means the ends of 2 line segments could pass through each other. It is up to you to specify a *cutoff* setting that is consistent with the length of the line segments you are using and the sub-particle cutoff settings.

For style *line/lj*, the following coefficients must be defined for each pair of atom types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart

commands:

- sizeI (distance units)
- sizeJ (distance units)
- epsilon (energy units)
- sigma (distance units)
- subcutoff (distance units)
- cutoff (distance units)

The *sizeI* and *sizeJ* coefficients are the sub-particle sizes for line particles of type I and type J. They are used to define the N sub-particles per segment as described above. These coefficients are actually stored on a per-type basis. Thus if there are multiple pair_coeff commmands that involve type I, as either the first or second atom type, you should use consistent values for sizeI or sizeJ in all of them. If you do not do this, the last value specified for sizeI will apply to all segments of type I. If typeI or typeJ refers to point particles, the corresponding sizeI or sizeJ is ignored; it can be set to 0.0.

The *epsilon*, *sigma*, and *subcutoff* coefficients are used to compute an LJ interactions between a pair of sub-particles on 2 line segments (of type I and J), or between a sub particle/point particle pair. As discussed above, the *subcutoff* and *cutoff* params are different. The latter is only used for building the neighbor list when the distance between centers of two line segments or one segment and a point particle is calculated.

The *cutoff* coefficient is optional. If not specified, the global cutoff is used.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, coeffiecients must be specified. No default mixing rules are used.

This pair style does not support the pair_modify shift, table, and tail options.

This pair style does not write its information to binary restart files.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This style is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Defining particles to be line segments so they participate in line/line or line/particle interactions requires the use the atom_style line command.

Related commands:

pair_coeff, pair_style tri/lj

Default: none

pair_style list command

Syntax:

```
pair_style list listfile cutoff keyword
```

- listfile = name of file with list of pairwise interactions
- cutoff = global cutoff (distance units)
- keyword = optional flag *nocheck* or *check* (default is *check*)

Examples:

```
pair_style list restraints.txt 200.0
pair_coeff * *

pair_style hybrid/overlay lj/cut 1.1225 list pair_list.txt 300.0
pair_coeff * * lj/cut 1.0 1.0
pair_coeff 3* 3* list
```

Description:

Style *list* computes interactions between explicitly listed pairs of atoms with the option to select functional form and parameters for each individual pair. Because the parameters are set in the list file, the pair_coeff command has no parameters (but still needs to be provided). The *check* and *nocheck* keywords enable/disable a test that checks whether all listed bonds were present and computed.

This pair style can be thought of as a hybrid between bonded, non-bonded, and restraint interactions. It will typically be used as an additional interaction within the *hybrid/overlay* pair style. It currently supports three interaction styles: a 12-6 Lennard-Jones, a Morse and a harmonic potential.

The format of the list file is as follows:

- one line per pair of atoms
- empty lines will be ignored
- comment text starts with a '#' character
- line syntax: *ID1 ID2 style coeffs cutoff*

```
ID1 = atom ID of first atom
ID2 = atom ID of second atom
style = style of interaction
coeffs = list of coeffs
cutoff = cutoff for interaction (optional)
```

The cutoff parameter is optional. If not specified, the global cutoff is used.

Here is an example file:

```
# this is a comment

15 259 lj126     1.0 1.0      50.0
15 603 morse    10.0 1.2 2.0  10.0 # and another comment
18 470 harmonic 50.0 1.2       5.0
```

The style *lj126* computes pairwise interactions with the formula

$$E = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \qquad r < r_c$$

and the coefficients:

- epsilon (energy units)
- sigma (distance units)

The style *morse* computes pairwise interactions with the formula

$$E = D_0 \left[e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)} \right] \qquad r < r_c$$

and the coefficients:

- D0 (energy units)
- alpha (1/distance units)
- r0 (distance units)

The style *harmonic* computes pairwise interactions with the formula

$$E = K(r - r_0)^2$$

and the coefficients:

- K (energy units)
- r0 (distance units)

Note that the usual 1/2 factor is included in K.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support mixing since all parameters are explicit for each pair.

The pair_modify shift option is supported by this pair style.

The pair_modify table and tail options are not relevant for this pair style.

This pair style does not write its information to binary restart files, so pair_style and pair_coeff commands need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style does not use a neighbor list and instead identifies atoms by their IDs. This has two consequences: 1) The cutoff has to be chosen sufficiently large, so that the second atom of a pair has to be a ghost atom on the same node on which the first atom is local; otherwise the interaction will be skipped. You can use the *check* option to detect, if interactions are missing. 2) Unlike other pair styles in LAMMPS, an atom I will not interact with multiple images of atom J (assuming the images are within the cutoff distance), but only with the nearest image.

This style is part of the USER-MISC package. It is only enabled if LAMMPS is build with that package. See the Making of LAMMPS section for more info.

Related commands:

pair_coeff, pair_style hybrid/overlay, pair_style lj/cut, pair_style morse, bond_style harmonic

Default: none

pair_style lj/cut command

pair_style lj/cut/cuda command

pair_style lj/cut/gpu command

pair_style lj/cut/intel command

pair_style lj/cut/kk command

pair_style lj/cut/opt command

pair_style lj/cut/omp command

pair_style lj/cut/coul/cut command

pair_style lj/cut/coul/cut/cuda command

pair_style lj/cut/coul/cut/gpu command

pair_style lj/cut/coul/cut/omp command

pair_style lj/cut/coul/debye command

pair_style lj/cut/coul/debye/cuda command

pair_style lj/cut/coul/debye/gpu command

pair_style lj/cut/coul/debye/kk command

pair_style lj/cut/coul/debye/omp command

pair_style lj/cut/coul/dsf command

pair_style lj/cut/coul/dsf/gpu command

pair_style lj/cut/coul/dsf/kk command

pair_style lj/cut/coul/dsf/omp command

pair_style lj/cut/coul/long command

pair_style lj/cut/coul/long/cs command

pair_style lj/cut/coul/long/cuda command

pair_style lj/cut/coul/long/gpu command

pair_style lj/cut/coul/long/intel command

pair_style lj/cut/coul/long/opt command

pair_style lj/cut/coul/long/omp command

pair_style lj/cut/coul/msm command

pair_style lj/cut/coul/msm/gpu command

pair_style lj/cut/coul/msm/omp command

pair_style lj/cut/tip4p/cut command

pair_style lj/cut/tip4p/cut/omp command

pair_style lj/cut/tip4p/long command

pair_style lj/cut/tip4p/long/omp command

pair_style lj/cut/tip4p/long/opt command

Syntax:

```
pair_style style args
```

- style = *lj/cut* or *lj/cut/coul/cut* or *lj/cut/coul/debye* or *lj/cut/coul/dsf* or *lj/cut/coul/long* or *lj/cut/coul/long/cs* or *lj/cut/coul/msm* or *lj/cut/tip4p/long*
- args = list of arguments for a particular style

```
lj/cut args = cutoff
    cutoff = global cutoff for Lennard Jones interactions (distance units)
  lj/cut/coul/cut args = cutoff (cutoff2)
    cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
  lj/cut/coul/debye args = kappa cutoff (cutoff2)
    kappa = inverse of the Debye length (inverse distance units)
    cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
  lj/cut/coul/dsf args = alpha cutoff (cutoff2)
    alpha = damping parameter (inverse distance units)
    cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (distance units)
  lj/cut/coul/long args = cutoff (cutoff2)
    cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

```
  lj/cut/coul/msm args = cutoff (cutoff2)
    cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
  lj/cut/tip4p/cut args = otype htype btype atype qdist cutoff (cutoff2)
    otype,htype = atom types for TIP4P O and H
    btype,atype = bond and angle types for TIP4P waters
    qdist = distance from O atom to massless charge (distance units)
    cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
  lj/cut/tip4p/long args = otype htype btype atype qdist cutoff (cutoff2)
    otype,htype = atom types for TIP4P O and H
    btype,atype = bond and angle types for TIP4P waters
    qdist = distance from O atom to massless charge (distance units)
    cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

Examples:

```
pair_style lj/cut 2.5
pair_coeff * * 1 1
pair_coeff 1 1 1 1.1 2.8

pair_style lj/cut/coul/cut 10.0
pair_style lj/cut/coul/cut 10.0 8.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0
pair_coeff 1 1 100.0 3.5 9.0 9.0

pair_style lj/cut/coul/debye 1.5 3.0
pair_style lj/cut/coul/debye 1.5 2.5 5.0
pair_coeff * * 1.0 1.0
pair_coeff 1 1 1.0 1.5 2.5
pair_coeff 1 1 1.0 1.5 2.5 5.0

pair_style lj/cut/coul/dsf 0.05 2.5 10.0
pair_coeff * * 1.0 1.0
pair_coeff 1 1 1.0 1.0 2.5

pair_style lj/cut/coul/long 10.0
pair_style lj/cut/coul/long/cs 10.0
pair_style lj/cut/coul/long 10.0 8.0
pair_style lj/cut/coul/long/cs 10.0 8.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0

pair_style lj/cut/coul/msm 10.0
pair_style lj/cut/coul/msm 10.0 8.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0

pair_style lj/cut/tip4p/cut 1 2 7 8 0.15 12.0
pair_style lj/cut/tip4p/cut 1 2 7 8 0.15 12.0 10.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0

pair_style lj/cut/tip4p/long 1 2 7 8 0.15 12.0
pair_style lj/cut/tip4p/long 1 2 7 8 0.15 12.0 10.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0
```

Description:

The *lj/cut* styles compute the standard 12/6 Lennard-Jones potential, given by

$$E = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right] \qquad r < r_c$$

Rc is the cutoff.

Style *lj/cut/coul/cut* adds a Coulombic pairwise interaction given by

$$E = \frac{C q_i q_j}{\epsilon r} \qquad r < r_c$$

where C is an energy-conversion constant, Qi and Qj are the charges on the 2 atoms, and epsilon is the dielectric constant which can be set by the dielectric command. If one cutoff is specified in the pair_style command, it is used for both the LJ and Coulombic terms. If two cutoffs are specified, they are used as cutoffs for the LJ and Coulombic terms respectively.

Style *lj/cut/coul/debye* adds an additional exp() damping factor to the Coulombic term, given by

$$E = \frac{C q_i q_j}{\epsilon r} \exp(-\kappa r) \qquad r < r_c$$

where kappa is the inverse of the Debye length. This potential is another way to mimic the screening effect of a polar solvent.

Style *lj/cut/coul/dsf* computes the Coulombic term via the damped shifted force model described in Fennell, given by:

$$E = q_i q_j \left[\frac{\mathrm{erfc}(\alpha r)}{r} - \frac{\mathrm{erfc}(\alpha r_c)}{r_c} + \left(\frac{\mathrm{erfc}(\alpha r_c)}{r_c^2} + \frac{2\alpha}{\sqrt{\pi}} \frac{\exp(-\alpha^2 r_c^2)}{r_c} \right) (r - r_c) \right] \qquad r$$

where *alpha* is the damping parameter and erfc() is the complementary error-function. This potential is essentially a short-range, spherically-truncated, charge-neutralized, shifted, pairwise *1/r* summation. The potential is based on Wolf summation, proposed as an alternative to Ewald summation for condensed phase systems where charge screening causes electrostatic interactions to become effectively short-ranged. In order for the electrostatic sum to be absolutely convergent, charge neutralization within the cutoff radius is enforced by shifting the potential through placement of image charges on the cutoff sphere. Convergence can often be improved by setting *alpha* to a small non-zero value.

Styles *lj/cut/coul/long* and *lj/cut/coul/msm* compute the same Coulombic interactions as style *lj/cut/coul/cut* except that an additional damping factor is applied to the Coulombic term so it can be used in conjunction with the kspace_style command and its *ewald* or *pppm* option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

Style *lj/cut/coul/long/cs* is identical to *lj/cut/coul/long* except that a term is added for the core/shell model to allow charges on core and shell particles to be separated by r = 0.0.

Styles *lj/cut/tip4p/cut* and *lj/cut/tip4p/long* implement the TIP4P water model of (Jorgensen), which introduces a massless site located a short distance away from the oxygen atom along the bisector of the HOH angle. The atomic types of the oxygen and hydrogen atoms, the bond and angle types for OH and HOH interactions, and the distance to the massless charge site are specified as pair_style arguments. Style *lj/cut/tip4p/cut* uses a cutoff for Coulomb interactions; style *lj/cut/tip4p/long* is for use with a long-range Coulombic solver (Ewald or PPPM).

NOTE: For each TIP4P water molecule in your system, the atom IDs for the O and 2 H atoms must be consecutive, with the O atom first. This is to enable LAMMPS to "find" the 2 H atoms associated with each O atom. For example, if the atom ID of an O atom in a TIP4P water molecule is 500, then its 2 H atoms must have IDs 501 and 502.

See the howto section for more information on how to use the TIP4P pair styles and lists of parameters to set. Note that the neighobr list cutoff for Coulomb interactions is effectively extended by a distance 2*qdist when using the TIP4P pair style, to account for the offset distance of the fictitious charges on O atoms in water molecules. Thus it is typically best in an efficiency sense to use a LJ cutoff >= Coulomb cutoff + 2*qdist, to shrink the size of the neighbor list. This leads to slightly larger cost for the long-range calculation, so you can test the trade-off for your model.

For all of the *lj/cut* pair styles, the following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- cutoff1 (distance units)
- cutoff2 (distance units)

Note that sigma is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum at 2^(1/6) sigma.

The latter 2 coefficients are optional. If not specified, the global LJ and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both LJ and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the LJ and Coulombic cutoffs for this type pair. You cannot specify 2 cutoffs for style *lj/cut*, since it has no Coulombic terms.

For *lj/cut/coul/long* and *lj/cut/coul/msm* and *lj/cut/tip4p/cut* and *lj/cut/tip4p/long* only the LJ cutoff can be specified since a Coulombic cutoff cannot be specified for an individual I,J type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/cut pair styles can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

All of the *lj/cut* pair styles support the pair_modify shift option for the energy of the Lennard-Jones portion of the pair interaction.

The *lj/cut/coul/long* and *lj/cut/tip4p/long* pair styles support the pair_modify table option since they can tabulate the short-range portion of the long-range Coulombic interaction.

All of the *lj/cut* pair styles support the pair_modify tail option for adding a long-range tail correction to the energy and pressure for the Lennard-Jones portion of the pair interaction.

All of the *lj/cut* pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

The *lj/cut* and *lj/cut/coul/long* pair styles support the use of the *inner*, *middle*, and *outer* keywords of the run_style respa command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. The other styles only support the *pair* keyword of run_style respa. See the run_style command for details.

Restrictions:

The *lj/cut/coul/long* and *lj/cut/tip4p/long* styles are part of the KSPACE package. The *lj/cut/tip4p/cut* style is part of the MOLECULE package. These styles are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info. Note that the KSPACE and MOLECULE packages are installed by default.

Related commands:

pair_coeff

Default: none

(Jorgensen) Jorgensen, Chandrasekhar, Madura, Impey, Klein, J Chem Phys, 79, 926 (1983).

(Fennell) C. J. Fennell, J. D. Gezelter, J Chem Phys, 124, 234104 (2006).

pair_style lj96/cut command

pair_style lj96/cut/cuda command

pair_style lj96/cut/gpu command

pair_style lj96/cut/omp command

Syntax:

```
pair_style lj96/cut cutoff
```

- cutoff = global cutoff for lj96/cut interactions (distance units)

Examples:

```
pair_style lj96/cut 2.5
pair_coeff * * 1.0 1.0 4.0
pair_coeff 1 1 1.0 1.0
```

Description:

The *lj96/cut* style compute a 9/6 Lennard-Jones potential, instead of the standard 12/6 potential, given by

$$E = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^9 - \left(\frac{\sigma}{r}\right)^6 \right] \qquad r < r_c$$

Rc is the cutoff.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global LJ cutoff specified in the pair_style command is used.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making

LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/cut pair styles can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style supports the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style supports the pair_modify tail option for adding a long-range tail correction to the energy and pressure of the pair interaction.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style supports the use of the *inner*, *middle*, and *outer* keywords of the run_style respa command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. See the run_style command for details.

Restrictions: none

Related commands:

pair_coeff

Default: none

pair_style lj/cubic command

pair_style lj/cubic/gpu command

pair_style lj/cubic/omp command

Syntax:

```
pair_style lj/cubic
```

Examples:

```
pair_style lj/cubic
pair_coeff * * 1.0 0.8908987
```

Description:

The *lj/cubic* style computes a truncated LJ interaction potential whose energy and force are continuous everywhere. Inside the inflection point the interaction is identical to the standard 12/6 Lennard-Jones potential. The LJ function outside the inflection point is replaced with a cubic function of distance. The energy, force, and second derivative are continuous at the inflection point. The cubic coefficient A3 is chosen so that both energy and force go to zero at the cutoff distance. Outside the cutoff distance the energy and force are zero.

$$
\begin{aligned}
E &= u_{LJ}(r) \qquad r \le r_s \\
&= u_{LJ}(r_s) + (r - r_s)u'_{LJ}(r_s) - \frac{1}{6}A_3(r - r_s)^3 \qquad r_s < r \le r_c \\
&= 0 \qquad r > r_c
\end{aligned}
$$

The location of the inflection point rs is defined by the LJ diameter, rs/sigma = (26/7)^1/6. The cutoff distance is defined by rc/rs = 67/48 or rc/sigma = 1.737.... The analytic expression for the the cubic coefficient A3*rmin^3/epsilon = 27.93... is given in the paper by Holian and Ravelo (Holian).

This potential is commonly used to study the shock mechanics of FCC solids, as in Ravelo et al. (Ravelo).

The following coefficients must be defined for each pair of atom types via the pair_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)

Note that sigma is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum, which is located at rmin = 2^(1/6)*sigma. In the above example, sigma = 0.8908987, so rmin = 1.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without

the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/cut pair styles can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

The lj/cubic pair style does not support the pair_modify shift option, since pair interaction is already smoothed to 0.0 at the cutoff.

The pair_modify table option is not relevant for this pair style.

The lj/cubic pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure, since there are no corrections for a potential that goes to 0.0 at the cutoff.

The lj/cubic pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

The lj/cubic pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions: none

Related commands:

pair_coeff

Default: none

(Holian) Holian and Ravelo, Phys Rev B, 51, 11275 (1995).

(Ravelo) Ravelo, Holian, Germann and Lomdahl, Phys Rev B, 70, 014103 (2004).

pair_style lj/expand command

pair_style lj/expand/cuda command

pair_style lj/expand/gpu command

pair_style lj/expand/omp command

Syntax:

```
pair_style lj/expand cutoff
```

- cutoff = global cutoff for lj/expand interactions (distance units)

Examples:

```
pair_style lj/expand 2.5
pair_coeff * * 1.0 1.0 0.5
pair_coeff 1 1 1.0 1.0 -0.2 2.0
```

Description:

Style *lj/expand* computes a LJ interaction with a distance shifted by delta which can be useful when particles are of different sizes, since it is different that using different sigma values in a standard LJ formula:

$$E = 4\epsilon \left[\left(\frac{\sigma}{r - \Delta} \right)^{12} - \left(\frac{\sigma}{r - \Delta} \right)^{6} \right] \qquad r < r_c + \Delta$$

Rc is the cutoff which does not include the delta distance. I.e. the actual force cutoff is the sum of cutoff + delta.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- delta (distance units)
- cutoff (distance units)

The delta values can be positive or negative. The last coefficient is optional. If not specified, the global LJ cutoff is used.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon, sigma, and shift coefficients and cutoff distance for this pair style can be mixed. Shift is always mixed via an *arithmetic* rule. The other coefficients are mixed according to the pair_modify mix value. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style supports the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style supports the pair_modify tail option for adding a long-range tail correction to the energy and pressure of the pair interaction.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions: none

Related commands:

pair_coeff

Default: none

pair_style lj/long/coul/long command

pair_style lj/long/coul/long/omp command

pair_style lj/long/coul/long/opt command

pair_style lj/long/tip4p/long command

Syntax:

```
pair_style style args
```

- style = *lj/long/coul/long* or *lj/long/tip4p/long*
- args = list of arguments for a particular style

```
lj/long/coul/long args = flag_lj flag_coul cutoff (cutoff2)
    flag_lj = long or cut or off
      long = use Kspace long-range summation for dispersion 1/r^6 term
      cut = use a cutoff on dispersion 1/r^6 term
      off = omit disperion 1/r^6 term entirely
    flag_coul = long or off
      long = use Kspace long-range summation for Coulombic 1/r term
      off = omit Coulombic term
    cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
  lj/long/tip4p/long args = flag_lj flag_coul otype htype btype atype qdist cutoff (cutoff2)
    flag_lj = long or cut
      long = use Kspace long-range summation for dispersion 1/r^6 term
      cut = use a cutoff
    flag_coul = long or off
      long = use Kspace long-range summation for Coulombic 1/r term
      off = omit Coulombic term
    otype,htype = atom types for TIP4P O and H
    btype,atype = bond and angle types for TIP4P waters
    qdist = distance from O atom to massless charge (distance units)
    cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

Examples:

```
pair_style lj/long/coul/long cut off 2.5
pair_style lj/long/coul/long cut long 2.5 4.0
pair_style lj/long/coul/long long long 2.5 4.0
pair_coeff * * 1 1
pair_coeff 1 1 1 3 4

pair_style lj/long/tip4p/long long long 1 2 7 8 0.15 12.0
pair_style lj/long/tip4p/long long long 1 2 7 8 0.15 12.0 10.0
pair_coeff * * 100.0 3.0
pair_coeff 1 1 100.0 3.5 9.0
```

Description:

Style *lj/long/coul/long* computes the standard 12/6 Lennard-Jones and Coulombic potentials, given by

$$E = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right] \qquad r < r_c$$

$$E = \frac{C q_i q_j}{\epsilon r} \qquad r < r_c$$

where C is an energy-conversion constant, Qi and Qj are the charges on the 2 atoms, epsilon is the dielectric constant which can be set by the dielectric command, and Rc is the cutoff. If one cutoff is specified in the pair_style command, it is used for both the LJ and Coulombic terms. If two cutoffs are specified, they are used as cutoffs for the LJ and Coulombic terms respectively.

The purpose of this pair style is to capture long-range interactions resulting from both attractive 1/r^6 Lennard-Jones and Coulombic 1/r interactions. This is done by use of the *flag_lj* and *flag_coul* settings. The In 't Veld paper has more details on when it is appropriate to include long-range 1/r^6 interactions, using this potential.

Style *lj/long/tip4p/long* implements the TIP4P water model of (Jorgensen), which introduces a massless site located a short distance away from the oxygen atom along the bisector of the HOH angle. The atomic types of the oxygen and hydrogen atoms, the bond and angle types for OH and HOH interactions, and the distance to the massless charge site are specified as pair_style arguments.

NOTE: For each TIP4P water molecule in your system, the atom IDs for the O and 2 H atoms must be consecutive, with the O atom first. This is to enable LAMMPS to "find" the 2 H atoms associated with each O atom. For example, if the atom ID of an O atom in a TIP4P water molecule is 500, then its 2 H atoms must have IDs 501 and 502.

See the howto section for more information on how to use the TIP4P pair style. Note that the neighobr list cutoff for Coulomb interactions is effectively extended by a distance 2*qdist when using the TIP4P pair style, to account for the offset distance of the fictitious charges on O atoms in water molecules. Thus it is typically best in an efficiency sense to use a LJ cutoff >= Coulomb cutoff + 2*qdist, to shrink the size of the neighbor list. This leads to slightly larger cost for the long-range calculation, so you can test the trade-off for your model.

If *flag_lj* is set to *long*, no cutoff is used on the LJ 1/r^6 dispersion term. The long-range portion can be calculated by using the kspace_style ewald/disp or pppm/disp commands. The specified LJ cutoff then determines which portion of the LJ interactions are computed directly by the pair potential versus which part is computed in reciprocal space via the Kspace style. If *flag_lj* is set to *cut*, the LJ interactions are simply cutoff, as with pair_style lj/cut.

If *flag_coul* is set to *long*, no cutoff is used on the Coulombic interactions. The long-range portion can calculated by using any of several kspace_style command options such as *pppm* or *ewald*. Note that if *flag_lj* is also set to long, then the *ewald/disp* or *pppm/disp* Kspace style needs to be used to perform the long-range calculations for both the LJ and Coulombic interactions. If *flag_coul* is set to *off*, Coulombic interactions are not computed.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- cutoff1 (distance units)
- cutoff2 (distance units)

Note that sigma is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum at 2^(1/6) sigma.

The latter 2 coefficients are optional. If not specified, the global LJ and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both LJ and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the LJ and Coulombic cutoffs for this type pair.

Note that if you are using *flag_lj* set to *long*, you cannot specify a LJ cutoff for an atom type pair, since only one global LJ cutoff is allowed. Similarly, if you are using *flag_coul* set to *long*, you cannot specify a Coulombic cutoff for an atom type pair, since only one global Coulombic cutoff is allowed.

For *lj/long/tip4p/long* only the LJ cutoff can be specified since a Coulombic cutoff cannot be specified for an individual I,J type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/long pair styles can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

These pair styles support the pair_modify shift option for the energy of the Lennard-Jones portion of the pair interaction, assuming *flag_lj* is *cut*.

These pair styles support the pair_modify table and table/disp options since they can tabulate the short-range portion of the long-range Coulombic and dispersion interactions.

Thes pair styles do not support the pair_modify tail option for adding a long-range tail correction to the Lennard-Jones portion of the energy and pressure.

These pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

The pair lj/long/coul/long styles support the use of the *inner*, *middle*, and *outer* keywords of the run_style respa command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. See the run_style command for details.

Restrictions:

These styles are part of the KSPACE package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info. Note that the KSPACE package is installed by default.

Related commands:

pair_coeff

Default: none

(In 't Veld) In 't Veld, Ismail, Grest, J Chem Phys (accepted) (2007).

pair_style lj/sf command

pair_style lj/sf/omp command

Syntax:

```
pair_style lj/sf cutoff
```

- cutoff = global cutoff for Lennard-Jones interactions (distance units)

Examples:

```
pair_style lj/sf 2.5
pair_coeff * * 1.0 1.0
pair_coeff 1 1 1.0 1.0 3.0
```

Description:

Style *lj/sf* computes a truncated and force-shifted LJ interaction (Shifted Force Lennard-Jones), so that both the potential and the force go continuously to zero at the cutoff (Toxvaerd):

$$
\begin{aligned}
F &= F_{\mathrm{LJ}}(r) - F_{\mathrm{LJ}}(r_{\mathrm{c}}) \qquad r < r_{\mathrm{c}} \\
E &= E_{\mathrm{LJ}}(r) - E_{\mathrm{LJ}}(r_{\mathrm{c}}) + (r - r_{\mathrm{c}}) F_{\mathrm{LJ}}(r_{\mathrm{c}}) \qquad r < r_{\mathrm{c}}
\end{aligned}
$$

$$
\text{with} \qquad E_{\mathrm{LJ}}(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \qquad \text{and} \qquad F_{\mathrm{LJ}}(r) = -E'_{\mathrm{LJ}}(r)
$$

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global LJ cutoff specified in the pair_style command is used.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for this pair style can be mixed. Rin is a cutoff value and is mixed like the cutoff. The default mix value is *geometric*. See the "pair_modify" command for details.

The pair_modify shift option is not relevant for this pair style, since the pair interaction goes to 0.0 at the cutoff.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure, since the energy of the pair interaction is smoothed to 0.0 at the cutoff.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff

Default: none

(Toxvaerd) Toxvaerd, Dyre, J Chem Phys, 134, 081102 (2011).

pair_style lj/smooth command

pair_style lj/smooth/cuda command

pair_style lj/smooth/omp command

Syntax:

```
pair_style lj/smooth Rin Rc
```

- Rin = inner cutoff beyond which force smoothing will be applied (distance units)
- Rc = outer cutoff for lj/smooth interactions (distance units)

Examples:

```
pair_style lj/smooth 8.0 10.0
pair_coeff * * 10.0 1.5
pair_coeff 1 1 20.0 1.3 7.0 9.0
```

Description:

Style *lj/smooth* computes a LJ interaction with a force smoothing applied between the inner and outer cutoff.

$$E = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \qquad r < r_{in}$$

$$F = C_1 + C_2(r - r_{in}) + C_3(r - r_{in})^2 + C_4(r - r_{in})^3 \qquad r_{in} < r < r_c$$

The polynomial coefficients C1, C2, C3, C4 are computed by LAMMPS to cause the force to vary smoothly from the inner cutoff Rin to the outer cutoff Rc.

At the inner cutoff the force and its 1st derivative will match the unsmoothed LJ formula. At the outer cutoff the force and its 1st derivative will be 0.0. The inner cutoff cannot be 0.0.

NOTE: this force smoothing causes the energy to be discontinuous both in its values and 1st derivative. This can lead to poor energy conservation and may require the use of a thermostat. Plot the energy and force resulting from this formula via the pair_write command to see the effect.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- innner (distance units)
- outer (distance units)

The last 2 coefficients are optional inner and outer cutoffs. If not specified, the global values for Rin and Rc are used.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon, sigma, Rin coefficients and the cutoff distance for this pair style can be mixed. Rin is a cutoff value and is mixed like the cutoff. The other coefficients are mixed according to the pair_modify mix option. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style supports the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure, since the energy of the pair interaction is smoothed to 0.0 at the cutoff.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions: none

Related commands:

pair_coeff, pair lj/smooth/linear

Default: none

pair_style lj/smooth/linear command

pair_style lj/smooth/linear/omp command

Syntax:

```
pair_style lj/smooth/linear Rc
```

- Rc = cutoff for lj/smooth/linear interactions (distance units)

Examples:

```
pair_style lj/smooth/linear 5.456108274435118
pair_coeff * * 0.7242785984051078 2.598146797350056
pair_coeff 1 1 20.0 1.3 9.0
```

Description:

Style *lj/smooth/linear* computes a LJ interaction that combines the standard 12/6 Lennard-Jones function and subtracts a linear term that includes the cutoff distance Rc, as in this formula:

$$\phi(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

$$E(r) = \phi(r) - \phi(R_c) - (r - R_c)\left.\frac{d\phi}{dr}\right|_{r=R_c} \qquad r < R_c$$

At the cutoff Rc, the energy and force (its 1st derivative) will be 0.0.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global value for Rc is used.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making

LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance can be mixed. The default mix value is geometric. See the "pair_modify" command for details.

This pair style does not support the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure, since the energy of the pair interaction is smoothed to 0.0 at the cutoff.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions: none

Related commands:

pair_coeff, pair lj/smooth

Default: none

pair_style lj/cut/soft command

pair_style lj/cut/soft/omp command

pair_style lj/cut/coul/cut/soft command

pair_style lj/cut/coul/cut/soft/omp command

pair_style lj/cut/coul/long/soft command

pair_style lj/cut/coul/long/soft/omp command

pair_style lj/cut/tip4p/long/soft command

pair_style lj/cut/tip4p/long/soft/omp command

pair_style lj/charmm/coul/long/soft command

pair_style lj/charmm/coul/long/soft/omp command

pair_style coul/cut/soft command

pair_style coul/cut/soft/omp command

pair_style coul/long/soft command

pair_style coul/long/soft/omp command

pair_style tip4p/long/soft command

pair_style tip4p/long/soft/omp command

Syntax:

```
pair_style style args
```

- style = *lj/cut/soft* or *lj/cut/coul/cut/soft* or *lj/cut/coul/long/soft* or *lj/cut/tip4p/long/soft* or *lj/charmm/coul/long/soft* or *coul/cut/soft* or *coul/long/soft* or *tip4p/long/soft*
- args = list of arguments for a particular style

```
lj/cut/soft args = n alpha_lj cutoff
    n, alpha_LJ = parameters of soft-core potential
    cutoff = global cutoff for Lennard-Jones interactions (distance units)
  lj/cut/coul/cut/soft args = n alpha_LJ alpha_C cutoff (cutoff2)
    n, alpha_LJ, alpha_C = parameters of soft-core potential
    cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
  lj/cut/coul/long/soft args = n alpha_LJ alpha_C cutoff
```

```
    n, alpha_LJ, alpha_C = parameters of the soft-core potential
    cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
  lj/cut/tip4p/long/soft args = otype htype btype atype qdist n alpha_LJ alpha_C cutoff (cutoff2)
    otype,htype = atom types for TIP4P O and H
    btype,atype = bond and angle types for TIP4P waters
    qdist = distance from O atom to massless charge (distance units)
    n, alpha_LJ, alpha_C = parameters of the soft-core potential
    cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
  lj/charmm/coul/long/soft args = n alpha_LJ alpha_C inner outer (cutoff)
    n, alpha_LJ, alpha_C = parameters of the soft-core potential
    inner, outer = global switching cutoffs for LJ (and Coulombic if only 5 args)
    cutoff = global cutoff for Coulombic (optional, outer is Coulombic cutoff if only 5 args)
  coul/cut/soft args = n alpha_C cutoff
    n, alpha_C = parameters of the soft-core potential
    cutoff = global cutoff for Coulomb interactions (distance units)
  coul/long/soft args = n alpha_C cutoff
    n, alpha_C = parameters of the soft-core potential
    cutoff = global cutoff for Coulomb interactions (distance units)
  tip4p/long/soft args = otype htype btype atype qdist n alpha_C cutoff
    otype,htype = atom types for TIP4P O and H
    btype,atype = bond and angle types for TIP4P waters
    qdist = distance from O atom to massless charge (distance units)
    n, alpha_C = parameters of the soft-core potential
    cutoff = global cutoff for Coulomb interactions (distance units)
```

Examples:

```
pair_style lj/cut/soft 2.0 0.5 9.5
pair_coeff * * 0.28 3.1 1.0
pair_coeff 1 1 0.28 3.1 1.0 9.5

pair_style lj/cut/coul/cut/soft 2.0 0.5 10.0 9.5
pair_style lj/cut/coul/cut/soft 2.0 0.5 10.0 9.5 9.5
pair_coeff * * 0.28 3.1 1.0
pair_coeff 1 1 0.28 3.1 0.5 10.0
pair_coeff 1 1 0.28 3.1 0.5 10.0 9.5

pair_style lj/cut/coul/long/soft 2.0 0.5 10.0 9.5
pair_style lj/cut/coul/long/soft 2.0 0.5 10.0 9.5 9.5
pair_coeff * * 0.28 3.1 1.0
pair_coeff 1 1 0.28 3.1 0.0 10.0
pair_coeff 1 1 0.28 3.1 0.0 10.0 9.5

pair_style lj/cut/tip4p/long/soft 1 2 7 8 0.15 2.0 0.5 10.0 9.8
pair_style lj/cut/tip4p/long/soft 1 2 7 8 0.15 2.0 0.5 10.0 9.8 9.5
pair_coeff * * 0.155 3.1536 1.0
pair_coeff 1 1 0.155 3.1536 1.0 9.5

pair_style lj/charmm/coul/long 2.0 0.5 10.0 8.0 10.0
pair_style lj/charmm/coul/long 2.0 0.5 10.0 8.0 10.0 9.0
pair_coeff * * 0.28 3.1 1.0
pair_coeff 1 1 0.28 3.1 1.0 0.14 3.1

pair_style coul/long/soft 1.0 10.0 9.5
pair_coeff * * 1.0
pair_coeff 1 1 1.0 9.5

pair_style tip4p/long/soft 1 2 7 8 0.15 2.0 0.5 10.0 9.8
pair_coeff * * 1.0
```

```
pair_coeff 1 1 1.0 9.5
```

Description:

The *lj/cut/soft* style and substyles compute the 12/6 Lennard-Jones and Coulomb potential modified by a soft core, in order to avoid singularities during free energy calculations when sites are created or anihilated (Beutler),

$$E = \lambda^n 4\epsilon \left\{ \frac{1}{\left[\alpha_{\mathrm{LJ}}(1-\lambda)^2 + \left(\frac{r}{\sigma}\right)^6\right]^2} - \frac{1}{\alpha_{\mathrm{LJ}}(1-\lambda)^2 + \left(\frac{r}{\sigma}\right)^6} \right\} \qquad r < r_c$$

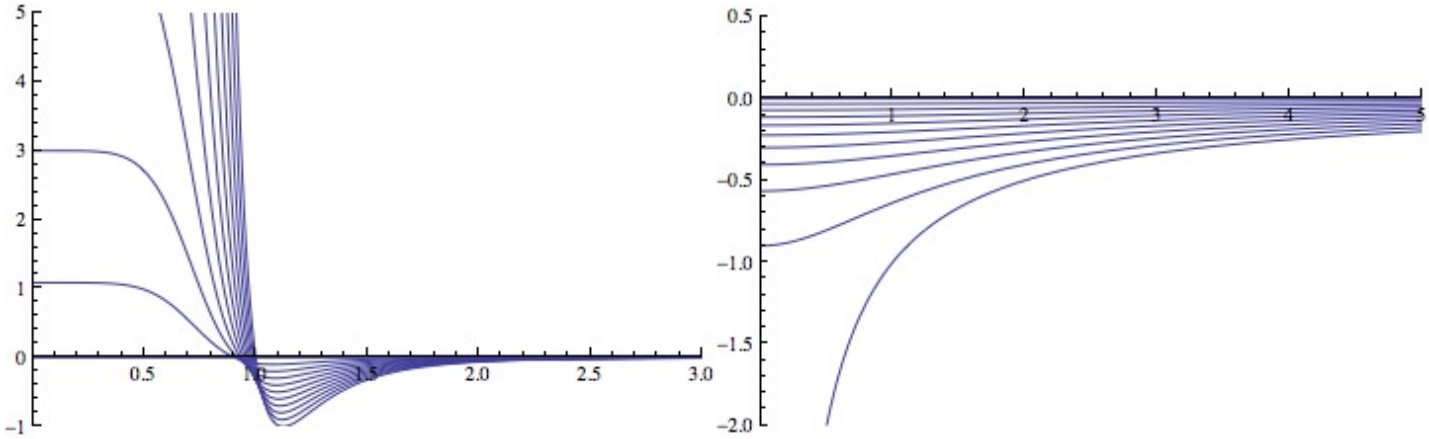
Coulomb interactions are also damped with a soft core at short distance,

$$E = \lambda^n \frac{C q_i q_j}{\epsilon \left[\alpha_{\mathrm{C}}(1-\lambda)^2 + r^2\right]^{1/2}} \qquad r < r_c$$

In the Coulomb part C is an energy-conversion constant, q_i and q_j are the charges on the 2 atoms, and epsilon is the dielectric constant which can be set by the dielectric command.

The coefficient lambda is an activation parameter. When lambda = 1 the pair potentiel is identical to a Lennard-Jones term or a Coulomb term or a combination of both. When lambda = 0 the interactions are deactivated. The transition between these two extrema is smoothed by a soft repulsive core in order to avoid singularities in potential energy and forces when sites are created or anihilated and can overlap (Beutler).

The paratemers n, alpha_LJ and alpha_C are set in the pair_style command, before the cutoffs. Usual choices for the exponent are n = 2 or n = 1. For the remaining coefficients alpha_LJ = 0.5 and alpha_C = 10 Angstrom^2 are appropriate choices. Plots of the LJ and Coulomb terms are shown below, for lambda ranging from 1 to 0 every 0.1.



For the *lj/cut/coul/cut/soft* or *lj/cut/coul/long/soft* pair styles, the following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- lambda (activation parameter between 0 and 1)

- cutoff1 (distance units)
- cutoff2 (distance units)

The latter two coefficients are optional. If not specified, the global LJ and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both LJ and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the LJ and Coulombic cutoffs for this type pair. You cannot specify 2 cutoffs for style *lj/cut/soft*, since it has no Coulombic terms. For the *coul/cut/soft* and *coul/long/soft* only lambda and the optional cutoff2 are to be specified.

Style *lj/cut/tip4p/long/soft* implements a soft-core version of the TIP4P water model. The usage of this pair style is documented in the pair_lj styles. The soft-core version introduces the lambda parameter to the list of arguments, after epsilon and sigma in the pair_coeff command. The paratemers n, alpha_LJ and alpha_C are set in the pair_style command, before the cutoffs.

Style *lj/charmm/coul/long/soft* implements a soft-core version of the CHARMM version of LJ interactions with an additional switching function S(r) that ramps the energy and force smoothly to zero between an inner and outer cutoff. The usage of this pair style is documented in the pair_charmm styles. The soft-core version introduces the lambda parameter to the list of arguments, after epsilon and sigma in the pair_coeff command (and before the optional eps14 and sigma14). The paratemers n, alpha_LJ and alpha_C are set in the pair_style command, before the cutoffs.

The *coul/cut/soft*, *coul/long/soft* and *tip4p/long/soft* substyles are designed to be combined with other pair potentials via the pair_style hybrid/overlay command. This is because they have no repulsive core. Hence, if used by themselves, there will be no repulsion to keep two oppositely charged particles from overlapping each other. In this case, if lambda = 1, a singularity may occur. These substyles are suitable to represent charges embedded in the Lennard-Jones radius of another site (for example hydrogen atoms in several water models).

NOTES: When using the core-softed Coulomb potentials with long-range solvers (*coul/long/soft*, *lj/cut/coul/long/soft*, etc.) in a free energy calculation in which sites holding electrostatic charges are being created or anihilated (using fix_adapt/fep and compute_fep) it is important to adapt both the lambda activation parameter (from 0 to 1, or the reverse) and the value of the charge (from 0 to its final value, or the reverse). This ensures that long-range electrostatic terms (kspace) are correct. It is not necessary to use core-softed Coulomb potentials if the van der Waals site is present during the free-energy route, thus avoiding overlap of the charges. Examples are provided in the LAMMPS source directory tree, under examples/USER/fep.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, tail correction, restart info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for this pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

These pair styles support the pair_modify shift option for the energy of the Lennard-Jones portion of the pair interaction.

These pair styles support the pair_modify tail option for adding a long-range tail correction to the energy and pressure for the Lennard-Jones portion of the pair interaction.

These pair styles write information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

Restrictions:

To avoid division by zero do not set sigma = 0; use the lambda parameter instead to activate/deactivate interactions, or use epsilon = 0 and sigma = 1. Alternatively, when sites do not interact though the Lennard-Jones term the *coul/long/soft* or similar substyle can be used via the pair_style hybrid/overlay command.

All of the plain *soft* pair styles are part of the USER-FEP package. The *long* styles also requires the KSPACE package to be installed. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, fix_adapt, fix_adapt/fep, compute_fep

Default: none

(Beutler) Beutler, Mark, van Schaik, Gerber, van Gunsteren, Chem Phys Lett, 222, 529 (1994).

pair_style lubricate command

pair_style lubricate/omp command

pair_style lubricate/poly command

pair_style lubricate/poly/omp command

Syntax:

```
pair_style style mu flaglog flagfld cutinner cutoff flagHI flagVF
```

- style = *lubricate* or *lubricate/poly*
- mu = dynamic viscosity (dynamic viscosity units)
- flaglog = 0/1 to exclude/include log terms in the lubrication approximation
- flagfld = 0/1 to exclude/include Fast Lubrication Dynamics (FLD) effects
- cutinner = inner cutoff distance (distance units)
- cutoff = outer cutoff for interactions (distance units)
- flagHI (optional) = 0/1 to exclude/include 1/r hydrodynamic interactions
- flagVF (optional) = 0/1 to exclude/include volume fraction corrections in the long-range isotropic terms

Examples: (all assume radius = 1)

```
pair_style lubricate 1.5 1 1 2.01 2.5
pair_coeff 1 1 2.05 2.8
pair_coeff * *

pair_style lubricate 1.5 1 1 2.01 2.5
pair_coeff * *
variable mu equal ramp(1,2)
fix 1 all adapt 1 pair lubricate mu * * v_mu
```

Description:

Styles *lubricate* and *lubricate/poly* compute hydrodynamic interactions between mono-disperse spherical particles in a pairwise fashion. The interactions have 2 components. The first is Ball-Melrose lubrication terms via the formulas in (Ball and Melrose)

$$\begin{aligned} W &= -a_{sq}\left|(v_1 - v_2) \bullet \mathbf{nn}\right|^2 - a_{sh}\left|(\omega_1 + \omega_2) \bullet (\mathbf{I} - \mathbf{nn}) - 2\Omega_N\right|^2 - \\ & \quad a_{pu}\left|(\omega_1 - \omega_2) \bullet (\mathbf{I} - \mathbf{nn})\right|^2 - a_{tw}\left|(\omega_1 - \omega_2) \bullet \mathbf{nn}\right|^2 \qquad r < r_c \end{aligned}$$

$$\Omega_N = \mathbf{n} \times (v_1 - v_2)/r$$

which represents the dissipation W between two nearby particles due to their relative velocities in the presence of a background solvent with viscosity *mu*. Note that this is dynamic viscosity which has units of mass/distance/time, not kinematic viscosity.

The Asq (squeeze) term is the strongest and is included if *flagHI* is set to 1 (default). It scales as 1/gap where gap is the separation between the surfaces of the 2 particles. The Ash (shear) and Apu (pump) terms are only included if *flaglog* is set to 1. They are the next strongest interactions, and the only other singular interaction, and scale as log(gap). Note that *flaglog* = 1 and *flagHI* = 0 is invalid, and will result in a warning message, after which *flagHI* will be set to 1. The Atw (twist) term is currently not included. It is typically a very small contribution to the lubrication forces.

The *flagHI* and *flagVF* settings are optional. Neither should be used, or both must be defined.

Cutinner sets the minimum center-to-center separation that will be used in calculations irrespective of the actual separation. *Cutoff* is the maximum center-to-center separation at which an interaction is computed. Using a *cutoff* less than 3 radii is recommended if *flaglog* is set to 1.

The other component is due to the Fast Lubrication Dynamics (FLD) approximation, described in (Kumar), which can be represented by the following equation

$$F^H = -R_{FU}(U - U^\infty) + R_{FE}E^\infty$$

where U represents the velocities and angular velocities of the particles, U^*infty* represents the velocity and the angular velocity of the undisturbed fluid, and E^*infty* represents the rate of strain tensor of the undisturbed fluid with viscosity *mu*. Again, note that this is dynamic viscosity which has units of mass/distance/time, not kinematic viscosity. Volume fraction corrections to R_FU are included as long as *flagVF* is set to 1 (default).

NOTE: When using the FLD terms, these pair styles are designed to be used with explicit time integration and a correspondingly small timestep. Thus either fix nve/sphere or fix nve/asphere should be used for time integration. To perform implicit FLD, see the pair_style lubricateU command.

Style *lubricate* requires monodisperse spherical particles; style *lubricate/poly* allows for polydisperse spherical particles.

The viscosity *mu* can be varied in a time-dependent manner over the course of a simluation, in which case in which case the pair_style setting for *mu* will be overridden. See the fix adapt command for details.

If the suspension is sheared via the fix deform command then the pair style uses the shear rate to adjust the hydrodynamic interactions accordingly. Volume changes due to fix deform are accounted for when computing the volume fraction corrections to R_FU.

When computing the volume fraction corrections to R_FU, the presence of walls (whether moving or stationary) will affect the volume fraction available to colloidal particles. This is currently accounted for with the following types of walls: wall/lj93, wall/lj126, wall/colloid, and wall/harmonic. For these wall styles, the correct volume fraction will be used when walls do not coincide with the box boundary, as well as when walls move and thereby cause a change in the volume fraction. Other wall styles will still work, but they will result in the volume fraction being computed based on the box boundaries.

Since lubrication forces are dissipative, it is usually desirable to thermostat the system at a constant temperature. If Brownian motion (at a constant temperature) is desired, it can be set using the pair_style brownian command.

These pair styles and the brownian style should use consistent parameters for *mu*, *flaglog*, *flagfld*, *cutinner*, *cutoff*, *flagHI* and *flagVF*.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- cutinner (distance units)
- cutoff (distance units)

The two coefficients are optional. If neither is specified, the two cutoffs specified in the pair_style command are used. Otherwise both must be specified.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in this section of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See this section of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the two cutoff distances for this pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style does not support the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

These styles are part of the FLD package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Only spherical monodisperse particles are allowed for pair_style lubricate.

Only spherical particles are allowed for pair_style lubricate/poly.

These pair styles will not restart exactly when using the read_restart command, though they should provide statistically similar results. This is because the forces they compute depend on atom velocities. See the read_restart command for more details.

Related commands:

pair_coeff, pair_style lubricateU

Default:

The default settings for the optional args are flagHI = 1 and flagVF = 1.

(Ball) Ball and Melrose, Physica A, 247, 444-472 (1997).

(Kumar) Kumar and Higdon, Phys Rev E, 82, 051401 (2010). See also his thesis for more details: A. Kumar, "Microscale Dynamics in Suspensions of Non-spherical Particles", Thesis, University of Illinois Urbana-Champaign, (2010). (https://www.ideals.illinois.edu/handle/2142/16032)

pair_style lubricateU command

pair_style lubricateU/poly command

Syntax:

```
pair_style style mu flaglog cutinner cutoff gdot flagHI flagVF
```

- style = *lubricateU* or *lubricateU/poly*
- mu = dynamic viscosity (dynamic viscosity units)
- flaglog = 0/1 to exclude/include log terms in the lubrication approximation
- cutinner = inner cut off distance (distance units)
- cutoff = outer cutoff for interactions (distance units)
- gdot = shear rate (1/time units)
- flagHI (optional) = 0/1 to exclude/include 1/r hydrodynamic interactions
- flagVF (optional) = 0/1 to exclude/include volume fraction corrections in the long-range isotropic terms

Examples: (all assume radius = 1)

```
pair_style lubricateU 1.5 1 2.01 2.5 0.01 1 1
pair_coeff 1 1 2.05 2.8
pair_coeff * *
```

Description:

Styles *lubricateU* and *lubricateU/poly* compute velocities and angular velocities such that the hydrodynamic interaction balances the force and torque due to all other types of interactions.

The interactions have 2 components. The first is Ball-Melrose lubrication terms via the formulas in (Ball and Melrose)

$$\begin{aligned} W &= -a_{sq}\left|(v_1 - v_2) \bullet \mathbf{nn}\right|^2 - a_{sh}\left|(\omega_1 + \omega_2) \bullet (\mathbf{I} - \mathbf{nn}) - 2\Omega_N\right|^2 - \\ & \quad a_{pu}\left|(\omega_1 - \omega_2) \bullet (\mathbf{I} - \mathbf{nn})\right|^2 - a_{tw}\left|(\omega_1 - \omega_2) \bullet \mathbf{nn}\right|^2 \qquad r < r_c \end{aligned}$$

$$\Omega_N = \mathbf{n} \times (v_1 - v_2)/r$$

which represents the dissipation W between two nearby particles due to their relative velocities in the presence of a background solvent with viscosity *mu*. Note that this is dynamic viscosity which has units of mass/distance/time, not kinematic viscosity.

The Asq (squeeze) term is the strongest and is included as long as *flagHI* is set to 1 (default). It scales as 1/gap where gap is the separation between the surfaces of the 2 particles. The Ash (shear) and Apu (pump) terms are only included if *flaglog* is set to 1. They are the next strongest interactions, and the only other singular interaction, and scale as log(gap). Note that *flaglog* = 1 and *flagHI* = 0 is invalid, and will result in a warning message, after

which *flagHI* will be set to 1. The Atw (twist) term is currently not included. It is typically a very small contribution to the lubrication forces.

The *flagHI* and *flagVF* settings are optional. Neither should be used, or both must be defined.

Cutinner sets the minimum center-to-center separation that will be used in calculations irrespective of the actual separation. *Cutoff* is the maximum center-to-center separation at which an interaction is computed. Using a *cutoff* less than 3 radii is recommended if *flaglog* is set to 1.

The other component is due to the Fast Lubrication Dynamics (FLD) approximation, described in (Kumar). The equation being solved to balance the forces and torques is

$$-R_{FU}(U - U^{\infty}) = -R_{FE}E^{\infty} - F^{rest}$$

where U represents the velocities and angular velocities of the particles, U^*infty* represents the velocities and the angular velocities of the undisturbed fluid, and E^*infty* represents the rate of strain tensor of the undisturbed fluid flow with viscosity *mu*. Again, note that this is dynamic viscosity which has units of mass/distance/time, not kinematic viscosity. Volume fraction corrections to R_FU are included if *flagVF* is set to 1 (default).

F*rest* represents the forces and torques due to all other types of interactions, e.g. Brownian, electrostatic etc. Note that this algorithm neglects the inertial terms, thereby removing the restriction of resolving the small interial time scale, which may not be of interest for colloidal particles. This pair style solves for the velocity such that the hydrodynamic force balances all other types of forces, thereby resulting in a net zero force (zero inertia limit). When defining this pair style, it must be defined last so that when this style is invoked all other types of forces have already been computed. For the same reason, it won't work if additional non-pair styles are defined (such as bond or Kspace forces) as they are calculated in LAMMPS after the pairwise interactions have been computed.

NOTE: When using these styles, the these pair styles are designed to be used with implicit time integration and a correspondingly larger timestep. Thus either fix nve/noforce should be used for spherical particles defined via atom_style sphere or fix nve/asphere/noforce should be used for spherical particles defined via atom_style ellipsoid. This is because the velocity and angular momentum of each particle is set by the pair style, and should not be reset by the time integration fix.

Style *lubricateU* requires monodisperse spherical particles; style *lubricateU/poly* allows for polydisperse spherical particles.

If the suspension is sheared via the fix deform command then the pair style uses the shear rate to adjust the hydrodynamic interactions accordingly. Volume changes due to fix deform are accounted for when computing the volume fraction corrections to R_FU.

When computing the volume fraction corrections to R_FU, the presence of walls (whether moving or stationary) will affect the volume fraction available to colloidal particles. This is currently accounted for with the following types of walls: wall/lj93, wall/lj126, wall/colloid, and "wall/harmonic_fix_wall.html". For these wall styles, the correct volume fraction will be used when walls do not coincide with the box boundary, as well as when walls move and thereby cause a change in the volume fraction. To use these wall styles with pair_style *lubricateU* or *lubricateU/poly*, the *fld yes* option must be specified in the fix wall command.

Since lubrication forces are dissipative, it is usually desirable to thermostat the system at a constant temperature. If Brownian motion (at a constant temperature) is desired, it can be set using the pair_style brownian command.

These pair styles and the brownian style should use consistent parameters for *mu*, *flaglog*, *flagfld*, *cutinner*, *cutoff*, *flagHI* and *flagVF*.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- cutinner (distance units)
- cutoff (distance units)

The two coefficients are optional. If neither is specified, the two cutoffs specified in the pair_style command are used. Otherwise both must be specified.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the two cutoff distances for this pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style does not support the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

These styles are part of the FLD package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Currently, these pair styles assume that all other types of forces/torques on the particles have been already been computed when it is invoked. This requires this style to be defined as the last of the pair styles, and that no fixes apply additional constraint forces. One exception is the fix wall/colloid commands, which has an "fld" option to apply their wall forces correctly.

Only spherical monodisperse particles are allowed for pair_style lubricateU.

Only spherical particles are allowed for pair_style lubricateU/poly.

For sheared suspensions, it is assumed that the shearing is done in the xy plane, with x being the velocity direction and y being the velocity-gradient direction. In this case, one must use fix deform with the same rate of shear (erate).

Related commands:

pair_coeff, pair_style lubricate

Default:

The default settings for the optional args are flagHI = 1 and flagVF = 1.

(Ball) Ball and Melrose, Physica A, 247, 444-472 (1997).

(Kumar) Kumar and Higdon, Phys Rev E, 82, 051401 (2010).

pair_style lj/mdf command

pair_style buck/mdf command

pair_style lennard/mdf command

Syntax:

```
pair_style style args
```

- style = *lj/mdf* or *buck/mdf* or *lennard/mdf*
- args = list of arguments for a particular style

```
  lj/mdf args = cutoff1 cutoff2
      cutoff1 = inner cutoff for the start of the tapering function
      cutoff1 = out cutoff for the end of the tapering function
    buck/mdf args = cutoff1 cutoff2
      cutoff1 = inner cutoff for the start of the tapering function
      cutoff1 = out cutoff for the end of the tapering function
    lennard/mdf args = cutoff1 cutoff2
      cutoff1 = inner cutoff for the start of the tapering function
      cutoff1 = out cutoff for the end of the tapering function
```

Examples:

```
pair_style lj/mdf 2.5 3.0
pair_coeff * * 1 1
pair_coeff 1 1 1 1.1 2.8 3.0 3.2

pair_style buck 2.5 3.0
pair_coeff * * 100.0 1.5 200.0
pair_coeff * * 100.0 1.5 200.0 3.0 3.5

pair_style lennard/mdf 2.5 3.0
pair_coeff * * 1 1
pair_coeff 1 1 1 1.1 2.8 3.0 3.2
```

Description:

The *lj/mdf*, *buck/mdf* and *lennard/mdf* compute the standard 12-6 Lennard-Jones and Buckingham potential with the addition of a taper function that ramps the energy and force smoothly to zero between an inner and outer cutoff.

The tapering, *f(r)*, is done by using the Mei, Davenport, Fernando function (Mei).

where

Here *r_m* is the inner cutoff radius and *r_cut* is the outer cutoff radius.

For the *lj/mdf* pair_style, the potential energy, *E(r)*, is the standard 12-6 Lennard-Jones written in the epsilon/sigma form:

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- r_m (distance units)
- r_*cut* (distance units)

For the *buck/mdf* pair_style, the potential energy, *E(r)*, is the standard 12-6 Lennard-Jones written in the epsilon/sigma form:

- A (energy units)
- \rho (distance units)
- C (energy-distance^6 units)
- r_m (distance units)
- r_*cut*$ (distance units)

For the *lennard/mdf* pair_style, the potential energy, *E(r)*, is the standard 12-6 Lennard-Jones written in the A/B form:

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- A (energy-distance^12 units)
- B (energy-distance^6 units)
- r_m (distance units)
- r_*cut* (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/cut pair styles can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

All of the *lj/cut* pair styles support the pair_modify shift option for the energy of the Lennard-Jones portion of the pair interaction.

The *lj/cut/coul/long* and *lj/cut/tip4p/long* pair styles support the pair_modify table option since they can tabulate the short-range portion of the long-range Coulombic interaction.

All of the *lj/cut* pair styles support the pair_modify tail option for adding a long-range tail correction to the energy and pressure for the Lennard-Jones portion of the pair interaction.

All of the *lj/cut* pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

The *lj/cut* and *lj/cut/coul/long* pair styles support the use of the *inner*, *middle*, and *outer* keywords of the run_style respa command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. The other styles only support the *pair* keyword of run_style respa. See the run_style command for details.

Restrictions:

These pair styles can only be used if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info on packages.

Related commands:

pair_coeff

Default: none

(Mei) Mei, Davenport, Fernando, Phys Rev B, 43 4653 (1991)

pair_style meam command

Syntax:

```
pair_style meam
```

Examples:

```
pair_style meam
pair_coeff * * ../potentials/library.meam Si ../potentials/si.meam Si
pair_coeff * * ../potentials/library.meam Ni Al NULL Ni Al Ni Ni
```

Description:

NOTE: The behavior of the MEAM potential for alloy systems has changed as of November 2010; see description below of the mixture_ref_t parameter

Style *meam* computes pairwise interactions for a variety of materials using modified embedded-atom method (MEAM) potentials (Baskes). Conceptually, it is an extension to the original EAM potentials which adds angular forces. It is thus suitable for modeling metals and alloys with fcc, bcc, hcp and diamond cubic structures, as well as covalently bonded materials like silicon and carbon.

In the MEAM formulation, the total energy E of a system of atoms is given by:

$$E = \sum_i \left\{ F_i(\bar{\rho}_i) + \frac{1}{2} \sum_{i \neq j} \phi_{ij}(r_{ij}) \right\}$$

where F is the embedding energy which is a function of the atomic electron density rho, and phi is a pair potential interaction. The pair interaction is summed over all neighbors J of atom I within the cutoff distance. As with EAM, the multi-body nature of the MEAM potential is a result of the embedding energy term. Details of the computation of the embedding and pair energies, as implemented in LAMMPS, are given in (Gullet) and references therein.

The various parameters in the MEAM formulas are listed in two files which are specified by the pair_coeff command. These are ASCII text files in a format consistent with other MD codes that implement MEAM potentials, such as the serial DYNAMO code and Warp. Several MEAM potential files with parameters for different materials are included in the "potentials" directory of the LAMMPS distribution with a ".meam" suffix. All of these are parameterized in terms of LAMMPS metal units.

Note that unlike for other potentials, cutoffs for MEAM potentials are not set in the pair_style or pair_coeff command; they are specified in the MEAM potential files themselves.

Only a single pair_coeff command is used with the *meam* style which specifies two MEAM files and the element(s) to extract information for. The MEAM elements are mapped to LAMMPS atom types by specifying N additional arguments after the 2nd filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- MEAM library file
- Elem1, Elem2, ...
- MEAM parameter file
- N element names = mapping of MEAM elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential files.

As an example, the potentials/library.meam file has generic MEAM settings for a variety of elements. The potentials/sic.meam file has specific parameter settings for a Si and C alloy system. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * library.meam Si C sic.meam Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The two filenames are for the library and parameter file respectively. The Si and C arguments (between the file names) are the two elements for which info will be extracted from the library file. The first three trailing Si arguments map LAMMPS atom types 1,2,3 to the MEAM Si element. The final C argument maps LAMMPS atom type 4 to the MEAM C element.

If the 2nd filename is specified as NULL, no parameter file is read, which simply means the generic parameters in the library file are used. Use of the NULL specification for the parameter file is discouraged for systems with more than a single element type (e.g. alloys), since the parameter file is expected to set element interaction terms that are not captured by the information in the library file.

If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *meam* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

The MEAM library file provided with LAMMPS has the name potentials/library.meam. It is the "meamf" file used by other MD codes. Aside from blank and comment lines (start with #) which can appear anywhere, it is formatted as a series of entries, each of which has 19 parameters and can span multiple lines:

elt, lat, z, ielement, atwt, alpha, b0, b1, b2, b3, alat, esub, asub, t0, t1, t2, t3, rozero, ibar

The "elt" and "lat" parameters are text strings, such as elt = Si or Cu and lat = dia or fcc. Because the library file is used by Fortran MD codes, these strings may be enclosed in single quotes, but this is not required. The other numeric parameters match values in the formulas above. The value of the "elt" string is what is used in the pair_coeff command to identify which settings from the library file you wish to read in. There can be multiple entries in the library file with the same "elt" value; LAMMPS reads the 1st matching entry it finds and ignores the rest.

Other parameters in the MEAM library file correspond to single-element potential parameters:

```
lat      = lattice structure of reference configuration
z        = number of nearest neighbors in the reference structure
ielement = atomic number
atwt     = atomic weight
alat     = lattice constant of reference structure
esub     = energy per atom (eV) in the reference structure at equilibrium
asub     = "A" parameter for MEAM (see e.g. (Baskes))
```

The alpha, b0, b1, b2, b3, t0, t1, t2, t3 parameters correspond to the standard MEAM parameters in the literature (Baskes) (the b parameters are the standard beta parameters). The rozero parameter is an element-dependent density scaling that weights the reference background density (see e.g. equation 4.5 in (Gullet)) and is typically

1.0 for single-element systems. The ibar parameter selects the form of the function G(Gamma) used to compute the electron density; options are

```
  0 => G = sqrt(1+Gamma)
  1 => G = exp(Gamma/2)
  2 => not implemented
  3 => G = 2/(1+exp(-Gamma))
  4 => G = sqrt(1+Gamma)
 -5 => G = +-sqrt(abs(1+Gamma))
```

If used, the MEAM parameter file contains settings that override or complement the library file settings. Examples of such parameter files are in the potentials directory with a ".meam" suffix. Their format is the same as is read by other Fortran MD codes. Aside from blank and comment lines (start with #) which can appear anywhere, each line has one of the following forms. Each line can also have a trailing comment (starting with #) which is ignored.

```
keyword = value
keyword(I) = value
keyword(I,J) = value
keyword(I,J,K) = value
```

The recognized keywords are as follows:

Ec, alpha, rho0, delta, lattce, attrac, repuls, nn2, Cmin, Cmax, rc, delr, augt1, gsmooth_factor, re

where

```
rc          = cutoff radius for cutoff function; default = 4.0
delr        = length of smoothing distance for cutoff function; default = 0.1
rho0(I)     = relative density for element I (overwrites value
              read from meamf file)
Ec(I,J)     = cohesive energy of reference structure for I-J mixture
delta(I,J)  = heat of formation for I-J alloy; if Ec_IJ is input as
              zero, then LAMMPS sets Ec_IJ = (Ec_II + Ec_JJ)/2 - delta_IJ
alpha(I,J)  = alpha parameter for pair potential between I and J (can
              be computed from bulk modulus of reference structure
re(I,J)     = equilibrium distance between I and J in the reference
              structure
Cmax(I,J,K) = Cmax screening parameter when I-J pair is screened
              by K (I<=J); default = 2.8
Cmin(I,J,K) = Cmin screening parameter when I-J pair is screened
              by K (I<=J); default = 2.0
lattce(I,J) = lattice structure of I-J reference structure:
                dia = diamond (interlaced fcc for alloy)
                fcc = face centered cubic
                bcc = body centered cubic
                dim = dimer
                b1  = rock salt (NaCl structure)
                hcp = hexagonal close-packed
                c11 = MoSi2 structure
                l12 = Cu3Au structure (lower case L, followed by 12)
                b2  = CsCl structure (interpenetrating simple cubic)
nn2(I,J)    = turn on second-nearest neighbor MEAM formulation for
              I-J pair (see for example (Lee)).
                0 = second-nearest neighbor formulation off
                1 = second-nearest neighbor formulation on
                default = 0
attrac(I,J) = additional cubic attraction term in Rose energy I-J pair potential
                default = 0
repuls(I,J) = additional cubic repulsive term in Rose energy I-J pair potential
                default = 0
```

```
zbl(I,J)     = blend the MEAM I-J pair potential with the ZBL potential for small
               atom separations (ZBL)
                 default = 1
gsmooth_factor  = factor determining the length of the G-function smoothing
                  region; only significant for ibar=0 or ibar=4.
                      99.0 = short smoothing region, sharp step
                      0.5  = long smoothing region, smooth step
                      default = 99.0
augt1           = integer flag for whether to augment t1 parameter by
                  3/5*t3 to account for old vs. new meam formulations;
                    0 = don't augment t1
                    1 = augment t1
                    default = 1
ialloy          = integer flag to use alternative averaging rule for t parameters,
                  for comparison with the DYNAMO MEAM code
                    0 = standard averaging (matches ialloy=0 in DYNAMO)
                    1 = alternative averaging (matches ialloy=1 in DYNAMO)
                    2 = no averaging of t (use single-element values)
                    default = 0
mixture_ref_t   = integer flag to use mixture average of t to compute the background
                  reference density for alloys, instead of the single-element values
                  (see description and warning elsewhere in this doc page)
                    0 = do not use mixture averaging for t in the reference density
                    1 = use mixture averaging for t in the reference density
                    default = 0
erose_form      = integer value to select the form of the Rose energy function
                  (see description below).
                    default = 0
emb_lin_neg     = integer value to select embedding function for negative densities
                    0 = F(rho)=0
                    1 = F(rho) = -asub*esub*rho (linear in rho, matches DYNAMO)
                    default = 0
bkgd_dyn        = integer value to select background density formula
                    0 = rho_bkgd = rho_ref_meam(a) (as in the reference structure)
                    1 = rho_bkgd = rho0_meam(a)*Z_meam(a) (matches DYNAMO)
                    default = 0
```

Rc, delr, re are in distance units (Angstroms in the case of metal units). Ec and delta are in energy units (eV in the case of metal units).

Each keyword represents a quantity which is either a scalar, vector, 2d array, or 3d array and must be specified with the correct corresponding array syntax. The indices I,J,K each run from 1 to N where N is the number of MEAM elements being used.

Thus these lines

```
rho0(2) = 2.25
alpha(1,2) = 4.37
```

set rho0 for the 2nd element to the value 2.25 and set alpha for the alloy interaction between elements 1 and 2 to 4.37.

The augt1 parameter is related to modifications in the MEAM formulation of the partial electron density function. In recent literature, an extra term is included in the expression for the third-order density in order to make the densities orthogonal (see for example (Wang), equation 3d); this term is included in the MEAM implementation in lammps. However, in earlier published work this term was not included when deriving parameters, including most of those provided in the library.meam file included with lammps, and to account for this difference the parameter t1 must be augmented by 3/5*t3. If augt1=1, the default, this augmentation is done automatically. When parameter values are fit using the modified density function, as in more recent literature, augt1 should be

set to 0.

The mixture_ref_t parameter is available to match results with those of previous versions of lammps (before January 2011). Newer versions of lammps, by default, use the single-element values of the t parameters to compute the background reference density. This is the proper way to compute these parameters. Earlier versions of lammps used an alloy mixture averaged value of t to compute the background reference density. Setting mixture_ref_t=1 gives the old behavior. WARNING: using mixture_ref_t=1 will give results that are demonstrably incorrect for second-neighbor MEAM, and non-standard for first-neighbor MEAM; this option is included only for matching with previous versions of lammps and should be avoided if possible.

The parameters attrac and repuls, along with the integer selection parameter erose_form, can be used to modify the Rose energy function used to compute the pair potential. This function gives the energy of the reference state as a function of interatomic spacing. The form of this function is:

```
astar = alpha * (r/re - 1.d0)
if erose_form = 0: erose = -Ec*(1+astar+a3*(astar**3)/(r/re))*exp(-astar)
if erose_form = 1: erose = -Ec*(1+astar+(-attrac+repuls/r)*(astar**3))*exp(-astar)
if erose_form = 2: erose = -Ec*(1 +astar + a3*(astar**3))*exp(-astar)
a3 = repuls, astar <0
a3 = attrac, astar >= 0
```

Most published MEAM parameter sets use the default values attrac=repulse=0. Setting repuls=attrac=delta corresponds to the form used in several recent published MEAM parameter sets, such as (Vallone)

NOTE: The default form of the erose expression in LAMMPS was corrected in March 2009. The current version is correct, but may show different behavior compared with earlier versions of lammps with the attrac and/or repuls parameters are non-zero. To obtain the previous default form, use erose_form = 1 (this form does not seem to appear in the literature). An alternative form (see e.g. (Lee2)) is available using erose_form = 2.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS with user-specifiable parameters as described above. You never need to specify a pair_coeff command with I != J arguments for this style.

This pair style does not support the pair_modify shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This style is part of the MEAM package. It is only enabled if LAMMPS was built with that package, which also requires the MEAM library be built and linked with LAMMPS. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_style eam, pair_style meam/spline

Default: none

(Baskes) Baskes, Phys Rev B, 46, 2727-2742 (1992).

(Gullet) Gullet, Wagner, Slepoy, SANDIA Report 2003-8782 (2003). This report may be accessed on-line via this link.

(Lee) Lee, Baskes, Phys. Rev. B, 62, 8564-8567 (2000).

(Lee2) Lee, Baskes, Kim, Cho. Phys. Rev. B, 64, 184102 (2001).

(Valone) Valone, Baskes, Martin, Phys. Rev. B, 73, 214209 (2006).

(Wang) Wang, Van Hove, Ross, Baskes, J. Chem. Phys., 121, 5410 (2004).

(ZBL) J.F. Ziegler, J.P. Biersack, U. Littmark, "Stopping and Ranges of Ions in Matter", Vol 1, 1985, Pergamon Press.

pair_style meam/spline

pair_style meam/spline/omp

Syntax:

```
pair_style meam/spline
```

Examples:

```
pair_style meam/spline
pair_coeff * * Ti.meam.spline Ti
pair_coeff * * Ti.meam.spline Ti Ti Ti
```

Description:

The *meam/spline* style computes pairwise interactions for metals using a variant of modified embedded-atom method (MEAM) potentials (Lenosky). The total energy E is given by

$$E = \sum_{ij} \phi(r_{ij}) + \sum_{i} U(\rho_i),$$

$$\rho_i = \sum_{j} \rho(r_{ij}) + \sum_{jk} f(r_{ij}) f(r_{ik}) g[\cos(\theta_{jik})]$$

where rho_i is the density at atom I, theta_jik is the angle between atoms J, I, and K centered on atom I. The five functions Phi, U, rho, f, and g are represented by cubic splines.

The cutoffs and the coefficients for these spline functions are listed in a parameter file which is specified by the pair_coeff command. Parameter files for different elements are included in the "potentials" directory of the LAMMPS distribution and have a ".meam.spline" file suffix. All of these files are parameterized in terms of LAMMPS metal units.

Note that unlike for other potentials, cutoffs for spline-based MEAM potentials are not set in the pair_style or pair_coeff command; they are specified in the potential files themselves.

Unlike the EAM pair style, which retrieves the atomic mass from the potential file, the spline-based MEAM potentials do not include mass information; thus you need to use the mass command to specify it.

Only a single pair_coeff command is used with the *meam/spline* style which specifies a potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of spline-based MEAM elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file.

As an example, imagine the Ti.meam.spline file has values for Ti. If your LAMMPS simulation has 3 atoms types and they are all to be treated with this potentials, you would use the following pair_coeff command:

```
pair_coeff * * Ti.meam.spline Ti Ti Ti
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The three Ti arguments map LAMMPS atom types 1,2,3 to the Ti element in the potential file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *meam/spline* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

NOTE: The *meam/spline* style currently supports only single-element MEAM potentials. It may be extended for alloy systems in the future.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

The current version of this pair style does not support multiple element types or mixing. It has been designed for pure elements only.

This pair style does not support the pair_modify shift, table, and tail options.

The *meam/spline* pair style does not write its information to binary restart files, since it is stored in an external potential parameter file. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

The *meam/spline* pair style can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style requires the newton setting to be "on" for pair interactions.

This pair style is only enabled if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_style meam

Default: none

(Lenosky) Lenosky, Sadigh, Alonso, Bulatov, de la Rubia, Kim, Voter, Kress, Modelling Simulation Materials Science Enginerring, 8, 825 (2000).

pair_style meam/sw/spline

pair_style meam/sw/spline/omp

Syntax:

```
pair_style meam/sw/spline
```

Examples:

```
pair_style meam/sw/spline
pair_coeff * * Ti.meam.sw.spline Ti
pair_coeff * * Ti.meam.sw.spline Ti Ti Ti
```

Description:

The *meam/sw/spline* style computes pairwise interactions for metals using a variant of modified embedded-atom method (MEAM) potentials (Lenosky) with an additional Stillinger-Weber (SW) term (Stillinger) in the energy. This form of the potential was first proposed by Nicklas, Fellinger, and Park (Nicklas). We refer to it as MEAM+SW. The total energy E is given by

$$
\begin{aligned}
E &= E_{MEAM} + E_{SW} \\
E_{MEAM} &= \sum_{IJ} \phi(r_{IJ}) + \sum_{I} U(\rho_I) \\
E_{SW} &= \sum_{I} \sum_{JK} F(r_{IJ})\, F(r_{IK})\, G(\cos(\theta_{JIK})) \\
\rho_I &= \sum_{J} \rho(r_{IJ}) + \sum_{JK} f(r_{IJ})\, f(r_{IK})\, g(\cos(\theta_{JIK}))
\end{aligned}
$$

where rho_I is the density at atom I, theta_JIK is the angle between atoms J, I, and K centered on atom I. The seven functions Phi, F, G, U, rho, f, and g are represented by cubic splines.

The cutoffs and the coefficients for these spline functions are listed in a parameter file which is specified by the pair_coeff command. Parameter files for different elements are included in the "potentials" directory of the LAMMPS distribution and have a ".meam.sw.spline" file suffix. All of these files are parameterized in terms of LAMMPS metal units.

Note that unlike for other potentials, cutoffs for spline-based MEAM+SW potentials are not set in the pair_style or pair_coeff command; they are specified in the potential files themselves.

Unlike the EAM pair style, which retrieves the atomic mass from the potential file, the spline-based MEAM+SW potentials do not include mass information; thus you need to use the mass command to specify it.

Only a single pair_coeff command is used with the meam/sw/spline style which specifies a potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional

arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of spline-based MEAM+SW elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file.

As an example, imagine the Ti.meam.sw.spline file has values for Ti. If your LAMMPS simulation has 3 atoms types and they are all to be treated with this potential, you would use the following pair_coeff command:

pair_coeff * * Ti.meam.sw.spline Ti Ti Ti

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The three Ti arguments map LAMMPS atom types 1,2,3 to the Ti element in the potential file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *meam/sw/spline* potential is used as part of the hybrid pair style. The NULL values are placeholders for atom types that will be used with other potentials.

NOTE: The *meam/sw/spline* style currently supports only single-element MEAM+SW potentials. It may be extended for alloy systems in the future.

Example input scripts that use this pair style are provided in the examples/USER/misc/meam_sw_spline directory.

Mixing, shift, table, tail correction, restart, rRESPA info:

The pair style does not support multiple element types or mixing. It has been designed for pure elements only.

This pair style does not support the pair_modify shift, table, and tail options.

The *meam/sw/spline* pair style does not write its information to binary restart files, since it is stored in an external potential parameter file. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

The *meam/sw/spline* pair style can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style requires the newton setting to be "on" for pair interactions.

This pair style is only enabled if LAMMPS was built with the USER-MISC package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_style meam, pair_style meam/spline

Default: none

(Lenosky) Lenosky, Sadigh, Alonso, Bulatov, de la Rubia, Kim, Voter, Kress, Modell. Simul. Mater. Sci. Eng. 8, 825 (2000).

(Stillinger) Stillinger, Weber, Phys. Rev. B 31, 5262 (1985).

(Nicklas) The spline-based MEAM+SW format was first devised and used to develop potentials for bcc transition metals by Jeremy Nicklas, Michael Fellinger, and Hyoungki Park at The Ohio State University.

pair_style mgpt command

Syntax:

```
pair_style mgpt
```

Examples:

```
pair_style mgpt
pair_coeff * * Ta6.8x.mgpt.parmin Ta6.8x.mgpt.potin Omega
cp ~/lammps/potentials/Ta6.8x.mgpt.parmin parmin
cp ~/lammps/potentials/Ta6.8x.mgpt.potin potin
pair_coeff * * parmin potin Omega volpress yes nbody 1234 precision double
pair_coeff * * parmin potin Omega volpress yes nbody 12
```

Description:

Within DFT quantum mechanics, generalized pseudopotential theory (GPT) (Moriarty1) provides a first-principles approach to multi-ion interatomic potentials in d-band transition metals, with a volume-dependent, real-space total-energy functional for the N-ion elemental bulk material in the form

$$E_{\rm tot}(\mathbf{R}_1 \ldots \mathbf{R}_N) = NE_{\rm vol}(\Omega) + \frac{1}{2}{\sum_{i,j}}' v_2(ij;\Omega) + \frac{1}{6}{\sum_{i,j,k}}' v_3(ijk;\Omega) + \frac{1}{24}{\sum_{i,j,k,l}}' v_4(ij$$

where the prime on each summation sign indicates the exclusion of all self-interaction terms from the summation. The leading volume term E_vol as well as the two-ion central-force pair potential v_2 and the three- and four-ion angular-force potentials, v_3 and v_4, depend explicitly on the atomic volume Omega, but are structure independent and transferable to all bulk ion configurations, either ordered or disordered, and with of without the presence of point and line defects. The simplified model GPT or MGPT (Moriarty2, Moriarty3), which retains the form of E_tot and permits more efficient large-scale atomistic simulations, derives from the GPT through a series of systematic approximations applied to E_vol and the potentials v_n that are valid for mid-period transition metals with nearly half-filled d bands.

Both analytic (Moriarty2) and matrix (Moriarty3) representations of MGPT have been developed. In the more general matrix representation, which can also be applied to f-band actinide metals and permits both canonical and non-canonical d/f bands, the multi-ion potentials are evaluated on the fly during a simulation through d- or f-state matrix multiplication, and the forces that move the ions are determined analytically. Fast matrix-MGPT algorithms have been developed independently by Glosli (Glosli, Moriarty3) and by Oppelstrup (Oppelstrup)

The *mgpt* pair style calculates forces, energies, and the total energy per atom, E_tot/N, using the Oppelstrup matrix-MGPT algorithm. Input potential and control data are entered through the pair_coeff command. Each material treated requires input parmin and potin potential files, as shown in the above examples, as well as specification by the user of the initial atomic volume Omega through pair_coeff. At the beginning of a time step in any simulation, the total volume of the simulation cell V should always be equal to Omega*N, where N is the number of metal ions present, taking into account the presence of any vacancies and/or interstitials in the case of a solid. In a constant-volume simulation, which is the normal mode of operation for the *mgpt* pair style, Omega, V and N all remain constant throughout the simulation and thus are equal to their initial values. In a constant-stress simulation, the cell volume V will change (slowly) as the simulation proceeds. After each time step, the atomic volume should be updated by the code as Omega = V/N. In addition, the volume term E_vol and the potentials

v_2, v_3 and v_4 have to be removed at the end of the time step, and then respecified at the new value of Omega. In all smulations, Omega must remain within the defined volume range for E_vol and the potentials for the given material.

The default option volpress yes in the pair_coeff command includes all volume derivatives of E_tot required to calculate the stress tensor and pressure correctly. The option volpress no disregards the pressure contribution resulting from the volume term E_vol, and can be used for testing and analysis purposes. The additional optional variable nbody controls the specific terms in E_tot that are calculated. The default option and the normal option for mid-period transition and actinide metals is nbody 1234 for which all four terms in E_tot are retained. The option nbody 12, for example, retains only the volume term and the two-ion pair potential term and can be used for GPT series-end transition metals that can be well described without v_3 and v_4. The nbody option can also be used to test or analyze the contribution of any of the four terms in E_tot to a given calculated property.

The *mgpt* pair style makes extensive use of matrix algebra and includes optimized kernels for the BlueGene/Q architecture and the Intel/AMD (x86) architectures. When compiled with the appropriate compiler and compiler switches (-msse3 on x86, and using the IBM XL compiler on BG/Q), these optimized routines are used automatically. For BG/Q machines, building with the default Makefile for that architecture (e.g., "make bgq") should enable the optimized algebra routines. For x-86 machines, the here provided Makefile.mpi_fastmgpt (build with "make mpi_fastmgpt") enables the fast algebra routines. The user will be informed in the output files of the matrix kernels in use. To further improve speed, on x86 the option precision single can be added to the pair_coeff command line, which improves speed (up to a factor of two) at the cost of doing matrix calculations with 7 digit precision instead of the default 16. For consistency the default option can be specified explicitly by the option precision double.

All remaining potential and control data are contained with the parmin and potin files, including cutoffs, atomic mass, and other basic MGPT variables. Specific MGPT potential data for the transition metals tantalum (Ta4 and Ta6.8x potentials), molybdenum (Mo5.2 potentials), and vanadium (V6.1 potentials) are contained in the LAMMPS potentials directory. The stored files are, respectively, Ta4.mgpt.parmin, Ta4.mgpt.potin, Ta6.8x.mgpt.parmin, Ta6.8x.mgpt.potin, Mo5.2.mgpt.parmin, Mo5.2.mgpt.potin, V6.1.mgpt.parmin, and V6.1.mgpt.potin . Useful corresponding informational "README" files on the Ta4, Ta6.8x, Mo5.2 and V6.1 potentials are also included in the potentials directory. These latter files indicate the volume mesh and range for each potential and give appropriate references for the potentials. It is expected that MGPT potentials for additional materials will be added over time.

Useful example MGPT scripts are given in the examples/USER/mgpt directory. These scripts show the necessary steps to perform constant-volume calculations and simulations. It is strongly recommended that the user work through and understand these examples before proceeding to more complex simulations.

NOTE: For good performance, LAMMPS should be built with the compiler flags "-O3 -msse3 -funroll-loops" when including this pair style. The src/MAKE/OPTIONS/Makefile.mpi_fastmgpt is an example machine Makefile with these options included as part of a standard MPI build. Note that as-is it will build with whatever low-level compiler (g++, icc, etc) is the default for your MPI installation.

Mixing, shift, table tail correction, restart:

This pair style does not support the pair_modify mix, shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you needs to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the USER-MGPT package and is only enabled if LAMMPS is built with that package. See the Making LAMMPS section for more info.

The MGPT potentials require the newtion setting to be "on" for pair style interactions.

The stored parmin and potin potential files provided with LAMMPS in the "potentials" directory are written in Rydberg atomic units, with energies in Rydbergs and distances in Bohr radii. The *mgpt* pair style converts Rydbergs to Hartrees to make the potential files compatible with LAMMPS electron units.

The form of E_tot used in the *mgpt* pair style is only appropriate for elemental bulk solids and liquids. This includes solids with point and extended defects such as vacancies, interstitials, grain boundaries and dislocations. Alloys and free surfaces, however, require significant modifications, which are not included in the *mgpt* pair style. Likewise, the *hybrid* pair style is not allowed, where MGPT would be used for some atoms but not for others.

Electron-thermal effects are not included in the standard MGPT potentials provided in the "potentials" directory, where the potentials have been constructed at zero electron temperature. Physically, electron-thermal effects may be important in 3d (e.g., V) and 4d (e.g., Mo) transition metals at high temperatures near melt and above. It is expected that temperature-dependent MGPT potentials for such cases will be added over time.

Related commands:

pair_coeff

Default:

The options defaults for the pair_coeff command are volpress yes, nbody 1234, and precision double.

(Moriarty1) Moriarty, Physical Review B, 38, 3199 (1988).

(Moriarty2) Moriarty, Physical Review B, 42, 1609 (1990). Moriarty, Physical Review B 49, 12431 (1994).

(Moriarty3) Moriarty, Benedict, Glosli, Hood, Orlikowski, Patel, Soderlind, Streitz, Tang, and Yang, Journal of Materials Research, 21, 563 (2006).

(Glosli) Glosli, unpublished, 2005. Streitz, Glosli, Patel, Chan, Yates, de Supinski, Sexton and Gunnels, Journal of Physics: Conference Series, 46, 254 (2006).

(Oppelstrup) Oppelstrup, unpublished, 2015. Oppelstrup and Moriarty, to be published.

pair_style mie/cut command

pair_style mie/cut/gpu command

Syntax:

```
pair_style mie/cut cutoff
```

- cutoff = global cutoff for mie/cut interactions (distance units)

Examples:

```
pair_style mie/cut 10.0
pair_coeff 1 1 0.72 3.40 23.00 6.66
pair_coeff 2 2 0.30 3.55 12.65 6.00
pair_coeff 1 2 0.46 3.32 16.90 6.31
```

Description:

The *mie/cut* style computes the Mie potential, given by

$$E = C\epsilon \left[\left(\frac{\sigma}{r} \right)^{\gamma_{rep}} - \left(\frac{\sigma}{r} \right)^{\gamma_{att}} \right] \qquad r < r_c$$

Rc is the cutoff and C is a function that depends on the repulsive and attractive exponents, given by:

$$C = \left(\frac{\gamma_{rep}}{\gamma_{rep} - \gamma_{att}} \right) \left(\frac{\gamma_{rep}}{\gamma_{att}} \right)^{\left(\frac{\gamma_{att}}{\gamma_{rep} - \gamma_{att}} \right)}$$

Note that for 12/6 exponents, C is equal to 4 and the formula is the same as the standard Lennard-Jones potential.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- epsilon (energy units)
- sigma (distance units)
- gammaR
- gammaA
- cutoff (distance units)

The last coefficient is optional. If not specified, the global cutoff specified in the pair_style command is used.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the mie/cut pair styles can be mixed. If not explicity defined, both the repulsive and attractive gamma exponents for different atoms will be calculated following the same mixing rule defined for distances. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style supports the pair_modify shift option for the energy of the pair interaction.

This pair style supports the pair_modify tail option for adding a long-range tail correction to the energy and pressure of the pair interaction.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style supports the use of the *inner*, *middle*, and *outer* keywords of the run_style respa command, meaning the pairwise forces can be partitioned by distance at different levels of the rRESPA hierarchy. See the run_style command for details.

Restrictions: none

Related commands:

pair_coeff

Default: none

(Mie) G. Mie, Ann Phys, 316, 657 (1903).

(Avendano) C. Avendano, T. Lafitte, A. Galindo, C. S. Adjiman, G. Jackson, E. Muller, J Phys Chem B, 115, 11154 (2011).

pair_modify command

Syntax:

```
pair_modify keyword values ...
```

- one or more keyword/value pairs may be listed
- keyword = *pair* or *shift* or *mix* or *table* or *table/disp* or *tabinner* or *tabinner/disp* or *tail* or *compute*

```
pair values = sub-style N special which wt1 wt2 wt3
    sub-style = sub-style of pair hybrid
    N = which instance of sub-style (only if sub-style is used multiple times)
    special which wt1 wt2 wt3 = override special_bonds settings (optional)
    which = lj/coul or lj or coul
    w1,w2,w3 = 1-2, 1-3, and 1-4 weights from 0.0 to 1.0 inclusive
  mix value = geometric or arithmetic or sixthpower
  shift value = yes or no
  table value = N
    2^N = # of values in table
  table/disp value = N
    2^N = # of values in table
  tabinner value = cutoff
    cutoff = inner cutoff at which to begin table (distance units)
  tabinner/disp value = cutoff
    cutoff = inner cutoff at which to begin table (distance units)
  tail value = yes or no
  compute value = yes or no
```

Examples:

pair_modify shift yes mix geometric pair_modify tail yes pair_modify table 12 pair_modify pair lj/cut compute no pair_modify pair lj/cut/coul/long 1 special lj/coul 0.0 0.0 0.0:pre

Description:

Modify the parameters of the currently defined pair style. Not all parameters are relevant to all pair styles.

If used, the *pair* keyword must appear first in the list of keywords. It can only be used with the hybrid and hybrid/overlay pair styles. It means that all the following parameters will only be modified for the specified sub-style. If the sub-style is defined multiple times, then an additional numeric argument *N* must also be specified, which is a number from 1 to M where M is the number of times the sub-style was listed in the pair_style hybrid command. The extra number indicates which instance of the sub-style the remaining keywords will be applied to. Note that if the *pair* keyword is not used, and the pair style is *hybrid* or *hybrid/overlay*, then all the specified keywords will be applied to all sub-styles.

The *special* keyword can only be used in conjunction with the *pair* keyword and must directly follow it. It allows to override the special_bonds settings for the specified sub-style. More details are given below.

The *mix* keyword affects pair coefficients for interactions between atoms of type I and J, when I != J and the coefficients are not explicitly set in the input script. Note that coefficients for I = J must be set explicitly, either in the input script via the "pair_coeff" command or in the "Pair Coeffs" section of the data file. For some pair styles it is not necessary to specify coefficients when I != J, since a "mixing" rule will create them from the I,I and J,J settings. The pair_modify *mix* value determines what formulas are used to compute the mixed coefficients. In

each case, the cutoff distance is mixed the same way as sigma.

Note that not all pair styles support mixing. Also, some mix options are not available for certain pair styles. See the doc page for individual pair styles for those restrictions. Note also that the pair_coeff command also can be to directly set coefficients for a specific I != J pairing, in which case no mixing is performed.

mix *geometric*

```
epsilon_ij = sqrt(epsilon_i * epsilon_j)
sigma_ij = sqrt(sigma_i * sigma_j)
```

mix *arithmetic*

```
epsilon_ij = sqrt(epsilon_i * epsilon_j)
sigma_ij = (sigma_i + sigma_j) / 2
```

mix *sixthpower*

```
epsilon_ij = (2 * sqrt(epsilon_i*epsilon_j) * sigma_i^3 * sigma_j^3) /
             (sigma_i^6 + sigma_j^6)
sigma_ij = ((sigma_i**6 + sigma_j**6) / 2) ^ (1/6)
```

The *shift* keyword determines whether a Lennard-Jones potential is shifted at its cutoff to 0.0. If so, this adds an energy term to each pairwise interaction which will be included in the thermodynamic output, but does not affect pair forces or atom trajectories. See the doc page for individual pair styles to see which ones support this option.

The *table* and *table/disp* keywords apply to pair styles with a long-range Coulombic term or long-range dispersion term respectively; see the doc page for individual styles to see which potentials support these options. If N is non-zero, a table of length 2^N is pre-computed for forces and energies, which can shrink their computational cost by up to a factor of 2. The table is indexed via a bit-mapping technique (Wolff) and a linear interpolation is performed between adjacent table values. In our experiments with different table styles (lookup, linear, spline), this method typically gave the best performance in terms of speed and accuracy.

The choice of table length is a tradeoff in accuracy versus speed. A larger N yields more accurate force computations, but requires more memory which can slow down the computation due to cache misses. A reasonable value of N is between 8 and 16. The default value of 12 (table of length 4096) gives approximately the same accuracy as the no-table (N = 0) option. For N = 0, forces and energies are computed directly, using a polynomial fit for the needed erfc() function evaluation, which is what earlier versions of LAMMPS did. Values greater than 16 typically slow down the simulation and will not improve accuracy; values from 1 to 8 give unreliable results.

The *tabinner* and *tabinner/disp* keywords set an inner cutoff above which the pairwise computation is done by table lookup (if tables are invoked), for the corresponding Coulombic and dispersion tables discussed with the *table* and *table/disp* keywords. The smaller the cutoff is set, the less accurate the table becomes (for a given number of table values), which can require use of larger tables. The default cutoff value is sqrt(2.0) distance units which means nearly all pairwise interactions are computed via table lookup for simulations with "real" units, but some close pairs may be computed directly (non-table) for simulations with "lj" units.

When the *tail* keyword is set to *yes*, certain pair styles will add a long-range VanderWaals tail "correction" to the energy and pressure. These corrections are bookkeeping terms which do not affect dynamics, unless a constant-pressure simulation is being performed. See the doc page for individual styles to see which support this option. These corrections are included in the calculation and printing of thermodynamic quantities (see the thermo_style command). Their effect will also be included in constant NPT or NPH simulations where the pressure influences the simulation box dimensions (e.g. the fix npt and fix nph commands). The formulas used for

the long-range corrections come from equation 5 of (Sun).

NOTE: The tail correction terms are computed at the beginning of each run, using the current atom counts of each atom type. If atoms are deleted (or lost) or created during a simulation, e.g. via the fix gcmc command, the correction factors are not re-computed. If you expect the counts to change dramatically, you can break a run into a series of shorter runs so that the correction factors are re-computed more frequently.

Several additional assumptions are inherent in using tail corrections, including the following:

- The simulated system is a 3d bulk homogeneous liquid. This option should not be used for systems that are non-liquid, 2d, have a slab geometry (only 2d periodic), or inhomogeneous.
- G(r), the radial distribution function (rdf), is unity beyond the cutoff, so a fairly large cutoff should be used (i.e. 2.5 sigma for an LJ fluid), and it is probably a good idea to verify this assumption by checking the rdf. The rdf is not exactly unity beyond the cutoff for each pair of interaction types, so the tail correction is necessarily an approximation.

  The tail corrections are computed at the beginning of each simulation run. If the number of atoms changes during the run, e.g. due to atoms leaving the simulation domain, or use of the fix gcmc command, then the corrections are not updates to relect the changed atom count. If this is a large effect in your simulation, you should break the long run into several short runs, so that the correction factors are re-computed multiple times.
- Thermophysical properties obtained from calculations with this option enabled will not be thermodynamically consistent with the truncated force-field that was used. In other words, atoms do not feel any LJ pair interactions beyond the cutoff, but the energy and pressure reported by the simulation include an estimated contribution from those interactions.

The *compute* keyword allows pairwise computations to be turned off, even though a pair_style is defined. This is not useful for running a real simulation, but can be useful for debugging purposes or for performing a rerun simulation, when you only wish to compute partial forces that do not include the pairwise contribution.

Two examples are as follows. First, this option allows you to perform a simulation with pair_style hybrid with only a subset of the hybrid sub-styles enabled. Second, this option allows you to perform a simulation with only long-range interactions but no short-range pairwise interactions. Doing this by simply not defining a pair style will not work, because the kspace_style command requires a Kspace-compatible pair style be defined.

Use of *special* keyword

The *special* keyword allows to override the 1-2, 1-3, and 1-4 exclusion settings for individual sub-styles of a hybrid pair style. It requires 4 arguments similar to the special_bonds command, *which* and wt1,wt2,wt3. The *which* argument can be *lj* to change the Lennard-Jones settings, *coul* to change the Coulombic settings, or *lj/coul* to change both to the same set of 3 values. The wt1,wt2,wt3 values are numeric weights from 0.0 to 1.0 inclusive, for the 1-2, 1-3, and 1-4 bond topology neighbors, respectively. The *special* keyword can only be used in conjunction with the *pair* keyword and has to directly follow it.

NOTE: The global settings specified by the special_bonds command affect the construction of neighbor lists. Weights of 0.0 (for 1-2, 1-3, or 1-4 neighbors) exclude those pairs from the neighbor list entirely. Weights of 1.0 store the neighbor with no weighting applied. Thus only global values different from exactly 0.0 or 1.0 can be overridden and an error is generated if the requested setting is not compatible with the global setting. Substituting 1.0e-10 for 0.0 and 0.9999999999 for 1.0 is usually a sufficient workaround in this case without causing a significant error.

Restrictions: none

You cannot use *shift* yes with *tail* yes, since those are conflicting options. You cannot use *tail* yes with 2d simulations.

Related commands:

pair_style, pair_coeff, thermo_style

Default:

The option defaults are mix = geometric, shift = no, table = 12, tabinner = sqrt(2.0), tail = no, and compute = yes.

Note that some pair styles perform mixing, but only a certain style of mixing. See the doc pages for individual pair styles for details.

(Wolff) Wolff and Rudd, Comp Phys Comm, 120, 200-32 (1999).

(Sun) Sun, J Phys Chem B, 102, 7338-7364 (1998).

pair_style morse command

pair_style morse/cuda command

pair_style morse/gpu command

pair_style morse/omp command

pair_style morse/opt command

Syntax:

```
pair_style morse cutoff
```

- cutoff = global cutoff for Morse interactions (distance units)

Examples:

```
pair_style morse 2.5
pair_coeff * * 100.0 2.0 1.5
pair_coeff 1 1 100.0 2.0 1.5 3.0
```

Description:

Style *morse* computes pairwise interactions with the formula

$$E = D_0 \left[e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)} \right] \qquad r < r_c$$

Rc is the cutoff.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- D0 (energy units)
- alpha (1/distance units)
- r0 (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global morse cutoff is used.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

None of these pair styles support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

All of these pair styles support the pair_modify shift option for the energy of the pair interaction.

The pair_modify table options is not relevant for the Morse pair styles.

None of these pair styles support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

All of these pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.

Restrictions: none

Related commands:

pair_coeff

Default: none

pair_style nb3b/harmonic command

pair_style nb3b/harmonic/omp command

Syntax:

```
pair_style nb3b/harmonic
```

Examples:

```
pair_style nb3b/harmonic
pair_coeff * * MgOH.nb3bharmonic Mg O H
```

Description:

This pair style computes a nonbonded 3-body harmonic potential for the energy E of a system of atoms as

$$E = K(\theta - \theta_0)^2$$

where *theta_0* is the equilibrium value of the angle and *K* is a prefactor. Note that the usual 1/2 factor is included in *K*. The form of the potential is identical to that used in angle_style *harmonic*, but in this case, the atoms do not need to be explicitly bonded.

Only a single pair_coeff command is used with this style which specifies a potential file with parameters for specified elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file.

As an example, imagine a file SiC.nb3b.harmonic has potential values for Si and C. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * SiC.nb3b.harmonic Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the potential file. The final C argument maps LAMMPS atom type 4 to the C element in the potential file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when the potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials. An example of a pair_coeff command for use with the *hybrid* pair style is:

pair_coeff * * nb3b/harmonic MgOH.nb3b.harmonic Mg O H

Three-body nonbonded harmonic files in the *potentials* directory of the LAMMPS distribution have a

".nb3b.harmonic" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements.

Each entry has six arguments. The first three are atom types as referenced in the LAMMPS input file. The first argument specifies the central atom. The fourth argument indicates the *K* parameter. The fifth argument indicates *theta_0*. The sixth argument indicates a separation cutoff in Angstroms.

For a given entry, if the second and third arguments are identical, then the entry is for a cutoff for the distance between types 1 and 2 (values for *K* and *theta_0* are irrelevant in this case).

For a given entry, if the first three arguments are all different, then the entry is for the *K* and *theta_0* parameters (the cutoff in this case is irrelevant).

It is *not* required that the potential file contain entries for all of the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

This pair style can only be used if LAMMPS was built with the MANYBODY package (which it is by default). See the Making LAMMPS section for more info on packages.

Related commands:

pair_coeff

Default: none

pair_style nm/cut command

pair_style nm/cut/coul/cut command

pair_style nm/cut/coul/long command

pair_style nm/cut/omp command

pair_style nm/cut/coul/cut/omp command

pair_style nm/cut/coul/long/omp command

Syntax:

```
pair_style style args
```

- style = *nm/cut* or *nm/cut/coul/cut* or *nm/cut/coul/long*
- args = list of arguments for a particular style

```
  nm/cut args = cutoff
      cutoff = global cutoff for Pair interactions (distance units)
    nm/cut/coul/cut args = cutoff (cutoff2)
      cutoff = global cutoff for Pair (and Coulombic if only 1 arg) (distance units)
      cutoff2 = global cutoff for Coulombic (optional) (distance units)
    nm/cut/coul/long args = cutoff (cutoff2)
      cutoff = global cutoff for Pair (and Coulombic if only 1 arg) (distance units)
      cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

Examples:

```
pair_style nm/cut 12.0
pair_coeff * * 0.01 5.4 8.0 7.0
pair_coeff 1 1 0.01 4.4 7.0 6.0

pair_style nm/cut/coul/cut 12.0 15.0
pair_coeff * * 0.01 5.4 8.0 7.0
pair_coeff 1 1 0.01 4.4 7.0 6.0

pair_style nm/cut/coul/long 12.0 15.0
pair_coeff * * 0.01 5.4 8.0 7.0
pair_coeff 1 1 0.01 4.4 7.0 6.0
```

Description:

Style *nm* computes site-site interactions based on the N-M potential by Clarke, mainly used for ionic liquids. A site can represent a single atom or a united-atom site. The energy of an interaction has the following form:

$$E = \frac{E_0}{(n-m)} \left[m \left(\frac{r_0}{r} \right)^n - n \left(\frac{r_0}{r} \right)^m \right] \qquad r < r_c$$

Rc is the cutoff.

Style *nm/cut/coul/cut* adds a Coulombic pairwise interaction given by

$$E = \frac{Cq_iq_j}{\epsilon r} \qquad r < r_c$$

where C is an energy-conversion constant, Qi and Qj are the charges on the 2 atoms, and epsilon is the dielectric constant which can be set by the dielectric command. If one cutoff is specified in the pair_style command, it is used for both the NM and Coulombic terms. If two cutoffs are specified, they are used as cutoffs for the NM and Coulombic terms respectively.

Styles *nm/cut/coul/long* compute the same Coulombic interactions as style *nm/cut/coul/cut* except that an additional damping factor is applied to the Coulombic term so it can be used in conjunction with the kspace_style command and its *ewald* or *pppm* option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

For all of the *nm* pair styles, the following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands.

- E0 (energy units)
- r0 (distance units)
- n (unitless)
- m (unitless)
- cutoff1 (distance units)
- cutoff2 (distance units)

The latter 2 coefficients are optional. If not specified, the global NM and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both NM and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the NM and Coulombic cutoffs for this type pair. You cannot specify 2 cutoffs for style *nm*, since it has no Coulombic terms.

For *nm/cut/coul/long* only the NM cutoff can be specified since a Coulombic cutoff cannot be specified for an individual I,J type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

All of the *nm* pair styles supports the pair_modify shift option for the energy of the pair interaction.

The *nm/cut/coul/long* pair styles support the pair_modify table option since they can tabulate the short-range portion of the long-range Coulombic interaction.

All of the *nm* pair styles support the pair_modify tail option for adding a long-range tail correction to the energy and pressure for the NM portion of the pair interaction.

All of the *nm* pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

All of the *nm* pair styles can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

These pair styles are part of the MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff

Default: none

(Clarke) Clarke and Smith, J Chem Phys, 84, 2290 (1986).

pair_style none command

Syntax:

```
pair_style none
```

Examples:

```
pair_style none
```

Description:

Using a pair style of none means pair forces are not computed.

With this choice, the force cutoff is 0.0, which means that only atoms within the neighbor skin distance (see the neighbor command) are communicated between processors. You must insure the skin distance is large enough to acquire atoms needed for computing bonds, angles, etc.

A pair style of *none* will also prevent pairwise neighbor lists from being built. However if the neighbor style is *bin*, data structures for binning are still allocated. If the neighbor skin distance is small, then these data structures can consume a large amount of memory. So you should either set the neighbor style to *nsq* or set the skin distance to a larger value.

Restrictions: none

Related commands: none

Default: none

pair_style peri/pmb command

pair_style peri/pmb/omp command

pair_style peri/lps command

pair_style peri/lps/omp command

pair_style peri/ves command

pair_style peri/eps command

Syntax:

```
pair_style style
```

style = *peri/pmb* or *peri/lps* or *peri/ves* or *peri/eps*:ul

Examples:

```
pair_style peri/pmb
pair_coeff * * 1.6863e22 0.0015001 0.0005 0.25

pair_style peri/lps
pair_coeff * * 14.9e9 14.9e9 0.0015001 0.0005 0.25

pair_style peri/ves
pair_coeff * * 14.9e9 14.9e9 0.0015001 0.0005 0.25 0.5 0.001

pair_style peri/eps
pair_coeff * * 14.9e9 14.9e9 0.0015001 0.0005 0.25 118.43
```

Description:

The peridynamic pair styles implement material models that can be used at the mescscopic and macroscopic scales. See this document for an overview of LAMMPS commands for Peridynamics modeling.

Style *peri/pmb* implements the Peridynamic bond-based prototype microelastic brittle (PMB) model.

Style *peri/lps* implements the Peridynamic state-based linear peridynamic solid (LPS) model.

Style *peri/ves* implements the Peridynamic state-based linear peridynamic viscoelastic solid (VES) model.

Style *peri/eps* implements the Peridynamic state-based elastic-plastic solid (EPS) model.

The canonical papers on Peridynamics are (Silling 2000) and (Silling 2007). The implementation of Peridynamics in LAMMPS is described in (Parks). Also see the PDLAMMPS user guide for more details about its implementation.

The peridynamic VES and EPS models in PDLAMMPS were implemented by R. Rahman and J. T. Foster at University of Texas at San Antonio. The original VES formulation is described in "(Mitchell2011)" and the original EPS formulation is in "(Mitchell2011a)". Additional PDF docs that describe the VES and EPS implementations are include in the LAMMPS distro in doc/PDF/PDLammps_VES.pdf and doc/PDF/PDLammps_EPS.pdf. For questions regarding the VES and EPS models in LAMMPS you can contact R. Rahman (rezwanur.rahman at utsa.edu).

The following coefficients must be defined for each pair of atom types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below.

For the *peri/pmb* style:

- c (energy/distance/volume^2 units)
- horizon (distance units)
- s00 (unitless)
- alpha (unitless)

C is the effectively a spring constant for Peridynamic bonds, the horizon is a cutoff distance for truncating interactions, and s00 and alpha are used as a bond breaking criteria. The units of c are such that c/distance = stiffness/volume^2, where stiffness is energy/distance^2 and volume is distance^3. See the users guide for more details.

For the *peri/lps* style:

- K (force/area units)
- G (force/area units)
- horizon (distance units)
- s00 (unitless)
- alpha (unitless)

K is the bulk modulus and G is the shear modulus. The horizon is a cutoff distance for truncating interactions, and s00 and alpha are used as a bond breaking criteria. See the users guide for more details.

For the *peri/ves* style:

- K (force/area units)
- G (force/area units)
- horizon (distance units)
- s00 (unitless)
- alpha (unitless)
- m_lambdai (unitless)
- m_taubi (unitless)

K is the bulk modulus and G is the shear modulus. The horizon is a cutoff distance for truncating interactions, and s00 and alpha are used as a bond breaking criteria. m_lambdai and m_taubi are the viscoelastic relaxation parameter and time constant, respectively. m_lambdai varies within zero to one. For very small values of m_lambdai the viscoelsatic model responds very similar to a linear elastic model. For details please see the description in "(Mtchell2011)".

For the *peri/eps* style:

K (force/area units) G (force/area units) horizon (distance units) s00 (unitless) alpha (unitless) m_yield_stress (force/area units)

K is the bulk modulus and G is the shear modulus. The horizon is a cutoff distance and s00 and alpha are used as a bond breaking criteria. m_yield_stress is the yield stress of the material. For details please see the description in "(Mtchell2011a)".

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

These pair styles do not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

These pair styles do not support the pair_modify shift option.

The pair_modify table and tail options are not relevant for these pair styles.

These pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.

Restrictions:

All of these styles are part of the PERI package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff

Default: none

(Parks) Parks, Lehoucq, Plimpton, Silling, Comp Phys Comm, 179(11), 777-783 (2008).

(Silling 2000) Silling, J Mech Phys Solids, 48, 175-209 (2000).

(Silling 2007) Silling, Epton, Weckner, Xu, Askari, J Elasticity, 88, 151-184 (2007).

(Mitchell2011) Mitchell. A non-local, ordinary-state-based viscoelasticity model for peridynamics. Sandia National Lab Report, 8064:1-28 (2011).

(Mitchell2011a) Mitchell. A Nonlocal, Ordinary, State-Based Plasticity Model for Peridynamics. Sandia National Lab Report, 3166:1-34 (2011).

pair_style polymorphic command

Syntax:

```
pair_style polymorphic
```

style = *polymorphic*

Examples:

```
pair_style polymorphic
pair_coeff * * TlBr_msw.polymorphic Tl Br
pair_coeff * * AlCu_eam.polymorphic Al Cu
pair_coeff * * GaN_tersoff.polymorphic Ga N
pair_coeff * * GaN_sw.polymorphic GaN
```

Description:

The *polymorphic* pair style computes a 3-body free-form potential (Zhou) for the energy E of a system of atoms as

$$E = \frac{1}{2} \sum_{i=1}^{i=N} \sum_{j=1}^{j=N} \left[(1 - \delta_{ij}) \cdot U_{IJ}\left(r_{ij}\right) - (1 - \eta_{ij}) \cdot F_{IJ}\left(r_{ij}\right) \cdot V_{IJ}\left(r_{ij}\right) \right]$$

$$X_{ij} = \sum_{k=i_1, k \neq i,j}^{i_N} W_{IK}\left(r_{ik}\right) \cdot G_{JIK}\left(\theta_{jik}\right) \cdot P_{IK}\left(\Delta r_{jik}\right)$$

$$\Delta r_{jik} = r_{ij} - \xi_{IJ} \cdot r_{ik}$$

where I, J, K represent species of atoms i, j, and k, i_1, ..., i_N represents a list of i's neighbors, delta_ij is a Direc constant (i.e., delta_ij = 1 when i = j, and delta_ij = 0 otherwise), eta_ij is similar constant that can be set either to eta_ij = delta_ij or eta_ij = 1 - delta_ij depending on the potential type, U_IJ(r_ij), V_IJ(r_ij), W_IK(r_ik) are pair functions, G_JIK(cos(theta)) is an angular function, P_IK(delta r_jik) is a function of atomic spacing differential delta r_jik = r_ij - xi_IJ*r_ik with xi_IJ being a pair-dependent parameter, and F_IJ(X_ij) is a function of the local environment variable X_ij. This generic potential is fully defined once the constants eta_ij and xi_IJ, and the six functions U_IJ(r_ij), V_IJ(r_ij), W_IK(r_ik), G_JIK(cos(theta)), P_IK(delta r_jik), and F_IJ(X_ij) are given. Note that these six functions are all one dimensional, and hence can be provided in an analytic or tabular form. This allows users to design different potentials solely based on a manipulation of these functions. For instance, the potential reduces to Stillinger-Weber potential (SW) if we set

$$\begin{cases} \eta_{ij}=\delta_{ij},\xi_{IJ}=0 \\ U_{IJ}(r)=A_{IJ}\cdot\epsilon_{IJ}\cdot\left(\frac{\sigma_{IJ}}{r}\right)^{q}\cdot\left[B_{IJ}\cdot\left(\frac{\sigma_{IJ}}{r}\right)^{p-q}-1\right]\cdot exp\left(\frac{\sigma_{IJ}}{r-a_{IJ}\cdot\sigma_{IJ}}\right) \\ V_{IJ}(r)=\sqrt{\lambda_{IJ}\cdot\epsilon_{IJ}}\cdot exp\left(\frac{\gamma_{IJ}\cdot\sigma_{IJ}}{r-a_{IJ}\cdot\sigma_{IJ}}\right) \\ F_{IJ}(X)=-X \\ P_{IJ}(\Delta r)=1 \\ W_{IJ}(r)=\sqrt{\lambda_{IJ}\cdot\epsilon_{IJ}}\cdot exp\left(\frac{\gamma_{IJ}\cdot\sigma_{IJ}}{r-a_{IJ}\cdot\sigma_{IJ}}\right) \\ G_{JIK}(\theta)=\left(cos\theta+\frac{1}{3}\right)^{2} \end{cases}$$

The potential reduces to Tersoff types of potential (Tersoff or Albe) if we set

$$\begin{cases} \eta_{ij}=\delta_{ij},\xi_{IJ}=1 \\ U_{IJ}(r)=\frac{D_{e,IJ}}{S_{IJ}-1}\cdot exp\left[-\beta_{IJ}\sqrt{2S_{IJ}\left(r-r_{e,IJ}\right)}\right]\cdot f_{c,IJ}(r) \\ V_{IJ}(r)=\frac{S_{IJ}\cdot D_{e,IJ}}{S_{IJ}-1}\cdot exp\left[-\beta_{IJ}\sqrt{\frac{2}{S_{IJ}}\left(r-r_{e,IJ}\right)}\right]\cdot f_{c,IJ}(r) \\ F_{IJ}(X)=(1+X)^{-\frac{1}{2}} \\ P_{IJ}(\Delta r)=exp\left(2\mu_{IK}\cdot\Delta r\right) \\ W_{IJ}(r)=f_{c,IK}(r) \\ G_{JIK}(\theta)=\gamma_{IK}\left[1+\frac{c_{IK}^{2}}{d_{IK}^{2}}-\frac{c_{IK}^{2}}{d_{IK}^{2}+(h_{IK}+cos\theta)^{2}}\right] \end{cases}$$

$$f_{c,IJ}=\begin{cases} 1, & r\le r_{s,IJ} \\ \frac{1}{2}+\frac{1}{2}cos\left[\frac{\pi\left(r-r_{s,IJ}\right)}{r_{c,IJ}-r_{s,IJ}}\right], & r_{s,IJ}<r<r_{c,IJ} \\ 0, & r\ge r_{c,IJ} \end{cases}$$

The potential reduces to Rockett-Tersoff (Wang) type if we set

$$
\begin{aligned}
&_{ij} = \delta_{ij}, \xi_{IJ} = 1 \\
&_{IJ}(r) = \begin{cases} A_{IJ} \cdot exp(-\lambda_{1,IJ} \cdot r) \cdot f_{c,IJ}(r), & r \le r_{s,1,IJ} \\ A_{IJ} \cdot exp(-\lambda_{1,IJ} \cdot r) \cdot f_{c,IJ}(r) \cdot f_{c,1,IJ}(r), & r_{s,1,IJ} < r < r_{c,1,IJ} \\ 0, & r \ge r_{c,1,IJ} \end{cases} \\
&_{IJ}(r) = \begin{cases} B_{IJ} \cdot exp(-\lambda_{2,IJ} \cdot r) \cdot f_{c,IJ}(r), & r \\ B_{IJ} \cdot exp(-\lambda_{2,IJ} \cdot r) \cdot f_{c,IJ}(r) + A_{IJ} \cdot exp(-\lambda_{1,IJ} \cdot r) \cdot \\ \quad f_{c,IJ}(r) \cdot [1 - f_{c,1,IJ}(r)], & r_{s,1,IJ} < r \\ B_{IJ} \cdot exp(-\lambda_{2,IJ} \cdot r) \cdot f_{c,IJ}(r) + A_{IJ} \cdot exp(-\lambda_{1,IJ} \cdot r) \cdot \\ \quad f_{c,IJ}(r) & r \end{cases} \\
&_{IJ}(X) = [1 + (\beta_{IJ} \cdot X)^{n_{IJ}}]^{-\frac{1}{2n_{IJ}}} \\
&_{IJ}(\Delta r) = exp(\lambda_{3,IK} \cdot \Delta r^3) \\
&_{IJ}(r) = f_{c,IK}(r) \\
&_{JIK}(\theta) = 1 + \frac{c_{IK}^2}{d_{IK}^2} - \frac{c_{IK}^2}{d_{IK}^2 + (h_{IK} + cos\theta)^2}
\end{aligned}
$$

$$
f_{c,IJ} = \begin{cases} 1, & r \le r_{s,IJ} \\ \frac{1}{2} + \frac{1}{2} cos\left[\frac{\pi\left(r - r_{s,IJ}\right)}{r_{c,IJ} - r_{s,IJ}}\right], & r_{s,IJ} < r < r_{c,IJ} \\ 0, & r \ge r_{c,IJ} \end{cases}
$$

$$
f_{c,1,IJ} = \begin{cases} 1, & r \le r_{s,1,IJ} \\ \frac{1}{2} + \frac{1}{2} cos\left[\frac{\pi\left(r - r_{s,1,IJ}\right)}{r_{c,1,IJ} - r_{s,1,IJ}}\right], & r_{s,1,IJ} < r < r_{c,1,IJ} \\ 0, & r \ge r_{c,1,IJ} \end{cases}
$$

The potential becomes embedded atom method (Daw) if we set

$$\begin{cases} \eta_{ij} = 1 - \delta_{ij}, \xi_{IJ} = 0 \\ U_{IJ}(r) = \phi_{IJ}(r) \\ V_{IJ}(r) = 1 \\ F_{II}(X) = -2F_I(X) \\ P_{IJ}(\Delta r) = 1 \\ W_{IJ}(r) = f_K(r) \\ G_{JIK}(\theta) = 1 \end{cases}$$

In the embedded atom method case, phi_IJ(r_ij) is the pair energy, F_I(X) is the embedding energy, X is the local electron density, and f_K(r) is the atomic electron density function.

If the tabulated functions are created using the parameters of sw, tersoff, and eam potentials, the polymorphic pair style will produce the same global properties (energies and stresses) and the same forces as the sw, tersoff, and eam pair styles. The polymorphic pair style also produces the same atom properties (energies and stresses) as the corresponding tersoff and eam pair styles. However, due to a different partition of global properties to atom properties, the polymorphic pair style will produce different atom properties (energies and stresses) as the sw pair style. This does not mean that polymorphic pair style is different from the sw pair style in this case. It just means that the definitions of the atom energies and atom stresses are different.

Only a single pair_coeff command is used with the polymorphic style which specifies an potential file for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of Tersoff elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file. Several files for polymorphic potentials are included in the potentials dir of the LAMMPS distro. They have a "poly" suffix.

As an example, imagine the SiC_tersoff.polymorphic file has tabulated functions for Si-C tersoff potential. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * SiC_tersoff.polymorphic Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the polymorphic file. The final C argument maps LAMMPS atom type 4 to the C element in the polymorphic file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when an polymorphic potential is used as part of the hybrid pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Potential files in the potentials directory of the LAMMPS distribution have a ".poly" suffix. At the beginning of the files, an unlimited number of lines starting with '#' are used to describe the potential and are ignored by LAMMPS. The next line lists two numbers:

```
ntypes eta
```

Here ntypes represent total number of species defined in the potential file, and eta = 0 or 1. The number ntypes must equal the total number of different species defined in the pair_coeff command. When eta = 1, eta_ij defined in the potential functions above is set to 1 - delta_ij, otherwise eta_ij is set to delta_ij. The next ntypes lines each lists two numbers and a character string representing atomic number, atomic mass, and name of the species of the ntypes elements:

```
atomic_number atomic-mass element (1)
atomic_number atomic-mass element (2)
...
atomic_number atomic-mass element (ntypes)
```

The next ntypes*(ntypes+1)/2 lines contain two numbers:

```
cut xi (1)
cut xi (2)
...
cut xi (ntypes*(ntypes+1)/2)
```

Here cut means the cutoff distance of the pair functions, xi is the same as defined in the potential functions above. The ntypes*(ntypes+1)/2 lines are related to the pairs according to the sequence of first ii (self) pairs, i = 1, 2, ..., ntypes, and then then ij (cross) pairs, i = 1, 2, ..., ntypes-1, and j = i+1, i+2, ..., ntypes (i.e., the sequence of the ij pairs follows 11, 22, ..., 12, 13, 14, ..., 23, 24, ...).

The final blocks of the potential file are the U, V, W, P, G, and F functions are listed sequentially. First, U functions are given for each of the ntypes*(ntypes+1)/2 pairs according to the sequence described above. For each of the pairs, nr values are listed. Next, similar arrays are given for V, W, and P functions. Then G functions are given for all the ntypes*ntypes*ntypes ijk triplets in a natural sequence i from 1 to ntypes, j from 1 to ntypes, and k from 1 to ntypes (i.e., ijk = 111, 112, 113, ..., 121, 122, 123 ..., 211, 212, ...). Each of the ijk functions contains ng values. Finally, the F functions are listed for all ntypes*(ntypes+1)/2 pairs, each containing nx values. Either analytic or tabulated functions can be specified. Currently, constant, exponential, sine and cosine analytic functions are available which are specified with: constant c1 , where f(x) = c1 exponential c1 c2 , where f(x) = c1 exp(c2*x) sine c1 c2 , where f(x) = c1 sin(c2*x) cos c1 c2 , where f(x) = c1 cos(c2*x) Tabulated functions are specified by spline n x1 x2, where n=number of point, (x1,x2)=range and then followed by n values evaluated uniformly over these argument ranges. The valid argument ranges of the functions are between 0 <= r <= cut for the U(r), V(r), W(r) functions, -cutmax <= delta_r <= cutmax for the P(delta_r) functions, -1 <= costheta <= 1 for the G(costheta) functions, and 0 <= X <= maxX for the F(X) functions.

Mixing, shift, table tail correction, restart:

This pair styles does not support the pair_modify shift, table, and tail options.

This pair style does not write their information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

Restrictions:

If using create_atoms command, atomic masses must be defined in the input script. If using read_data, atomic masses must be defined in the atomic structure data file.

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

This pair potential requires the newton setting to be "on" for pair interactions.

The potential files provided with LAMMPS (see the potentials directory) are parameterized for metal units. You can use any LAMMPS units, but you would need to create your own potential files.

Related commands:

pair_coeff

(Zhou) X. W. Zhou, M. E. Foster, R. E. Jones, P. Yang, H. Fan, and F. P. Doty, J. Mater. Sci. Res., 4, 15 (2015).

(SW) F. H. Stillinger-Weber, and T. A. Weber, Phys. Rev. B, 31, 5262 (1985).

(Tersoff) J. Tersoff, Phys. Rev. B, 39, 5566 (1989).

(Albe) K. Albe, K. Nordlund, J. Nord, and A. Kuronen, Phys. Rev. B, 66, 035205 (2002).

(Wang) J. Wang, and A. Rockett, Phys. Rev. B, 43, 12571 (1991).

(Daw) M. S. Daw, and M. I. Baskes, Phys. Rev. B, 29, 6443 (1984).

pair_style quip command

Syntax:

```
pair_style quip
```

Examples:

```
pair_style      quip
pair_coeff      * * gap_example.xml "Potential xml_label=GAP_2014_5_8_60_17_10_38_466" 14
pair_coeff      * * sw_example.xml "IP SW" 14
```

Description:

Style *quip* provides an interface for calling potential routines from the QUIP package. QUIP is built separately, and then linked to LAMMPS. The most recent version of the QUIP package can be downloaded from GitHub: https://github.com/libAtoms/QUIP. The interface is chiefly intended to be used to run Gaussian Approximation Potentials (GAP), which are described in the following publications: (Bartok et al) and (PhD thesis of Bartok).

Only a single pair_coeff command is used with the *quip* style that specifies a QUIP potential file containing the parameters of the potential for all needed elements in XML format. This is followed by a QUIP initialization string. Finally, the QUIP elements are mapped to LAMMPS atom types by specifying N atomic numbers, where N is the number of LAMMPS atom types:

- QUIP filename
- QUIP initialization string
- N atomic numbers = mapping of QUIP elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file.

A QUIP potential is fully specified by the filename which contains the parameters of the potential in XML format, the initialisation string, and the map of atomic numbers.

GAP potentials can be obtained from the Data repository section of http://www.libatoms.org, where the appropriate initialisation strings are also advised. The list of atomic numbers must be matched to the LAMMPS atom types specified in the LAMMPS data file or elsewhere.

Two examples input scripts are provided in the examples/USER/quip directory.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the pair_modify mix, shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the USER-QUIP package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

QUIP potentials are parametrized in electron-volts and Angstroms and therefore should be used with LAMMPS metal units.

Related commands:

pair_coeff

(Bartok_2010) AP Bartok, MC Payne, R Kondor, and G Csanyi, Physical Review Letters 104, 136403 (2010).

(Bartok_PhD) A Bartok-Partay, PhD Thesis, University of Cambridge, (2010).

pair_style reax command

Syntax:

```
pair_style reax hbcut hbnewflag tripflag precision
```

- hbcut = hydrogen-bond cutoff (optional) (distance units)
- hbnewflag = use old or new hbond function style (0 or 1) (optional)
- tripflag = apply stabilization to all triple bonds (0 or 1) (optional)
- precision = precision for charge equilibration (optional)

Examples:

```
pair_style reax
pair_style reax 10.0 0 1 1.0e-5
pair_coeff * * ffield.reax 3 1 2 2
pair_coeff * * ffield.reax 3 NULL NULL 3
```

Description:

Style *reax* computes the ReaxFF potential of van Duin, Goddard and co-workers. ReaxFF uses distance-dependent bond-order functions to represent the contributions of chemical bonding to the potential energy. There is more than one version of ReaxFF. The version implemented in LAMMPS uses the functional forms documented in the supplemental information of the following paper: (Chenoweth). The version integrated into LAMMPS matches the most up-to-date version of ReaxFF as of summer 2010.

WARNING: pair style reax is now deprecated and will soon be retired. Users should switch to pair_style reax/c. The *reax* style differs from the *reax/c* style in the lo-level implementation details. The *reax* style is a Fortran library, linked to LAMMPS. The *reax/c* style was initially implemented as stand-alone C code and is now integrated into LAMMPS as a package.

LAMMPS requires that a file called ffield.reax be provided, containing the ReaxFF parameters for each atom type, bond type, etc. The format is identical to the ffield file used by van Duin and co-workers. The filename is required as an argument in the pair_coeff command. Any value other than "ffield.reax" will be rejected (see below).

LAMMPS provides several different versions of ffield.reax in its potentials dir, each called potentials/ffield.reax.label. These are documented in potentials/README.reax. The default ffield.reax contains parameterizations for the following elements: C, H, O, N, S.

NOTE: We do not distribute a wide variety of ReaxFF force field files with LAMMPS. Adri van Duin's group at PSU is the central repository for this kind of data as they are continuously deriving and updating parameterizations for different classes of materials. You can visit their WWW site at http://www.engr.psu.edu/adri, register as a "new user", and then submit a request to their group describing material(s) you are interested in modeling with ReaxFF. They can tell you what is currently available or what it would take to create a suitable ReaxFF parameterization.

The format of these files is identical to that used originally by van Duin. We have tested the accuracy of *pair_style reax* potential against the original ReaxFF code for the systems mentioned above. You can use other ffield files for specific chemical systems that may be available elsewhere (but note that their accuracy may not have been tested).

The *hbcut*, *hbnewflag*, *tripflag*, and *precision* settings are optional arguments. If none are provided, default settings are used: *hbcut* = 6 (which is Angstroms in real units), *hbnewflag* = 1 (use new hbond function style), *tripflag* = 1 (apply stabilization to all triple bonds), and *precision* = 1.0e-6 (one part in 10^6). If you wish to override any of these defaults, then all of the settings must be specified.

Two examples using *pair_style reax* are provided in the examples/reax sub-directory, along with corresponding examples for pair_style reax/c.

Use of this pair style requires that a charge be defined for every atom since the *reax* pair style performs a charge equilibration (QEq) calculation. See the atom_style and read_data commands for details on how to specify charges.

The thermo variable *evdwl* stores the sum of all the ReaxFF potential energy contributions, with the exception of the Coulombic and charge equilibration contributions which are stored in the thermo variable *ecoul*. The output of these quantities is controlled by the thermo command.

This pair style tallies a breakdown of the total ReaxFF potential energy into sub-categories, which can be accessed via the compute pair command as a vector of values of length 14. The 14 values correspond to the following sub-categories (the variable names in italics match those used in the ReaxFF FORTRAN library):

1. *eb* = bond energy
2. *ea* = atom energy
3. *elp* = lone-pair energy
4. *emol* = molecule energy (always 0.0)
5. *ev* = valence angle energy
6. *epen* = double-bond valence angle penalty
7. *ecoa* = valence angle conjugation energy
8. *ehb* = hydrogen bond energy
9. *et* = torsion energy
10. *eco* = conjugation energy
11. *ew* = van der Waals energy
12. *ep* = Coulomb energy
13. *efi* = electric field energy (always 0.0)
14. *eqeq* = charge equilibration energy

To print these quantities to the log file (with descriptive column headings) the following commands could be included in an input script:

```
compute reax all pair reax
variable eb      equal c_reax[1]
variable ea      equal c_reax[2]
...
variable eqeq    equal c_reax[14]
thermo_style custom step temp epair v_eb v_ea ... v_eqeq
```

Only a single pair_coeff command is used with the *reax* style which specifies a ReaxFF potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N indices = mapping of ReaxFF elements to atom types

The specification of the filename and the mapping of LAMMPS atom types recognized by the ReaxFF is done

differently than for other LAMMPS potentials, due to the non-portable difficulty of passing character strings (e.g. filename, element names) between C++ and Fortran.

The filename has to be "ffield.reax" and it has to exist in the directory you are running LAMMPS in. This means you cannot prepend a path to the file in the potentials dir. Rather, you should copy that file into the directory you are running from. If you wish to use another ReaxFF potential file, then name it "ffield.reax" and put it in the directory you run from.

In the ReaxFF potential file, near the top, after the general parameters, is the atomic parameters section that contains element names, each with a couple dozen numeric parameters. If there are M elements specified in the *ffield* file, think of these as numbered 1 to M. Each of the N indices you specify for the N atom types of LAMMPS atoms must be an integer from 1 to M. Atoms with LAMMPS type 1 will be mapped to whatever element you specify as the first index value, etc. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a ReaxFF potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

NOTE: Currently the reax pair style cannot be used as part of the *hybrid* pair style. Some additional changes still need to be made to enable this.

As an example, say your LAMMPS simulation has 4 atom types and the elements are ordered as C, H, O, N in the *ffield* file. If you want the LAMMPS atom type 1 and 2 to be C, type 3 to be N, and type 4 to be H, you would use the following pair_coeff command:

```
pair_coeff * * ffield.reax 1 1 4 2
```

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the pair_modify mix, shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

The ReaxFF potential files provided with LAMMPS in the potentials directory are parameterized for real units. You can use the ReaxFF potential with any LAMMPS units, but you would need to create your own potential file with coefficients listed in the appropriate units if your simulation doesn't use "real" units.

Related commands:

pair_coeff, pair_style reax/c, fix_reax_bonds

Default:

The keyword defaults are *hbcut* = 6, *hbnewflag* = 1, *tripflag* = 1, *precision* = 1.0e-6.

(Chenoweth_2008) Chenoweth, van Duin and Goddard, Journal of Physical Chemistry A, 112, 1040-1053 (2008).

pair_style reax/c command

Syntax:

```
pair_style reax/c cfile keyword value
```

- cfile = NULL or name of a control file
- zero or more keyword/value pairs may be appended

```
keyword = checkqeq or lgvdw or safezone or mincap
  checkqeq value = yes or no = whether or not to require qeq/reax fix
  lgvdw value = yes or no = whether or not to use a low gradient vdW correction
  safezone = factor used for array allocation
  mincap = minimum size for array allocation
```

Examples:

```
pair_style reax/c NULL
pair_style reax/c controlfile checkqeq no
pair_style reax/c NULL lgvdw yes
pair_style reax/c NULL safezone 1.6 mincap 100
pair_coeff * * ffield.reax C H O N
```

Description:

Style *reax/c* computes the ReaxFF potential of van Duin, Goddard and co-workers. ReaxFF uses distance-dependent bond-order functions to represent the contributions of chemical bonding to the potential energy. There is more than one version of ReaxFF. The version implemented in LAMMPS uses the functional forms documented in the supplemental information of the following paper: (Chenoweth et al., 2008). The version integrated into LAMMPS matches the most up-to-date version of ReaxFF as of summer 2010. For more technical details about the pair reax/c implementation of ReaxFF, see the (Aktulga) paper.

The *reax/c* style differs from the pair_style reax command in the lo-level implementation details. The *reax* style is a Fortran library, linked to LAMMPS. The *reax/c* style was initially implemented as stand-alone C code and is now integrated into LAMMPS as a package.

LAMMPS provides several different versions of ffield.reax in its potentials dir, each called potentials/ffield.reax.label. These are documented in potentials/README.reax. The default ffield.reax contains parameterizations for the following elements: C, H, O, N, S.

The format of these files is identical to that used originally by van Duin. We have tested the accuracy of *pair_style reax/c* potential against the original ReaxFF code for the systems mentioned above. You can use other ffield files for specific chemical systems that may be available elsewhere (but note that their accuracy may not have been tested).

NOTE: We do not distribute a wide variety of ReaxFF force field files with LAMMPS. Adri van Duin's group at PSU is the central repository for this kind of data as they are continuously deriving and updating parameterizations for different classes of materials. You can visit their WWW site at http://www.engr.psu.edu/adri, register as a "new user", and then submit a request to their group describing material(s) you are interested in modeling with ReaxFF. They can tell you what is currently available or what it would take to create a suitable ReaxFF parameterization.

The *cfile* setting can be specified as NULL, in which case default settings are used. A control file can be specified which defines values of control variables. Some control variables are global parameters for the ReaxFF potential. Others define certain performance and output settings. Each line in the control file specifies the value for a control variable. The format of the control file is described below.

NOTE: The LAMMPS default values for the ReaxFF global parameters correspond to those used by Adri van Duin's stand-alone serial code. If these are changed by setting control variables in the control file, the results from LAMMPS and the serial code will not agree.

Two examples using *pair_style reax/c* are provided in the examples/reax sub-directory, along with corresponding examples for pair_style reax.

Use of this pair style requires that a charge be defined for every atom. See the atom_style and read_data commands for details on how to specify charges.

The ReaxFF parameter files provided were created using a charge equilibration (QEq) model for handling the electrostatic interactions. Therefore, by default, LAMMPS requires that the fix qeq/reax command be used with *pair_style reax/c* when simulating a ReaxFF model, to equilibrate charge each timestep. Using the keyword *checkqeq* with the value *no* turns off the check for *fix qeq/reax*, allowing a simulation to be run without charge equilibration. In this case, the static charges you assign to each atom will be used for computing the electrostatic interactions in the system. See the fix qeq/reax command for details.

Using the optional keyword *lgvdw* with the value *yes* turns on the low-gradient correction of the ReaxFF/C for long-range London Dispersion, as described in the (Liu) paper. Force field file *ffield.reax.lg* is designed for this correction, and is trained for several energetic materials (see "Liu"). When using lg-correction, recommended value for parameter *thb* is 0.01, which can be set in the control file. Note: Force field files are different for the original or lg corrected pair styles, using wrong ffield file generates an error message.

Optional keywords *safezone* and *mincap* are used for allocating reax/c arrays. Increase these values can avoid memory problems, such as segmentation faults and bondchk failed errors, that could occur under certain conditions.

The thermo variable *evdwl* stores the sum of all the ReaxFF potential energy contributions, with the exception of the Coulombic and charge equilibration contributions which are stored in the thermo variable *ecoul*. The output of these quantities is controlled by the thermo command.

This pair style tallies a breakdown of the total ReaxFF potential energy into sub-categories, which can be accessed via the compute pair command as a vector of values of length 14. The 14 values correspond to the following sub-categories (the variable names in italics match those used in the original FORTRAN ReaxFF code):

1. *eb* = bond energy
2. *ea* = atom energy
3. *elp* = lone-pair energy
4. *emol* = molecule energy (always 0.0)
5. *ev* = valence angle energy
6. *epen* = double-bond valence angle penalty
7. *ecoa* = valence angle conjugation energy
8. *ehb* = hydrogen bond energy
9. *et* = torsion energy
10. *eco* = conjugation energy
11. *ew* = van der Waals energy
12. *ep* = Coulomb energy

13. *efi* = electric field energy (always 0.0)
14. *eqeq* = charge equilibration energy

To print these quantities to the log file (with descriptive column headings) the following commands could be included in an input script:

```
compute reax all pair reax/c
variable eb      equal c_reax[1]
variable ea      equal c_reax[2]
...
variable eqeq    equal c_reax[14]
thermo_style custom step temp epair v_eb v_ea ... v_eqeq
```

Only a single pair_coeff command is used with the *reax/c* style which specifies a ReaxFF potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N indices = ReaxFF elements

The filename is the ReaxFF potential file. Unlike for the *reax* pair style, any filename can be used.

In the ReaxFF potential file, near the top, after the general parameters, is the atomic parameters section that contains element names, each with a couple dozen numeric parameters. If there are M elements specified in the *ffield* file, think of these as numbered 1 to M. Each of the N indices you specify for the N atom types of LAMMPS atoms must be an integer from 1 to M. Atoms with LAMMPS type 1 will be mapped to whatever element you specify as the first index value, etc. If a mapping value is specified as NULL, the mapping is not performed. This can be used when the *reax/c* style is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

As an example, say your LAMMPS simulation has 4 atom types and the elements are ordered as C, H, O, N in the *ffield* file. If you want the LAMMPS atom type 1 and 2 to be C, type 3 to be N, and type 4 to be H, you would use the following pair_coeff command:

```
pair_coeff * * ffield.reax C C N H
```

The format of a line in the control file is as follows:

```
variable_name value
```

and it may be followed by an "!" character and a trailing comment.

If the value of a control variable is not specified, then default values are used. What follows is the list of variables along with a brief description of their use and default values.

simulation_name: Output files produced by *pair_style reax/c* carry this name + extensions specific to their contents. Partial energies are reported with a ".pot" extension, while the trajectory file has ".trj" extension.

tabulate_long_range: To improve performance, long range interactions can optionally be tabulated (0 means no tabulation). Value of this variable denotes the size of the long range interaction table. The range from 0 to long range cutoff (defined in the *ffield* file) is divided into *tabulate_long_range* points. Then at the start of simulation, we fill in the entries of the long range interaction table by computing the energies and forces resulting from van der Waals and Coulomb interactions between every possible atom type pairs present in the input system. During the simulation we consult to the long range interaction table to estimate the energy and forces between a pair of

atoms. Linear interpolation is used for estimation. (default value = 0)

energy_update_freq: Denotes the frequency (in number of steps) of writes into the partial energies file. (default value = 0)

nbrhood_cutoff: Denotes the near neighbors cutoff (in Angstroms) regarding the bonded interactions. (default value = 5.0)

hbond_cutoff: Denotes the cutoff distance (in Angstroms) for hydrogen bond interactions.(default value = 7.5. Value of 0.0 turns off hydrogen bonds)

bond_graph_cutoff: is the threshold used in determining what is a physical bond, what is not. Bonds and angles reported in the trajectory file rely on this cutoff. (default value = 0.3)

thb_cutoff: cutoff value for the strength of bonds to be considered in three body interactions. (default value = 0.001)

thb_cutoff_sq: cutoff value for the strength of bond order products to be considered in three body interactions. (default value = 0.00001)

write_freq: Frequency of writes into the trajectory file. (default value = 0)

traj_title: Title of the trajectory - not the name of the trajectory file.

atom_info: 1 means print only atomic positions + charge (default = 0)

atom_forces: 1 adds net forces to atom lines in the trajectory file (default = 0)

atom_velocities: 1 adds atomic velocities to atoms line (default = 0)

bond_info: 1 prints bonds in the trajectory file (default = 0)

angle_info: 1 prints angles in the trajectory file (default = 0)

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the pair_modify mix, shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the USER-REAXC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

The ReaxFF potential files provided with LAMMPS in the potentials directory are parameterized for real units. You can use the ReaxFF potential with any LAMMPS units, but you would need to create your own potential file with coefficients listed in the appropriate units if your simulation doesn't use "real" units.

Related commands:

pair_coeff, fix qeq/reax, fix reax/c/bonds, fix reax/c/species, pair_style reax

Default:

The keyword defaults are checkqeq = yes, lgvdw = no, safezone = 1.2, mincap = 50.

(Chenoweth_2008) Chenoweth, van Duin and Goddard, Journal of Physical Chemistry A, 112, 1040-1053 (2008).

(Aktulga) Aktulga, Fogarty, Pandit, Grama, Parallel Computing, 38, 245-259 (2012).

(Liu) L. Liu, Y. Liu, S. V. Zybin, H. Sun and W. A. Goddard, Journal of Physical Chemistry A, 115, 11016-11022 (2011).

pair_style resquared command

pair_style resquared/gpu command

pair_style resquared/omp command

Syntax:

```
pair_style resquared cutoff
```

- cutoff = global cutoff for interactions (distance units)

Examples:

```
pair_style resquared 10.0
pair_coeff * * 1.0 1.0 1.7 3.4 3.4 1.0 1.0 1.0
```

Description:

Style *resquared* computes the RE-squared anisotropic interaction (Everaers), (Babadi) between pairs of ellipsoidal and/or spherical Lennard-Jones particles. For ellipsoidal interactions, the potential considers the ellipsoid as being comprised of small spheres of size sigma. LJ particles are a single sphere of size sigma. The distinction is made to allow the pair style to make efficient calculations of ellipsoid/solvent interactions.

Details for the equations used are given in the references below and in this supplementary document.

Use of this pair style requires the NVE, NVT, or NPT fixes with the *asphere* extension (e.g. fix nve/asphere) in order to integrate particle rotation. Additionally, atom_style ellipsoid should be used since it defines the rotational state and the size and shape of each ellipsoidal particle.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- A12 = Energy Prefactor/Hamaker constant (energy units)
- sigma = atomic interaction diameter (distance units)
- epsilon_i_a = relative well depth of type I for side-to-side interactions
- epsilon_i_b = relative well depth of type I for face-to-face interactions
- epsilon_i_c = relative well depth of type I for end-to-end interactions
- epsilon_j_a = relative well depth of type J for side-to-side interactions
- epsilon_j_b = relative well depth of type J for face-to-face interactions
- epsilon_j_c = relative well depth of type J for end-to-end interactions
- cutoff (distance units)

The parameters used depend on the type of the interacting particles, i.e. ellipsoids or LJ spheres. The type of a particle is determined by the diameters specified for its 3 shape paramters. If all 3 shape parameters = 0.0, then the particle is treated as an LJ sphere. The epsilon_i_* or epsilon_j_* parameters are ignored for LJ spheres. If the 3 shape paraemters are > 0.0, then the particle is treated as an ellipsoid (even if the 3 parameters are equal to each other).

A12 specifies the energy prefactor which depends on the types of the two interacting particles.

For ellipsoid/ellipsoid interactions, the interaction is computed by the formulas in the supplementary docuement referenced above. A12 is the Hamaker constant as described in (Everaers). In LJ units:

$$A_{12} = 4\pi^2 \epsilon_{\mathrm{LJ}} (\rho\sigma^3)^2$$

where rho gives the number density of the spherical particles composing the ellipsoids and epsilon_LJ determines the interaction strength of the spherical particles.

For ellipsoid/LJ sphere interactions, the interaction is also computed by the formulas in the supplementary docuement referenced above. A12 has a modifed form (see here for details):

$$A_{12} = 4\pi^2 \epsilon_{\mathrm{LJ}} (\rho\sigma^3)$$

For ellipsoid/LJ sphere interactions, a correction to the distance- of-closest approach equation has been implemented to reduce the error from two particles of disparate sizes; see this supplementary document.

For LJ sphere/LJ sphere interactions, the interaction is computed using the standard Lennard-Jones formula, which is much cheaper to compute than the ellipsoidal formulas. A12 is used as epsilon in the standard LJ formula:

$$A_{12} = \epsilon_{\mathrm{LJ}}$$

and the specified *sigma* is used as the sigma in the standard LJ formula.

When one of both of the interacting particles are ellipsoids, then *sigma* specifies the diameter of the continuous distribution of constituent particles within each ellipsoid used to model the RE-squared potential. Note that this is a different meaning for *sigma* than the pair_style gayberne potential uses.

The epsilon_i and epsilon_j coefficients are defined for atom types, not for pairs of atom types. Thus, in a series of pair_coeff commands, they only need to be specified once for each atom type.

Specifically, if any of epsilon_i_a, epsilon_i_b, epsilon_i_c are non-zero, the three values are assigned to atom type I. If all the epsilon_i values are zero, they are ignored. If any of epsilon_j_a, epsilon_j_b, epsilon_j_c are non-zero, the three values are assigned to atom type J. If all three epsilon_i values are zero, they are ignored. Thus the typical way to define the epsilon_i and epsilon_j coefficients is to list their values in "pair_coeff I J" commands when I = J, but set them to 0.0 when I != J. If you do list them when I != J, you should insure they are consistent with their values in other pair_coeff commands.

Note that if this potential is being used as a sub-style of pair_style hybrid, and there is no "pair_coeff I I" setting made for RE-squared for a particular type I (because I-I interactions are computed by another hybrid pair potential), then you still need to insure the epsilon a,b,c coefficients are assigned to that type in a "pair_coeff I J" command.

For large uniform molecules it has been shown that the epsilon_*_* energy parameters are approximately representable in terms of local contact curvatures (Everaers):

$$\epsilon_a = \sigma \cdot \frac{a}{b \cdot c}; \epsilon_b = \sigma \cdot \frac{b}{a \cdot c}; \epsilon_c = \sigma \cdot \frac{c}{a \cdot b}$$

where a, b, and c give the particle diameters.

The last coefficient is optional. If not specified, the global cutoff specified in the pair_style command is used.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance can be mixed, but only for sphere pairs. The default mix value is *geometric*. See the "pair_modify" command for details. Other type pairs cannot be mixed, due to the different meanings of the energy prefactors used to calculate the interactions and the implicit dependence of the ellipsoid-sphere interaction on the equation for the Hamaker constant presented here. Mixing of sigma and epsilon followed by calculation of the energy prefactors using the equations above is recommended.

This pair styles supports the pair_modify shift option for the energy of the Lennard-Jones portion of the pair interaction, but only for sphere-sphere interactions. There is no shifting performed for ellipsoidal interactions due to the anisotropic dependence of the interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords of the run_style command.

Restrictions:

This style is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This pair style requires that atoms be ellipsoids as defined by the atom_style ellipsoid command.

Particles acted on by the potential can be finite-size aspherical or spherical particles, or point particles. Spherical particles have all 3 of their shape parameters equal to each other. Point particles have all 3 of their shape parameters equal to 0.0.

The distance-of-closest-approach approximation used by LAMMPS becomes less accurate when high-aspect ratio ellipsoids are used.

Related commands:

pair_coeff, fix nve/asphere, compute temp/asphere, pair_style gayberne

Default: none

(Everaers) Everaers and Ejtehadi, Phys Rev E, 67, 041710 (2003).

(Berardi) Babadi, Ejtehadi, Everaers, J Comp Phys, 219, 770-779 (2006).

pair_style lj/sdk command

pair_style lj/sdk/gpu command

pair_style lj/sdk/kk command

pair_style lj/sdk/omp command

pair_style lj/sdk/coul/long command

pair_style lj/sdk/coul/long/gpu command

pair_style lj/sdk/coul/long/omp command

Syntax:

```
pair_style style args
```

- style = *lj/sdk* or *lj/sdk/coul/long*
- args = list of arguments for a particular style

```
lj/sdk args = cutoff
    cutoff = global cutoff for Lennard Jones interactions (distance units)
  lj/sdk/coul/long args = cutoff (cutoff2)
    cutoff = global cutoff for LJ (and Coulombic if only 1 arg) (distance units)
    cutoff2 = global cutoff for Coulombic (optional) (distance units)
```

Examples:

```
pair_style lj/sdk 2.5
pair_coeff 1 1 lj12_6 1 1.1 2.8

pair_style lj/sdk/coul/long 10.0
pair_style lj/sdk/coul/long 10.0 12.0
pair_coeff 1 1 lj9_6 100.0 3.5 12.0
```

Description:

The *lj/sdk* styles compute a 9/6, 12/4, or 12/6 Lennard-Jones potential, given by

$$E = \frac{27}{4}\epsilon\left[\left(\frac{\sigma}{r}\right)^9 - \left(\frac{\sigma}{r}\right)^6\right] \qquad r < r_c$$

$$E = \frac{3\sqrt{3}}{2}\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^4\right] \qquad r < r_c$$

$$E = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right] \qquad r < r_c$$

as required for the SDK Coarse-grained MD parametrization discussed in (Shinoda) and (DeVane). Rc is the cutoff.

Style *lj/sdk/coul/long* computes the adds Coulombic interactions with an additional damping factor applied so it can be used in conjunction with the kspace_style command and its *ewald* or *pppm* or *pppm/cg* option. The Coulombic cutoff specified for this style means that pairwise interactions within this distance are computed directly; interactions outside that distance are computed in reciprocal space.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- cg_type (lj9_6, lj12_4, or lj12_6)
- epsilon (energy units)
- sigma (distance units)
- cutoff1 (distance units)

Note that sigma is defined in the LJ formula as the zero-crossing distance for the potential, not as the energy minimum. The prefactors are chosen so that the potential minimum is at -epsilon.

The latter 2 coefficients are optional. If not specified, the global LJ and Coulombic cutoffs specified in the pair_style command are used. If only one cutoff is specified, it is used as the cutoff for both LJ and Coulombic interactions for this type pair. If both coefficients are specified, they are used as the LJ and Coulombic cutoffs for this type pair.

For *lj/sdk/coul/long* only the LJ cutoff can be specified since a Coulombic cutoff cannot be specified for an individual I,J type pair. All type pairs use the same global Coulombic cutoff specified in the pair_style command.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp* or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP, and OPT packages respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, and rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of the lj/sdk pair styles *cannot* be mixed, since different pairs may have different exponents. So all parameters for all pairs have to be specified explicitly through the "pair_coeff" command. Defining then in a data file is also not supported, due to limitations of that file format.

All of the lj/sdk pair styles support the pair_modify shift option for the energy of the Lennard-Jones portion of the pair interaction.

The *lj/sdk/coul/long* pair styles support the pair_modify table option since they can tabulate the short-range portion of the long-range Coulombic interaction.

All of the lj/sdk pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

The lj/sdk and lj/cut/coul/long pair styles do not support the use of the *inner*, *middle*, and *outer* keywords of the run_style respa command.

Restrictions:

All of the lj/sdk pair styles are part of the USER-CG-CMM package. The *lj/sdk/coul/long* style also requires the KSPACE package to be built (which is enabled by default). They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, angle_style sdk

Default: none

(Shinoda) Shinoda, DeVane, Klein, Mol Sim, 33, 27 (2007).

(DeVane) Shinoda, DeVane, Klein, Soft Matter, 4, 2453-2462 (2008).

pair_style smd/hertz command

Syntax:

```
pair_style smd/hertz scale_factor
```

Examples:

pair_style smd/hertz 1.0 pair_coeff 1 1

Description:

The *smd/hertz* style calculates contact forces between SPH particles belonging to different physical bodies.

The contact forces are calculated using a Hertz potential, which evaluates the overlap between two particles (whose spatial extents are defined via its contact radius). The effect is that a particles cannot penetrate into each other. The parameter has units of pressure and should equal roughly one half of the Young's modulus (or bulk modulus in the case of fluids) of the material model associated with the SPH particles.

The parameter *scale_factor* can be used to scale the particles' contact radii. This can be useful to control how close particles can approach each other. Usually, *scale_factor*=1.0.

Mixing, shift, table, tail correction, restart, rRESPA info:

No mixing is performed automatically. Currently, no part of USER-SMD supports restarting nor minimization. rRESPA does not apply to this pair style.

Restrictions:

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff

Default: none

---

pair_style smd/tlsph command

Syntax:

```
pair_style smd/tlsph args
```

Examples:

pair_style smd/tlsph

Description:

The *smd/tlsph* style computes particle interactions according to continuum mechanics constitutive laws and a Total-Lagrangian Smooth-Particle Hydrodynamics algorithm.

This pair style is invoked with the following command:

```
pair_style smd/tlsph
pair_coeff i j *COMMON rho0 E nu Q1 Q2 hg Cp &
               *END
```

Here, *i* and *j* denote the *LAMMPS* particle types for which this pair style is defined. Note that *i* and *j* must be equal, i.e., no *tlsph* cross interactions between different particle types are allowed. In contrast to the usual *LAMMPS pair coeff* definitions, which are given solely a number of floats and integers, the *tlsph pair coeff* definition is organised using keywords. These keywords mark the beginning of different sets of parameters for particle properties, material constitutive models, and damage models. The *pair coeff* line must be terminated with the **END* keyword. The use the line continuation operator *&* is recommended. A typical invocation of the *tlsph* for a solid body would consist of an equation of state for computing the pressure (the diagonal components of the stress tensor), and a material model to compute shear stresses (the off-diagonal components of the stress tensor). Damage and failure models can also be added.

Please see the SMD user guide for a complete listing of the possible keywords and material models.

Mixing, shift, table, tail correction, restart, rRESPA info:

No mixing is performed automatically. Currently, no part of USER-SMD supports restarting nor minimization. rRESPA does not apply to this pair style.

Restrictions:

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff

Default: none

---

pair_style smd/tri_surface command

Syntax:

```
pair_style smd/tri_surface scale_factor
```

Examples:

pair_style smd/tri_surface 1.0 pair_coeff 1 1

Description:

The *smd/tri_surface* style calculates contact forces between SPH particles and a rigid wall boundary defined via the smd/wall_surface fix.

The contact forces are calculated using a Hertz potential, which evaluates the overlap between a particle (whose spatial extents are defined via its contact radius) and the triangle. The effect is that a particle cannot penetrate into the triangular surface. The parameter has units of pressure and should equal roughly one half of the Young's modulus (or bulk modulus in the case of fluids) of the material model associated with the SPH particle

The parameter *scale_factor* can be used to scale the particles' contact radii. This can be useful to control how close particles can approach the triangulated surface. Usually, *scale_factor*=1.0.

Mixing, shift, table, tail correction, restart, rRESPA info:

No mixing is performed automatically. Currently, no part of USER-SMD supports restarting nor minimization. rRESPA does not apply to this pair style.

Restrictions:

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff

Default: none

---

pair_style smd/ulsph command

Syntax:

```
pair_style smd/ulsph args
```

- these keywords must be given

  keyword = **DENSITY_SUMMATION* or **DENSITY_CONTINUITY* and **VELOCITY_GRADIENT* or **NO_VELOCITY_GRADIENT* and **GRADIENT_CORRECTION* or **NO_GRADIENT_CORRECTION*

Examples:

pair_style smd/ulsph *DENSITY_CONTINUITY *VELOCITY_GRADIENT *NO_GRADIENT_CORRECTION

Description:

The *smd/ulsph* style computes particle interactions according to continuum mechanics constitutive laws and an updated Lagrangian Smooth-Particle Hydrodynamics algorithm.

This pair style is invoked similar to the following command:

```
pair_style smd/ulsph *DENSITY_CONTINUITY *VELOCITY_GRADIENT *NO_GRADIENT_CORRECTION
pair_coeff i j *COMMON rho0 c0 Q1 Cp hg &
               *END
```

Here, *i* and *j* denote the *LAMMPS* particle types for which this pair style is defined. Note that *i* and *j* can be different, i.e., *ulsph* cross interactions between different particle types are allowed. However, *i--i* respectively *j--j* pair_coeff lines have to preceed a cross interaction. In contrast to the usual *LAMMPS pair coeff* definitions, which are given solely a number of floats and integers, the *ulsph pair coeff* definition is organised using keywords. These keywords mark the beginning of different sets of parameters for particle properties, material constitutive models, and damage models. The *pair coeff* line must be terminated with the **END* keyword. The use the line continuation operator *&* is recommended. A typical invocation of the *ulsph* for a solid body would consist of an equation of state for computing the pressure (the diagonal components of the stress tensor), and a material model to compute shear stresses (the off-diagonal components of the stress tensor).

Note that the use of *GRADIENT_CORRECTION can lead to severe numerical instabilities. For a general fluid simulation, *NO_GRADIENT_CORRECTION is recommended.

Please see the SMD user guide for a complete listing of the possible keywords and material models.

Mixing, shift, table, tail correction, restart, rRESPA info:

No mixing is performed automatically. Currently, no part of USER-SMD supports restarting nor minimization. rRESPA does not apply to this pair style.

Restrictions:

This fix is part of the USER-SMD package. It is only enabled if LAMMPS was built with that package. See the

Making LAMMPS section for more info.

Related commands:

pair_coeff

Default: none

---

pair_style smtbq command

Syntax:

```
pair_style smtbq
```

Examples:

```
pair_style smtbq
pair_coeff * * ffield.smtbq.Al2O3 O Al
```

Description:

This pair stylecomputes a variable charge SMTB-Q (Second-Moment tight-Binding QEq) potential as described in SMTB-Q_1 and SMTB-Q_2. Briefly, the energy of metallic-oxygen systems is given by three contributions:

$$
\begin{aligned}
E_{tot} &= E_{ES} + E_{OO} + E_{MO} \\
E_{ES} &= \sum_i \left[\chi_i^0 Q_i + \frac{1}{2} J_i^0 Q_i^2 + \frac{1}{2} \sum_{j \neq i} J_{ij}(r_{ij}) f_{cut}^{R_{coul}}(r_{ij}) Q_i Q_j \right] \\
E_{OO} &= \sum_{i,j}^{i,j=O} \left[C exp(-\frac{r_{ij}}{\rho}) - D f_{cut}^{r_1^{OO} r_2^{OO}}(r_{ij}) exp(B r_{ij}) \right] \\
E_{MO} &= \sum_i E_{cov}^i + \sum_{j \neq i} A f_{cut}^{r_{c1} r_{c2}}(r_{ij}) exp\left[-p(\frac{r_{ij}}{r_0} - 1) \right]
\end{aligned}
$$

where E_{tot} is the total potential energy of the system, E_{ES} is the electrostatic part of the total energy, E_{OO} is the interaction between oxygens and E_{MO} is a short-range interaction between metal and oxygen atoms. This interactions depend on interatomic distance r_{ij} and/or the charge Q_i of atoms i. Cut-off function enables smooth convergence to zero interaction.

The parameters appearing in the upper expressions are set in the ffield.SMTBQ.Syst file where Syst corresponds to the selected system (e.g. field.SMTBQ.Al2O3). Exemples for TiO_2, Al_2O_3 are provided. A single pair_coeff command is used with the SMTBQ styles which provides the path to the potential file with parameters for needed elements. These are mapped to LAMMPS atom types by specifying additional arguments after the potential filename in the pair_coeff command. Note that atom type 1 must always correspond to oxygen atoms. As an example, to simulate a TiO2 system, atom type 1 has to be oxygen and atom type 2 Ti. The following pair_coeff command should then be used:

```
pair_coeff * * PathToLammps/potentials/ffield.smtbq.TiO2 O Ti
```

The electrostatic part of the energy consists of two components

self-energy of atom i in the form of a second order charge dependent polynomial and a long-range Coulombic electrostatic interaction. The latter uses the wolf summation method described in Wolf, spherically truncated at a

longer cutoff, R_{coul}. The charge of each ion is modeled by an orbital Slater which depends on the principal quantum number (n) of the outer orbital shared by the ion.

Interaction between oxygen, E_{OO}, consists of two parts, an attractive and a repulsive part. The attractive part is effective only at short range (< r_2^{OO}). The attractive contribution was optimized to study surfaces reconstruction (e.g. SMTB-Q_2 in TiO_2) and is not necessary for oxide bulk modeling. The repulsive part is the Pauli interaction between the electron clouds of oxygen. The Pauli repulsion and the coulombic electrostatic interaction have same cut off value. In the ffield.SMTBQ.Syst, the keyword *'buck'* allows to consider only the repulsive O-O interactions. The keyword *'buckPlusAttr'* allows to consider the repulsive and the attractive O-O interactions.

The short-range interaction between metal-oxygen, E_{MO} is based on the second moment approximation of the density of states with a N-body potential for the band energy term, E^i_{cov}, and a Born-Mayer type repulsive terms as indicated by the keyword *'second_moment'* in the ffield.SMTBQ.Syst. The energy band term is given by:

$$E^{(i=M,O)}_{cov} = -\left\{\eta_i(\mu\xi^0)^2 f_{cut}^{r_{c1}r_{c2}}(r_{ij})\left(\sum_{j(j=O,M)} exp[-2q(\frac{r_{ij}}{r_0}-1)]\right)\delta Q_i\left(2\frac{n_0}{\eta_i}-\delta Q\right.\right.$$

$$\delta Q_i = |Q_i^F| - |Q_i|$$

where &#951$_i$ is the stoichiometry of atom i, &#948Q_i is the charge delocalization of atom i, compared to its formal charge Q^F_i. n_0, the number of hybridized orbitals, is calculated with to the atomic orbitals shared d_i and the stoichiometry &#951$_i$. r_{c1} and r_{c2} are the two cutoff radius around the fourth neighbors in the cutoff function.

In the formalism used here, &#958^0 is the energy parameter. &#958^0 is in tight-binding approximation the hopping integral between the hybridized orbitals of the cation and the anion. In the literature we find many ways to write the hopping integral depending on whether one takes the point of view of the anion or cation. These are equivalent vision. The correspondence between the two visions is explained in appendix A of the article in the $SrTiO_3$ SMTB-Q_3 (parameter &#946 shown in this article is in fact the &#946$_O$). To summarize the relationship between the hopping integral &#958^0 and the others, we have in an oxide C_nO_m the following relationship:

$$\xi^0 = \frac{\xi_O}{m} = \frac{\xi_C}{n}$$

$$\frac{\beta_O}{\sqrt{m}} = \frac{\beta_C}{\sqrt{n}} = \xi^0\frac{\sqrt{m}+\sqrt{n}}{2}$$

Thus parameter &#956, indicated above, is given by : &#956 = (&#8730n + &#8730m) &#8260 2

The potential offers the possibility to consider the polarizability of the electron clouds of oxygen by changing the slater radius of the charge density around the oxygens through the parameters *rBB, rB and rS* in the ffield.SMTBQ.Syst. This change in radius is performed according to the method developed by E. Maras SMTB-Q_2. This method needs to determine the number of nearest neighbors around the oxygen. This calculation is based on first (r_{1n}) and second (r_{2n}) distances neighbors.

The SMTB-Q potential is a variable charge potential. The equilibrium charge on each atom is calculated by the electronegativity equalization (QEq) method. See Rick for further detail. One can adjust the frequency, the

maximum number of iterative loop and the convergence of the equilibrium charge calculation. To obtain the energy conservation in NVE thermodynamic ensemble, we recommend to use a convergence parameter in the interval 10^{-5} - 10^{-6} eV.

The ffield.SMTBQ.Syst files are provided for few systems. They consist of nine parts and the lines beginning with '#' are comments (note that the number of comment lines matter). The first sections are on the potential parameters and others are on the simulation options and might be modified. Keywords are character type and must be enclosed in quotation marks (").

1) Number of different element in the oxide:

- N_{elem}= 2 or 3
- Divided line

2) Atomic parameters

For the anion (oxygen)

- Name of element (char) and stoichiometry in oxide
- Formal charge and mass of element
- Principal quantic number of outer orbital (*n*), electronegativity (*&#967⁰ᵢ*) and hardness (J^0_i)
- Ionic radius parameters : max coordination number (*coordBB* = 6 by default), bulk coordination number *(coordB)*, surface coordination number *(coordS)* and *rBB, rB and rS* the slater radius for each coordination number. (**note : If you don't want to change the slater radius, use three identical radius values**)
- Number of orbital shared by the element in the oxide (d_i)
- Divided line

For each cations (metal):

- Name of element (char) and stoichiometry in oxide
- Formal charge and mass of element
- Number of electron in outer orbital *(ne)*, electronegativity (*&#967⁰ᵢ*), hardness (J^0_i) and r_{Salter} the slater radius for the cation.
- Number of orbitals shared by the elements in the oxide (d_i)
- Divided line

3) Potential parameters:

- Keyword for element1, element2 and interaction potential ('second_moment' or 'buck' or 'buckPlusAttr') between element 1 and 2. If the potential is 'second_moment', specify 'oxide' or 'metal' for metal-oxygen or metal-metal interactions respectively.
- Potential parameter:

```
       If type of potential is 'second_moment': A (eV), p, &#9580 (eV) and q
  rc1 (&#197), rc2 (&#197) and r0 (&#197)
       If type of potential is 'buck': A (eV) and &#961 (&#197)
       If type of potential is 'buckPlusAttr': A (eV) and &#961 (&#197)
  D (eV), B (&#197-1), r100 (&#197) and r200 (&#197)
```

- Divided line

4) Tables parameters:

- Cutoff radius for the Coulomb interaction (R_{coul})
- Starting radius (r_{min} = 1,18845 &#197) and increments (dr = 0,001 &#197) for creating the potential table.
- Divided line

5) Rick model parameter:

- *Nevery* : parameter to set the frequency (*1/Nevery*) of the charge resolution. The charges are evaluated each *Nevery* time steps.
- Max number of iterative loop (*loopmax*) and precision criterion (*prec*) in eV of the charge resolution
- Divided line

6) Coordination parameter:

- First (r_{1n}) and second (r_{2n}) neighbor distances in &#197
- Divided line

7) Charge initialization mode:

- Keyword (*QInitMode*) and initial oxygen charge (Q_{init}). If keyword = 'true', all oxygen charges are initially set equal to Q_{init}. The charges on the cations are initially set in order to respect the neutrality of the box. If keyword = 'false', all atom charges are initially set equal to 0 if you use "create_atom"#create_atom command or the charge specified in the file structure using read_data command.
- Divided line

8) Mode for the electronegativity equalization (Qeq)

- Keyword mode:

```
QEqAll  (one QEq group)                 |   no parameters
QEqAllParallel (several QEq groups)     |   no parameters
Surface                 |   zlim   (QEq only for z>zlim)
```

- Parameter if necessary
- Divided line

9) Verbose

- If you want the code to work in verbose mode or not : 'true' or 'false'
- If you want to print or not in file 'Energy_component.txt' the three main contributions to the energy of the system according to the description presented above : 'true' or 'false' and N_{Energy}. This option writes in file every N_{Energy} time step. If the value is 'false' then N_{Energy} = 0. The file take into account the possibility to have several QEq group g then it writes: time step, number of atoms in group g, electrostatic part of energy, E_{ES}, the interaction between oxygen, E_{OO}, and short range metal-oxygen interaction, E_{MO}.
- If you want to print in file 'Electroneg_component.txt' the electronegativity component (&#8706E_{tot} &#8260&#8706Q_i) or not: 'true' or 'false' and $N_{Electroneg}$.This option writes in file every $N_{Electroneg}$ time step. If the value is 'false' then $N_{Electroneg}$ = 0. The file consist in atom number i, atom type (1 for oxygen and # higher than 1 for metal), atom position: x, y and z, atomic charge of atom i, electrostatic part of atom i electronegativity, covalent part of atom i electronegativity, the hopping integral of atom i $(Z\&\#946^2)_i$ and box electronegativity.

NOTE: This last option slows down the calculation dramatically. Use only with a single processor simulation.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the pair_modify mix, shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you needs to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restriction:

This pair style is part of the USER-SMTBQ package and is only enabled if LAMMPS is built with that package. See the Making LAMMPS section for more info.

This potential requires using atom type 1 for oxygen and atom type higher than 1 for metal atoms.

This pair style requires the newton setting to be "on" for pair interactions.

The SMTB-Q potential files provided with LAMMPS (see the potentials directory) are parameterized for metal units.

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(SMTB-Q_1) N. Salles, O. Politano, E. Amzallag, R. Tetot, Comput. Mater. Sci. 111 (2016) 181-189

(SMTB-Q_2) E. Maras, N. Salles, R. Tetot, T. Ala-Nissila, H. Jonsson, J. Phys. Chem. C 2015, 119, 10391-10399

(SMTB-Q_3) R. Tetot, N. Salles, S. Landron, E. Amzallag, Surface Science 616, 19-8722 28 (2013)

(Wolf) D. Wolf, P. Keblinski, S. R. Phillpot, J. Eggebrecht, J Chem Phys, 110, 8254 (1999).

(Rick) S. W. Rick, S. J. Stuart, B. J. Berne, J Chem Phys 101, 6141 (1994).

pair_style snap command

Syntax:

```
pair_style snap
```

Examples:

```
pair_style snap
pair_coeff * * snap InP.snapcoeff In P InP.snapparam In In P P
```

Description:

Style *snap* computes interactions using the spectral neighbor analysis potential (SNAP) (Thompson). Like the GAP framework of Bartok et al. (Bartok2010), (Bartok2013) it uses bispectrum components to characterize the local neighborhood of each atom in a very general way. The mathematical definition of the bispectrum calculation used by SNAP is identical to that used of compute sna/atom. In SNAP, the total energy is decomposed into a sum over atom energies. The energy of atom *i* is expressed as a weighted sum over bispectrum components.

$$E^i_{SNAP}(B^i_1, ...B^i_K) = \beta^{\alpha_i}_0 + \sum_{k=1}^{K} \beta^{\alpha_i}_k B^i_k$$

where *B_k^i* is the *k*-th bispectrum component of atom *i*, and *beta_k^alpha_i* is the corresponding linear coefficient that depends on *alpha_i*, the SNAP element of atom *i*. The number of bispectrum components used and their definitions depend on the values of *twojmax* and *diagonalstyle* defined in the SNAP parameter file described below. The bispectrum calculation is described in more detail in compute sna/atom.

Note that unlike for other potentials, cutoffs for SNAP potentials are not set in the pair_style or pair_coeff command; they are specified in the SNAP potential files themselves.

Only a single pair_coeff command is used with the *snap* style which specifies two SNAP files and the list SNAP element(s) to be extracted. The SNAP elements are mapped to LAMMPS atom types by specifying N additional arguments after the 2nd filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- SNAP element file
- Elem1, Elem2, ...
- SNAP parameter file
- N element names = mapping of SNAP elements to atom types

As an example, if a LAMMPS indium phosphide simulation has 4 atoms types, with the first two being indium and the 3rd and 4th being phophorous, the pair_coeff command would look like this:

```
pair_coeff * * snap InP.snapcoeff In P InP.snapparam In In P P
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The two filenames are for the element and parameter files, respectively. The 'In' and 'P' arguments (between the file names) are the two elements which will be extracted from the element file. The two trailing 'In' arguments map LAMMPS atom types 1 and 2 to the

SNAP 'In' element. The two trailing 'P' arguments map LAMMPS atom types 3 and 4 to the SNAP 'P' element.

If a SNAP mapping value is specified as NULL, the mapping is not performed. This can be used when a *snap* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

The name of the SNAP element file usually ends in the ".snapcoeff" extension. It may contain coefficients for many SNAP elements. Only those elements listed in the pair_coeff command are extracted. The name of the SNAP parameter file usually ends in the ".snapparam" extension. It contains a small number of parameters that define the overall form of the SNAP potential. See the pair_coeff doc page for alternate ways to specify the path for these files.

Quite commonly, SNAP potentials are combined with one or more other LAMMPS pair styles using the *hybrid/overlay* pair style. As an example, the SNAP tantalum potential provided in the LAMMPS potentials directory combines the *snap* and *zbl* pair styles. It is invoked by the following commands:

```
variable zblcutinner equal 4
variable zblcutouter equal 4.8
variable zblz equal 73
pair_style hybrid/overlay &
zbl ${zblcutinner} ${zblcutouter} snap
pair_coeff * * zbl 0.0
pair_coeff 1 1 zbl ${zblz}
pair_coeff * * snap ../potentials/Ta06A.snapcoeff Ta &
../potentials/Ta06A.snapparam Ta
```

It is convenient to keep these commands in a separate file that can be inserted in any LAMMPS input script using the include command.

The top of the SNAP element file can contain any number of blank and comment lines (start with #), but follows a strict format after that. The first non-blank non-comment line must contain two integers:

- nelem = Number of elements
- ncoeff = Number of coefficients

This is followed by one block for each of the *nelem* elements. The first line of each block contains three entries:

- Element symbol (text string)
- R = Element radius (distance units)
- w = Element weight (dimensionless)

This line is followed by *ncoeff* coefficients, one per line.

The SNAP parameter file can contain blank and comment lines (start with #) anywhere. Each non-blank non-comment line must contain one keyword/value pair. The required keywords are *rcutfac* and *twojmax*. Optional keywords are *rfac0*, *rmin0*, *diagonalstyle*, and *switchflag*.

The default values for these keywords are

- *rfac0* = 0.99363
- *rmin0* = 0.0
- *diagonalstyle* = 3
- *switchflag* = 0

Detailed definitions of these keywords are given on the compute sna/atom doc page.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS with user-specifiable parameters as described above. You never need to specify a pair_coeff command with I != J arguments for this style.

This pair style does not support the pair_modify shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This style is part of the SNAP package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

compute sna/atom, compute snad/atom, compute snav/atom

Default: none

(Thompson) Thompson, Swiler, Trott, Foiles, Tucker, under review, preprint available at arXiv:1409.3880

(Bartok2010) Bartok, Payne, Risi, Csanyi, Phys Rev Lett, 104, 136403 (2010).

(Bartok2013) Bartok, Gillan, Manby, Csanyi, Phys Rev B 87, 184115 (2013).

pair_style soft command

pair_style soft/gpu command

pair_style soft/omp command

Syntax:

```
pair_style soft cutoff
```

- cutoff = global cutoff for soft interactions (distance units)

Examples:

```
pair_style soft 2.5
pair_coeff * * 10.0
pair_coeff 1 1 10.0 3.0

pair_style soft 2.5
pair_coeff * * 0.0
variable prefactor equal ramp(0,30)
fix 1 all adapt 1 pair soft a * * v_prefactor
```

Description:

Style *soft* computes pairwise interactions with the formula

$$E = A \left[1 + \cos\left(\frac{\pi r}{r_c}\right)\right] \qquad r < r_c$$

It is useful for pushing apart overlapping atoms, since it does not blow up as r goes to 0. A is a pre-factor that can be made to vary in time from the start to the end of the run (see discussion below), e.g. to start with a very soft potential and slowly harden the interactions over time. Rc is the cutoff. See the fix nve/limit command for another way to push apart overlapping atoms.

The following coefficients must be defined for each pair of atom types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- A (energy units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global soft cutoff is used.

NOTE: The syntax for pair_coeff with a single A coeff is different in the current version of LAMMPS than in older versions which took two values, Astart and Astop, to ramp between them. This functionality is now available in a more general form through the fix adapt command, as explained below. Note that if you use an old input script and specify Astart and Astop without a cutoff, then LAMMPS will interpret that as A and a cutoff,

which is probabably not what you want.

The fix adapt command can be used to vary A for one or more pair types over the course of a simulation, in which case pair_coeff settings for A must still be specified, but will be overridden. For example these commands will vary the prefactor A for all pairwise interactions from 0.0 at the beginning to 30.0 at the end of a run:

```
variable prefactor equal ramp(0,30)
fix 1 all adapt 1 pair soft a * * v_prefactor
```

Note that a formula defined by an equal-style variable can use the current timestep, elapsed time in the current run, elapsed time since the beginning of a series of runs, as well as access other variables.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the A coefficient and cutoff distance for this pair style can be mixed. A is always mixed via a *geometric* rule. The cutoff is mixed according to the pair_modify mix value. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style does not support the pair_modify shift option, since the pair interaction goes to 0.0 at the cutoff.

The pair_modify table and tail options are not relevant for this pair style.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions: none

Related commands:

pair_coeff, fix nve/limit, fix adapt

Default: none

pair_style sph/heatconduction command

Syntax:

```
pair_style sph/heatconduction
```

Examples:

```
pair_style sph/heatconduction
pair_coeff * * 1.0 2.4
```

Description:

The sph/heatconduction style computes heat transport between SPH particles. The transport model is the diffusion euqation for the internal energy.

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above.

- D diffusion coefficient (length^2/time units)
- h kernel function cutoff (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the pair_modify shift, table, and tail options.

This style does not write information to binary restart files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_sph/rhosum

Default: none

pair_style sph/idealgas command

Syntax:

```
pair_style sph/idealgas
```

Examples:

```
pair_style sph/idealgas
pair_coeff * * 1.0 2.4
```

Description:

The sph/idealgas style computes pressure forces between particles according to the ideal gas equation of state:

$$p = (\gamma - 1)\rho e$$

where gamma = 1.4 is the heat capacity ratio, rho is the local density, and e is the internal energy per unit mass. This pair style also computes Monaghan's artificial viscosity to prevent particles from interpentrating (Monaghan).

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above.

- nu artificial viscosity (no units)
- h kernel function cutoff (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the pair_modify shift, table, and tail options.

This style does not write information to binary restart files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_sph/rhosum

Default: none

(Monaghan) Monaghan and Gingold, Journal of Computational Physics, 52, 374-389 (1983).

pair_style sph/lj command

Syntax:

```
pair_style sph/lj
```

Examples:

```
pair_style sph/lj
pair_coeff * * 1.0 2.4
```

Description:

The sph/lj style computes pressure forces between particles according to the Lennard-Jones equation of state, which is computed according to Ree's 1980 polynomial fit (Ree). The Lennard-Jones parameters epsilon and sigma are set to unity. This pair style also computes Monaghan's artificial viscosity to prevent particles from interpentrating (Monaghan).

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above.

- nu artificial viscosity (no units)
- h kernel function cutoff (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the pair_modify shift, table, and tail options.

This style does not write information to binary restart files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

As noted above, the Lennard-Jones parameters epsilon and sigma are set to unity.

This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_sph/rhosum

Default: none

(Ree) Ree, Journal of Chemical Physics, 73, 5401 (1980).

(Monaghan) Monaghan and Gingold, Journal of Computational Physics, 52, 374-389 (1983).

pair_style sph/rhosum command

Syntax:

```
pair_style sph/rhosum Nstep
```

- Nstep = timestep interval

Examples:

```
pair_style sph/rhosum 10
pair_coeff * * 2.4
```

Description:

The sph/rhosum style computes the local particle mass density rho for SPH particles by kernel function interpolation, every Nstep timesteps.

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above.

- h (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the pair_modify shift, table, and tail options.

This style does not write information to binary restart files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_sph/taitwater

Default: none

pair_style sph/taitwater command

Syntax:

```
pair_style sph/taitwater
```

Examples:

```
pair_style sph/taitwater
pair_coeff * * 1000.0 1430.0 1.0 2.4
```

Description:

The sph/taitwater style computes pressure forces between SPH particles according to Tait's equation of state:

$$p = B[(\frac{\rho}{\rho_0})^\gamma - 1]$$

where gamma = 7 and B = c_0^2 rho_0 / gamma, with rho_0 being the reference density and c_0 the reference speed of sound.

This pair style also computes Monaghan's artificial viscosity to prevent particles from interpentrating (Monaghan).

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above.

- rho0 reference density (mass/volume units)
- c0 reference soundspeed (distance/time units)
- nu artificial viscosity (no units)
- h kernel function cutoff (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the pair_modify shift, table, and tail options.

This style does not write information to binary restart files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_sph/rhosum

Default: none

(Monaghan) Monaghan and Gingold, Journal of Computational Physics, 52, 374-389 (1983).

pair_style sph/taitwater/morris command

Syntax:

```
pair_style sph/taitwater/morris
```

Examples:

```
pair_style sph/taitwater/morris
pair_coeff * * 1000.0 1430.0 1.0 2.4
```

Description:

The sph/taitwater/morris style computes pressure forces between SPH particles according to Tait's equation of state:

$$p = B[(\frac{\rho}{\rho_0})^\gamma - 1]$$

where gamma = 7 and B = c_0^2 rho_0 / gamma, with rho_0 being the reference density and c_0 the reference speed of sound.

This pair style also computes laminar viscosity (Morris).

See this PDF guide to using SPH in LAMMPS.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above.

- rho0 reference density (mass/volume units)
- c0 reference soundspeed (distance/time units)
- nu dynamic viscosity (mass*distance/time units)
- h kernel function cutoff (distance units)

Mixing, shift, table, tail correction, restart, rRESPA info:

This style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

This style does not support the pair_modify shift, table, and tail options.

This style does not write information to binary restart files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the USER-SPH package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Related commands:

pair_coeff, pair_sph/rhosum

Default: none

(Morris) Morris, Fox, Zhu, J Comp Physics, 136, 214-226 (1997).

pair_style srp command

Syntax:

pair_style srp cutoff btype dist keyword value ...

- cutoff = global cutoff for SRP interactions (distance units)
- btype = bond type to apply SRP interactions to (can be wildcard, see below)
- distance = *min* or *mid*
- zero or more keyword/value pairs may be appended
- keyword = *exclude*

```
bptype value = atom type for bond particles
  exclude value = yes or no
```

Examples:

```
pair_style hybrid dpd 1.0 1.0 12345 srp 0.8 1 mid exclude yes
pair_coeff 1 1 dpd 60.0 4.5 1.0
pair_coeff 1 2 none
pair_coeff 2 2 srp 100.0 0.8

pair_style hybrid dpd 1.0 1.0 12345 srp 0.8 * min exclude yes
pair_coeff 1 1 dpd 60.0 50 1.0
pair_coeff 1 2 none
pair_coeff 2 2 srp 40.0

pair_style hybrid srp 0.8 2 mid
pair_coeff 1 1 none
pair_coeff 1 2 none
pair_coeff 2 2 srp 100.0 0.8
```

Description:

Style *srp* computes a soft segmental repulsive potential (SRP) that acts between pairs of bonds. This potential is useful for preventing bonds from passing through one another when a soft non-bonded potential acts between beads in, for example, DPD polymer chains. An example input script that uses this command is provided in examples/USER/srp.

Bonds of specified type *btype* interact with one another through a bond-pairwise potential, such that the force on bond *i* due to bond *j* is as follows

$$F_{ij}^{SRP} = C(1 - r/r_c)\hat{r}_{ij} \qquad r < r_c$$

where *r* and *rij* are the distance and unit vector between the two bonds. Note that *btype* can be specified as an asterisk "*", which case the interaction is applied to all bond types. The *mid* option computes *r* and *rij* from the midpoint distance between bonds. The *min* option computes *r* and *rij* from the minimum distance between bonds. The force acting on a bond is mapped onto the two bond atoms according to the lever rule,

$$
\begin{aligned}
F_{i1}^{SRP} &= F_{ij}^{SRP}(L) \\
F_{i2}^{SRP} &= F_{ij}^{SRP}(1-L)
\end{aligned}
$$

where L is the normalized distance from the atom to the point of closest approach of bond i and j. The *mid* option takes L as 0.5 for each interaction as described in (Sirk).

The following coefficients must be defined via the pair_coeff command as in the examples above, or in the data file or restart file read by the read_data or read_restart commands:

- C (force units)
- rc (distance units)

The last coefficient is optional. If not specified, the global cutoff is used.

NOTE: Pair style srp considers each bond of type *btype* to be a fictitious "particle" of type *bptype*, where *bptype* is either the largest atom type in the system, or the type set by the *bptype* flag. Any actual existing particles with this atom type will be deleted at the beginning of a run. This means you must specify the number of types in your system accordingly; usually to be one larger than what would normally be the case, e.g. via the create_box or by changing the header in your data file. The ficitious "bond particles" are inserted at the beginning of the run, and serve as placeholders that define the position of the bonds. This allows neighbor lists to be constructed and pairwise interactions to be computed in almost the same way as is done for actual particles. Because bonds interact only with other bonds, pair_style hybrid should be used to turn off interactions between atom type *bptype* and all other types of atoms. An error will be flagged if pair_style hybrid is not used.

The optional *exclude* keyword determines if forces are computed between first neighbor (directly connected) bonds. For a setting of *no*, first neighbor forces are computed; for *yes* they are not computed. A setting of *no* cannot be used with the *min* option for distance calculation because the the minimum distance between directly connected bonds is zero.

Pair style *srp* turns off normalization of thermodynamic properties by particle number, as if the command thermo_modify norm no had been issued.

The pairwise energy associated with style *srp* is shifted to be zero at the cutoff distance *rc*.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair styles does not support mixing.

This pair style does not support the pair_modify shift option for the energy of the pair interaction. Note that as discussed above, the energy term is already shifted to be 0.0 at the cutoff distance *rc*.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style writes global and per-atom information to binary restart files. Pair srp should be used with pair_style hybrid, thus the pair_coeff commands need to be specified in the input script when reading a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the USER-MISC package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This pair style must be used with pair_style hybrid.

This pair style requires the newton command to be *on* for non-bonded interactions.

Related commands:

pair_style hybrid, pair_coeff, pair dpd

Default:

The default keyword value is exclude = yes.

(Sirk) Sirk TW, Sliozberg YR, Brennan JK, Lisal M, Andzelm JW, J Chem Phys, 136 (13) 134903, 2012.

pair_style command

Syntax:

```
pair_style style args
```

- style = one of the styles from the list below
- args = arguments used by a particular style

Examples:

```
pair_style lj/cut 2.5
pair_style eam/alloy
pair_style hybrid lj/charmm/coul/long 10.0 eam
pair_style table linear 1000
pair_style none
```

Description:

Set the formula(s) LAMMPS uses to compute pairwise interactions. In LAMMPS, pair potentials are defined between pairs of atoms that are within a cutoff distance and the set of active interactions typically changes over time. See the bond_style command to define potentials between pairs of bonded atoms, which typically remain in place for the duration of a simulation.

In LAMMPS, pairwise force fields encompass a variety of interactions, some of which include many-body effects, e.g. EAM, Stillinger-Weber, Tersoff, REBO potentials. They are still classified as "pairwise" potentials because the set of interacting atoms changes with time (unlike molecular bonds) and thus a neighbor list is used to find nearby interacting atoms.

Hybrid models where specified pairs of atom types interact via different pair potentials can be setup using the *hybrid* pair style.

The coefficients associated with a pair style are typically set for each pair of atom types, and are specified by the pair_coeff command or read from a file by the read_data or read_restart commands.

The pair_modify command sets options for mixing of type I-J interaction coefficients and adding energy offsets or tail corrections to Lennard-Jones potentials. Details on these options as they pertain to individual potentials are described on the doc page for the potential. Likewise, info on whether the potential information is stored in a restart file is listed on the potential doc page.

In the formulas listed for each pair style, E is the energy of a pairwise interaction between two atoms separated by a distance r. The force between the atoms is the negative derivative of this expression.

If the pair_style command has a cutoff argument, it sets global cutoffs for all pairs of atom types. The distance(s) can be smaller or larger than the dimensions of the simulation box.

Typically, the global cutoff value can be overridden for a specific pair of atom types by the pair_coeff command. The pair style settings (including global cutoffs) can be changed by a subsequent pair_style command using the same style. This will reset the cutoffs for all atom type pairs, including those previously set explicitly by a pair_coeff command. The exceptions to this are that pair_style *table* and *hybrid* settings cannot be reset. A new pair_style command for these styles will wipe out all previously specified pair_coeff values.

Here is an alphabetic list of pair styles defined in LAMMPS. They are also given in more compact form in the pair section of this page.

Click on the style to display the formula it computes, arguments specified in the pair_style command, and coefficients specified by the associated pair_coeff command.

There are also additional pair styles (not listed here) submitted by users which are included in the LAMMPS distribution. The list of these with links to the individual styles are given in the pair section of this page.

There are also additional accelerated pair styles (not listed here) included in the LAMMPS distribution for faster performance on CPUs and GPUs. The list of these with links to the individual styles are given in the pair section of this page.

- pair_style none - turn off pairwise interactions
- pair_style hybrid - multiple styles of pairwise interactions
- pair_style hybrid/overlay - multiple styles of superposed pairwise interactions

- pair_style adp - angular dependent potential (ADP) of Mishin
- pair_style airebo - AIREBO potential of Stuart
- pair_style beck - Beck potential
- pair_style body - interactions between body particles
- pair_style bop - BOP potential of Pettifor
- pair_style born - Born-Mayer-Huggins potential
- pair_style born/coul/long - Born-Mayer-Huggins with long-range Coulombics
- pair_style born/coul/long/cs - Born-Mayer-Huggins with long-range Coulombics and core/shell
- pair_style born/coul/msm - Born-Mayer-Huggins with long-range MSM Coulombics
- pair_style born/coul/wolf - Born-Mayer-Huggins with Coulombics via Wolf potential
- pair_style brownian - Brownian potential for Fast Lubrication Dynamics
- pair_style brownian/poly - Brownian potential for Fast Lubrication Dynamics with polydispersity
- pair_style buck - Buckingham potential
- pair_style buck/coul/cut - Buckingham with cutoff Coulomb
- pair_style buck/coul/long - Buckingham with long-range Coulombics
- pair_style buck/coul/long/cs - Buckingham with long-range Coulombics and core/shell
- pair_style buck/coul/msm - Buckingham long-range MSM Coulombics
- pair_style buck/long/coul/long - long-range Buckingham with long-range Coulombics
- pair_style colloid - integrated colloidal potential
- pair_style comb - charge-optimized many-body (COMB) potential
- pair_style comb3 - charge-optimized many-body (COMB3) potential
- pair_style coul/cut - cutoff Coulombic potential
- pair_style coul/debye - cutoff Coulombic potential with Debye screening
- pair_style coul/dsf - Coulombics via damped shifted forces
- pair_style coul/long - long-range Coulombic potential
- pair_style coul/long/cs - long-range Coulombic potential and core/shell
- pair_style coul/msm - long-range MSM Coulombics
- pair_style coul/msm - Coulombics via Streitz/Mintmire Slater orbitals
- pair_style coul/wolf - Coulombics via Wolf potential
- pair_style dpd - dissipative particle dynamics (DPD)
- pair_style dpd/tstat - DPD thermostatting
- pair_style dsmc - Direct Simulation Monte Carlo (DSMC)
- pair_style eam - embedded atom method (EAM)
- pair_style eam/alloy - alloy EAM

- pair_style eam/fs - Finnis-Sinclair EAM
- pair_style eim - embedded ion method (EIM)
- pair_style gauss - Gaussian potential
- pair_style gayberne - Gay-Berne ellipsoidal potential
- pair_style gran/hertz/history - granular potential with Hertzian interactions
- pair_style gran/hooke - granular potential with history effects
- pair_style gran/hooke/history - granular potential without history effects
- pair_style hbond/dreiding/lj - DREIDING hydrogen bonding LJ potential
- pair_style hbond/dreiding/morse - DREIDING hydrogen bonding Morse potential
- pair_style kim - interface to potentials provided by KIM project
- pair_style lcbop - long-range bond-order potential (LCBOP)
- pair_style line/lj - LJ potential between line segments
- pair_style lj/charmm/coul/charmm - CHARMM potential with cutoff Coulomb
- pair_style lj/charmm/coul/charmm/implicit - CHARMM for implicit solvent
- pair_style lj/charmm/coul/long - CHARMM with long-range Coulomb
- pair_style lj/charmm/coul/msm - CHARMM with long-range MSM Coulombics
- pair_style lj/class2 - COMPASS (class 2) force field with no Coulomb
- pair_style lj/class2/coul/cut - COMPASS with cutoff Coulomb
- pair_style lj/class2/coul/long - COMPASS with long-range Coulomb
- pair_style lj/cubic - LJ with cubic after inflection point
- pair_style lj/cut - cutoff Lennard-Jones potential with no Coulomb
- pair_style lj/cut/coul/cut - LJ with cutoff Coulomb
- pair_style lj/cut/coul/debye - LJ with Debye screening added to Coulomb
- pair_style lj/cut/coul/dsf - LJ with Coulombics via damped shifted forces
- pair_style lj/cut/coul/long - LJ with long-range Coulombics
- pair_style lj/cut/coul/long/cs - LJ with long-range Coulombics and core/shell
- pair_style lj/cut/coul/msm - LJ with long-range MSM Coulombics
- pair_style lj/cut/dipole/cut - point dipoles with cutoff
- pair_style lj/cut/dipole/long - point dipoles with long-range Ewald
- pair_style lj/cut/tip4p/cut - LJ with cutoff Coulomb for TIP4P water
- pair_style lj/cut/tip4p/long - LJ with long-range Coulomb for TIP4P water
- pair_style lj/expand - Lennard-Jones for variable size particles
- pair_style lj/gromacs - GROMACS-style Lennard-Jones potential
- pair_style lj/gromacs/coul/gromacs - GROMACS-style LJ and Coulombic potential
- pair_style lj/long/coul/long - long-range LJ and long-range Coulombics
- pair_style lj/long/dipole/long - long-range LJ and long-range point dipoles
- pair_style lj/long/tip4p/long - long-range LJ and long-range Coulomb for TIP4P water
- pair_style lj/smooth - smoothed Lennard-Jones potential
- pair_style lj/smooth/linear - linear smoothed Lennard-Jones potential
- pair_style lj96/cut - Lennard-Jones 9/6 potential
- pair_style lubricate - hydrodynamic lubrication forces
- pair_style lubricate/poly - hydrodynamic lubrication forces with polydispersity
- pair_style lubricateU - hydrodynamic lubrication forces for Fast Lubrication Dynamics
- pair_style lubricateU/poly - hydrodynamic lubrication forces for Fast Lubrication with polydispersity
- pair_style meam - modified embedded atom method (MEAM)
- pair_style mie/cut - Mie potential
- pair_style morse - Morse potential
- pair_style nb3b/harmonic - nonbonded 3-body harmonic potential
- pair_style nm/cut - N-M potential
- pair_style nm/cut/coul/cut - N-M potential with cutoff Coulomb
- pair_style nm/cut/coul/long - N-M potential with long-range Coulombics
- pair_style peri/eps - peridynamic EPS potential

- pair_style peri/lps - peridynamic LPS potential
- pair_style peri/pmb - peridynamic PMB potential
- pair_style peri/ves - peridynamic VES potential
- pair_style polymorphic - polymorphic 3-body potential
- pair_style reax - ReaxFF potential
- pair_style rebo - 2nd generation REBO potential of Brenner
- pair_style resquared - Everaers RE-Squared ellipsoidal potential
- pair_style snap - SNAP quantum-accurate potential
- pair_style soft - Soft (cosine) potential
- pair_style sw - Stillinger-Weber 3-body potential
- pair_style table - tabulated pair potential
- pair_style tersoff - Tersoff 3-body potential
- pair_style tersoff/mod - modified Tersoff 3-body potential
- pair_style tersoff/zbl - Tersoff/ZBL 3-body potential
- pair_style tip4p/cut - Coulomb for TIP4P water w/out LJ
- pair_style tip4p/long - long-range Coulombics for TIP4P water w/out LJ
- pair_style tri/lj - LJ potential between triangles
- pair_style vashishta - Vashishta 2-body and 3-body potential
- pair_style yukawa - Yukawa potential
- pair_style yukawa/colloid - screened Yukawa potential for finite-size particles
- pair_style zbl - Ziegler-Biersack-Littmark potential

Restrictions:

This command must be used before any coefficients are set by the pair_coeff, read_data, or read_restart commands.

Some pair styles are part of specific packages. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info on packages. The doc pages for individual pair potentials tell if it is part of a package.

Related commands:

pair_coeff, read_data, pair_modify, kspace_style, dielectric, pair_write

Default:

```
pair_style none
```

pair_style sw command

pair_style sw/cuda command

pair_style sw/gpu command

pair_style sw/intel command

pair_style sw/kk command

pair_style sw/omp command

Syntax:

```
pair_style sw
```

Examples:

```
pair_style sw
pair_coeff * * si.sw Si
pair_coeff * * GaN.sw Ga N Ga
```

Description:

The *sw* style computes a 3-body Stillinger-Weber potential for the energy E of a system of atoms as

$$E = \sum_i \sum_{j>i} \phi_2(r_{ij}) + \sum_i \sum_{j \neq i} \sum_{k>j} \phi_3(r_{ij}, r_{ik}, \theta_{ijk})$$

$$\phi_2(r_{ij}) = A_{ij}\epsilon_{ij} \left[B_{ij}(\frac{\sigma_{ij}}{r_{ij}})^{p_{ij}} - (\frac{\sigma_{ij}}{r_{ij}})^{q_{ij}} \right] \exp\left(\frac{\sigma_{ij}}{r_{ij} - a_{ij}\sigma_{ij}}\right)$$

$$\phi_3(r_{ij}, r_{ik}, \theta_{ijk}) = \lambda_{ijk}\epsilon_{ijk} \left[\cos\theta_{ijk} - \cos\theta_{0ijk}\right]^2 \exp\left(\frac{\gamma_{ij}\sigma_{ij}}{r_{ij} - a_{ij}\sigma_{ij}}\right) \exp\left(\frac{\gamma_{ik}\sigma}{r_{ik} - a}\right.$$

where phi2 is a two-body term and phi3 is a three-body term. The summations in the formula are over all neighbors J and K of atom I within a cutoff distance = a*sigma.

Only a single pair_coeff command is used with the *sw* style which specifies a Stillinger-Weber potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of SW elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file.

As an example, imagine a file SiC.sw has Stillinger-Weber values for Si and C. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * SiC.sw Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the SW file. The final C argument maps LAMMPS atom type 4 to the C element in the SW file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *sw* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Stillinger-Weber files in the *potentials* directory of the LAMMPS distribution have a ".sw" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to the two-body and three-body coefficients in the formula above:

- element 1 (the center atom in a 3-body interaction)
- element 2
- element 3
- epsilon (energy units)
- sigma (distance units)
- a
- lambda
- gamma
- costheta0
- A
- B
- p
- q
- tol

The A, B, p, and q parameters are used only for two-body interactions. The lambda and costheta0 parameters are used only for three-body interactions. The epsilon, sigma and a parameters are used for both two-body and three-body interactions. gamma is used only in the three-body interactions, but is defined for pairs of atoms. The non-annotated parameters are unitless.

LAMMPS introduces an additional performance-optimization parameter tol that is used for both two-body and three-body interactions. In the Stillinger-Weber potential, the interaction energies become negligibly small at atomic separations substantially less than the theoretical cutoff distances. LAMMPS therefore defines a virtual cutoff distance based on a user defined tolerance tol. The use of the virtual cutoff distance in constructing atom neighbor lists can significantly reduce the neighbor list sizes and therefore the computational cost. LAMMPS provides a *tol* value for each of the three-body entries so that they can be separately controlled. If tol = 0.0, then the standard Stillinger-Weber cutoff is used.

The Stillinger-Weber potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries.

For a single-element simulation, only a single entry is required (e.g. SiSiSi). For a two-element simulation, the file must contain 8 entries (for SiSiSi, SiSiC, SiCSi, SiCC, CSiSi, CSiC, CCSi, CCC), that specify SW parameters for all permutations of the two elements interacting in three-body configurations. Thus for 3 elements, 27 entries

would be required, etc.

As annotated above, the first element in the entry is the center atom in a three-body interaction. Thus an entry for SiCC means a Si atom with 2 C atoms as neighbors. The parameter values used for the two-body interaction come from the entry where the 2nd and 3rd elements are the same. Thus the two-body parameters for Si interacting with C, comes from the SiCC entry. The three-body parameters can in principle be specific to the three elements of the configuration. In the literature, however, the three-body parameters are usually defined by simple formulas involving two sets of pair-wise parameters, corresponding to the ij and ik pairs, where i is the center atom. The user must ensure that the correct combining rule is used to calculate the values of the threebody parameters for alloys. Note also that the function phi3 contains two exponential screening factors with parameter values from the ij pair and ik pairs. So phi3 for a C atom bonded to a Si atom and a second C atom will depend on the three-body parameters for the CSiC entry, and also on the two-body parameters for the CCC and CSiSi entries. Since the order of the two neighbors is arbitrary, the threebody parameters for entries CSiC and CCSi should be the same. Similarly, the two-body parameters for entries SiCC and CSiSi should also be the same. The parameters used only for two-body interactions (A, B, p, and q) in entries whose 2nd and 3rd element are different (e.g. SiCSi) are not used for anything and can be set to 0.0 if desired. This is also true for the parameters in phi3 that are taken from the ij and ik pairs (sigma, a, gamma)

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

When using the USER-INTEL package with this style, there is an additional 5 to 10 percent performance improvement when the Stillinger-Weber parameters p and q are set to 4 and 0 respectively. These parameters are common for modeling silicon and water.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above from values in the potential file.

This pair style does not support the pair_modify shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

This pair style requires the newton setting to be "on" for pair interactions.

The Stillinger-Weber potential files provided with LAMMPS (see the potentials directory) are parameterized for metal units. You can use the SW potential with any LAMMPS units, but you would need to create your own SW potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

Related commands:

pair_coeff

Default: none

(Stillinger) Stillinger and Weber, Phys Rev B, 31, 5262 (1985).

pair_style table command

pair_style table/gpu command

pair_style table/kk command

pair_style table/omp command

Syntax:

```
pair_style table style N keyword ...
```

- style = *lookup* or *linear* or *spline* or *bitmap* = method of interpolation
- N = use N values in *lookup*, *linear*, *spline* tables
- N = use 2^N values in *bitmap* tables
- zero or more keywords may be appended
- keyword = *ewald* or *pppm* or *msm* or *dispersion* or *tip4p*

Examples:

```
pair_style table linear 1000
pair_style table linear 1000 pppm
pair_style table bitmap 12
pair_coeff * 3 morse.table ENTRY1
pair_coeff * 3 morse.table ENTRY1 7.0
```

Description:

Style *table* creates interpolation tables of length *N* from pair potential and force values listed in a file(s) as a function of distance. The files are read by the pair_coeff command.

The interpolation tables are created by fitting cubic splines to the file values and interpolating energy and force values at each of *N* distances. During a simulation, these tables are used to interpolate energy and force values as needed. The interpolation is done in one of 4 styles: *lookup*, *linear*, *spline*, or *bitmap*.

For the *lookup* style, the distance between 2 atoms is used to find the nearest table entry, which is the energy or force.

For the *linear* style, the pair distance is used to find 2 surrounding table values from which an energy or force is computed by linear interpolation.

For the *spline* style, a cubic spline coefficients are computed and stored at each of the *N* values in the table. The pair distance is used to find the appropriate set of coefficients which are used to evaluate a cubic polynomial which computes the energy or force.

For the *bitmap* style, the N means to create interpolation tables that are 2^N in length. The pair distance is used to index into the table via a fast bit-mapping technique due to (Wolff), and a linear interpolation is performed between adjacent table values.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above.

- filename
- keyword
- cutoff (distance units)

The filename specifies a file containing tabulated energy and force values. The keyword specifies a section of the file. The cutoff is an optional coefficient. If not specified, the outer cutoff in the table itself (see below) will be used to build an interpolation table that extend to the largest tabulated distance. If specified, only file values up to the cutoff are used to create the interpolation table. The format of this file is described below.

If your tabulated potential(s) are designed to be used as the short-range part of one of the long-range solvers specified by the kspace_style command, then you must use one or more of the optional keywords listed above for the pair_style command. These are *ewald* or *pppm* or *msm* or *dispersion* or *tip4p*. This is so LAMMPS can insure the short-range potential and long-range solver are compatible with each other, as it does for other short-range pair styles, such as pair_style lj/cut/coul/long. Note that it is up to you to insure the tabulated values for each pair of atom types has the correct functional form to be compatible with the matching long-range solver.

Here are some guidelines for using the pair_style table command to best effect:

- Vary the number of table points; you may need to use more than you think to get good resolution.
- Always use the pair_write command to produce a plot of what the final interpolated potential looks like. This can show up interpolation "features" you may not like.
- Start with the linear style; it's the style least likely to have problems.
- Use *N* in the pair_style command equal to the "N" in the tabulation file, and use the "RSQ" or "BITMAP" parameter, so additional interpolation is not needed. See discussion below.
- Make sure that your tabulated forces and tabulated energies are consistent (dE/dr = -F) along the entire range of r values.
- Use as large an inner cutoff as possible. This avoids fitting splines to very steep parts of the potential.

The format of a tabulated file is a series of one or more sections, defined as follows (without the parenthesized comments):

```
# Morse potential for Fe    (one or more comment or blank lines)

MORSE_FE                    (keyword is first text on line)
N 500 R 1.0 10.0            (N, R, RSQ, BITMAP, FPRIME parameters)
                            (blank)
1 1.0 25.5 102.34           (index, r, energy, force)
2 1.02 23.4 98.5
...
500 10.0 0.001 0.003
```

A section begins with a non-blank line whose 1st character is not a "#"; blank lines or lines starting with "#" can be used as comments between sections. The first line begins with a keyword which identifies the section. The line can contain additional text, but the initial text must match the argument specified in the pair_coeff command. The next line lists (in any order) one or more parameters for the table. Each parameter is a keyword followed by one or more numeric values.

The parameter "N" is required and its value is the number of table entries that follow. Note that this may be different than the *N* specified in the pair_style table command. Let Ntable = *N* in the pair_style command, and Nfile = "N" in the tabulated file. What LAMMPS does is a preliminary interpolation by creating splines using the Nfile tabulated values as nodal points. It uses these to interpolate as needed to generate energy and force values at

Ntable different points. The resulting tables of length Ntable are then used as described above, when computing energy and force for individual pair distances. This means that if you want the interpolation tables of length Ntable to match exactly what is in the tabulated file (with effectively no preliminary interpolation), you should set Ntable = Nfile, and use the "RSQ" or "BITMAP" parameter. The internal table abscissa is RSQ (separation distance squared).

All other parameters are optional. If "R" or "RSQ" or "BITMAP" does not appear, then the distances in each line of the table are used as-is to perform spline interpolation. In this case, the table values can be spaced in *r* uniformly or however you wish to position table values in regions of large gradients.

If used, the parameters "R" or "RSQ" are followed by 2 values *rlo* and *rhi*. If specified, the distance associated with each energy and force value is computed from these 2 values (at high accuracy), rather than using the (low-accuracy) value listed in each line of the table. The distance values in the table file are ignored in this case. For "R", distances uniformly spaced between *rlo* and *rhi* are computed; for "RSQ", squared distances uniformly spaced between *rlo***rlo* and *rhi***rhi* are computed.

If used, the parameter "BITMAP" is also followed by 2 values *rlo* and *rhi*. These values, along with the "N" value determine the ordering of the N lines that follow and what distance is associated with each. This ordering is complex, so it is not documented here, since this file is typically produced by the pair_write command with its *bitmap* option. When the table is in BITMAP format, the "N" parameter in the file must be equal to 2^M where M is the value specified in the pair_style command. Also, a cutoff parameter cannot be used as an optional 3rd argument in the pair_coeff command; the entire table extent as specified in the file must be used.

If used, the parameter "FPRIME" is followed by 2 values *fplo* and *fphi* which are the derivative of the force at the innermost and outermost distances listed in the table. These values are needed by the spline construction routines. If not specified by the "FPRIME" parameter, they are estimated (less accurately) by the first 2 and last 2 force values in the table. This parameter is not used by BITMAP tables.

Following a blank line, the next N lines list the tabulated values. On each line, the 1st value is the index from 1 to N, the 2nd value is r (in distance units), the 3rd value is the energy (in energy units), and the 4th is the force (in force units). The r values must increase from one line to the next (unless the BITMAP parameter is specified).

Note that one file can contain many sections, each with a tabulated potential. LAMMPS reads the file section by section until it finds one that matches the specified keyword.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

The pair_modify shift, table, and tail options are not relevant for this pair style.

This pair style writes the settings for the "pair_style table" command to binary restart files, so a pair_style command does not need to specified in an input script that reads a restart file. However, the coefficient information is not stored in the restart file, since it is tabulated in the potential files. Thus, pair_coeff commands do need to be specified in the restart input script.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions: none

Related commands:

pair_coeff

Default: none

(Wolff) Wolff and Rudd, Comp Phys Comm, 120, 200-32 (1999).

pair_style tersoff command

pair_style tersoff/table command

pair_style tersoff/cuda

pair_style tersoff/gpu

pair_style tersoff/intel

pair_style tersoff/kk

pair_style tersoff/omp

pair_style tersoff/table/omp command

Syntax:

```
pair_style style
```

style = *tersoff* or *tersoff/table* or *tersoff/cuda* or *tersoff/gpu* or *tersoff/omp* or *tersoff/table/omp*

Examples:

```
pair_style tersoff
pair_coeff * * Si.tersoff Si
pair_coeff * * SiC.tersoff Si C Si

pair_style tersoff/table
pair_coeff * * SiCGe.tersoff Si(D)
```

Description:

The *tersoff* style computes a 3-body Tersoff potential (Tersoff_1) for the energy E of a system of atoms as

$$
\begin{aligned}
E &= \frac{1}{2}\sum_i \sum_{j \neq i} V_{ij} \\
V_{ij} &= f_C(r_{ij}) \left[f_R(r_{ij}) + b_{ij} f_A(r_{ij}) \right] \\
f_C(r) &= \begin{cases} 1 & : \quad r < R - D \\ \frac{1}{2} - \frac{1}{2} \sin\left(\frac{\pi}{2} \frac{r-R}{D} \right) & : \quad R - D < r < R + D \\ 0 & : \quad r > R + D \end{cases} \\
f_R(r) &= A \exp(-\lambda_1 r) \\
f_A(r) &= -B \exp(-\lambda_2 r) \\
b_{ij} &= (1 + \beta^n {\zeta_{ij}}^n)^{-\frac{1}{2n}} \\
\zeta_{ij} &= \sum_{k \neq i,j} f_C(r_{ik}) g(\theta_{ijk}) \exp\left[{\lambda_3}^m (r_{ij} - r_{ik})^m \right] \\
g(\theta) &= \gamma_{ijk} \left(1 + \frac{c^2}{d^2} - \frac{c^2}{[d^2 + (\cos\theta - \cos\theta_0)^2]} \right)
\end{aligned}
$$

where f_R is a two-body term and f_A includes three-body interactions. The summations in the formula are over all neighbors J and K of atom I within a cutoff distance = R + D.

The *tersoff/table* style uses tabulated forms for the two-body, environment and angular functions. Linear interpolation is performed between adjacent table entries. The table length is chosen to be accurate within 10^-6 with respect to the *tersoff* style energy. The *tersoff/table* should give better performance in terms of speed.

Only a single pair_coeff command is used with the *tersoff* style which specifies a Tersoff potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of Tersoff elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file.

As an example, imagine the SiC.tersoff file has Tersoff values for Si and C. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * SiC.tersoff Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the Tersoff file. The final C argument maps LAMMPS atom type

4 to the C element in the Tersoff file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *tersoff* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Tersoff files in the *potentials* directory of the LAMMPS distribution have a ".tersoff" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to coefficients in the formula above:

- element 1 (the center atom in a 3-body interaction)
- element 2 (the atom bonded to the center atom)
- element 3 (the atom influencing the 1-2 bond in a bond-order sense)
- m
- gamma
- lambda3 (1/distance units)
- c
- d
- costheta0 (can be a value < -1 or > 1)
- n
- beta
- lambda2 (1/distance units)
- B (energy units)
- R (distance units)
- D (distance units)
- lambda1 (1/distance units)
- A (energy units)

The n, beta, lambda2, B, lambda1, and A parameters are only used for two-body interactions. The m, gamma, lambda3, c, d, and costheta0 parameters are only used for three-body interactions. The R and D parameters are used for both two-body and three-body interactions. The non-annotated parameters are unitless. The value of m must be 3 or 1.

The Tersoff potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries.

For a single-element simulation, only a single entry is required (e.g. SiSiSi). For a two-element simulation, the file must contain 8 entries (for SiSiSi, SiSiC, SiCSi, SiCC, CSiSi, CSiC, CCSi, CCC), that specify Tersoff parameters for all permutations of the two elements interacting in three-body configurations. Thus for 3 elements, 27 entries would be required, etc.

As annotated above, the first element in the entry is the center atom in a three-body interaction and it is bonded to the 2nd atom and the bond is influenced by the 3rd atom. Thus an entry for SiCC means Si bonded to a C with another C atom influencing the bond. Thus three-body parameters for SiCSi and SiSiC entries will not, in general, be the same. The parameters used for the two-body interaction come from the entry where the 2nd element is repeated. Thus the two-body parameters for Si interacting with C, comes from the SiCC entry.

The parameters used for a particular three-body interaction come from the entry with the corresponding three elements. The parameters used only for two-body interactions (n, beta, lambda2, B, lambda1, and A) in entries whose 2nd and 3rd element are different (e.g. SiCSi) are not used for anything and can be set to 0.0 if desired.

Note that the twobody parameters in entries such as SiCC and CSiSi are often the same, due to the common use of symmetric mixing rules, but this is not always the case. For example, the beta and n parameters in Tersoff_2 (Tersoff_2) are not symmetric.

We chose the above form so as to enable users to define all commonly used variants of the Tersoff potential. In particular, our form reduces to the original Tersoff form when m = 3 and gamma = 1, while it reduces to the form of Albe et al. when beta = 1 and m = 1. Note that in the current Tersoff implementation in LAMMPS, m must be specified as either 3 or 1. Tersoff used a slightly different but equivalent form for alloys, which we will refer to as Tersoff_2 potential (Tersoff_2). The *tersoff/table* style implements Tersoff_2 parameterization only.

LAMMPS parameter values for Tersoff_2 can be obtained as follows: gamma_ijk = omega_ik, lambda3 = 0 and the value of m has no effect. The parameters for species i and j can be calculated using the Tersoff_2 mixing rules:

$$
\begin{aligned}
\lambda_1^{i,j} &= \frac{1}{2}(\lambda_1^i + \lambda_1^j) \\
\lambda_2^{i,j} &= \frac{1}{2}(\lambda_2^i + \lambda_2^j) \\
A_{i,j} &= (A_i A_j)^{1/2} \\
B_{i,j} &= \chi_{ij}(B_i B_j)^{1/2} \\
R_{i,j} &= (R_i R_j)^{1/2} \\
S_{i,j} &= (S_i S_j)^{1/2}
\end{aligned}
$$

Tersoff_2 parameters R and S must be converted to the LAMMPS parameters R and D (R is different in both forms), using the following relations: R=(R'+S')/2 and D=(S'-R')/2, where the primes indicate the Tersoff_2 parameters.

In the potentials directory, the file SiCGe.tersoff provides the LAMMPS parameters for Tersoff's various versions of Si, as well as his alloy parameters for Si, C, and Ge. This file can be used for pure Si, (three different versions), pure C, pure Ge, binary SiC, and binary SiGe. LAMMPS will generate an error if this file is used with any combination involving C and Ge, since there are no entries for the GeC interactions (Tersoff did not publish parameters for this cross-interaction.) Tersoff files are also provided for the SiC alloy (SiC.tersoff) and the GaN (GaN.tersoff) alloys.

Many thanks to Rutuparna Narulkar, David Farrell, and Xiaowang Zhou for helping clarify how Tersoff parameters for alloys have been defined in various papers.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above from values in the potential file.

This pair style does not support the pair_modify shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

This pair style requires the newton setting to be "on" for pair interactions.

The Tersoff potential files provided with LAMMPS (see the potentials directory) are parameterized for metal units. You can use the Tersoff potential with any LAMMPS units, but you would need to create your own Tersoff potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

Related commands:

pair_coeff

Default: none

(Tersoff_1) J. Tersoff, Phys Rev B, 37, 6991 (1988).

(Albe) J. Nord, K. Albe, P. Erhart, and K. Nordlund, J. Phys.: Condens. Matter, 15, 5649(2003).

(Tersoff_2) J. Tersoff, Phys Rev B, 39, 5566 (1989); errata (PRB 41, 3248)

pair_style tersoff/mod command

pair_style tersoff/mod/kk command

pair_style tersoff/mod/omp command

Syntax:

```
pair_style tersoff/mod
```

Examples:

```
pair_style tersoff/mod
pair_coeff * * Si.tersoff.mod Si Si
```

Description:

The *tersoff/mod* style computes a bond-order type interatomic potential (Kumagai) based on a 3-body Tersoff potential (Tersoff_1), (Tersoff_2) with modified cutoff function and angular-dependent term, giving the energy E of a system of atoms as

$$
\begin{aligned}
E &= \frac{1}{2}\sum_i \sum_{j \neq i} V_{ij} \\
V_{ij} &= f_C(r_{ij}) \left[f_R(r_{ij}) + b_{ij} f_A(r_{ij}) \right] \\
f_C(r) &= \begin{cases} 1 & : \quad r < R - D \\ \frac{1}{2} - \frac{9}{16}\sin\left(\frac{\pi}{2}\frac{r-R}{D}\right) - \frac{1}{16}\sin\left(\frac{3\pi}{2}\frac{r-R}{D}\right) & : \quad R - D < r < R + D \\ 0 & : \quad r > R + D \end{cases} \\
f_R(r) &= A \exp(-\lambda_1 r) \\
f_A(r) &= -B \exp(-\lambda_2 r) \\
b_{ij} &= (1 + {\zeta_{ij}}^{\eta})^{-\frac{1}{2n}} \\
\zeta_{ij} &= \sum_{k \neq i,j} f_C(r_{ik}) g(\theta_{ijk}) \exp\left[\alpha (r_{ij} - r_{ik})^{\beta}\right] \\
g(\theta) &= c_1 + g_o(\theta) g_a(\theta) \\
g_o(\theta) &= \frac{c_2 (h - \cos\theta)^2}{c_3 + (h - \cos\theta)^2} \\
g_a(\theta) &= 1 + c_4 \exp\left[-c_5 (h - \cos\theta)^2\right]
\end{aligned}
$$

where f_R is a two-body term and f_A includes three-body interactions. The summations in the formula are over all neighbors J and K of atom I within a cutoff distance = R + D.

The modified cutoff function f_C proposed by (Murty) and having a continuous second-order differential is employed. The angular-dependent term g(theta) was modified to increase the flexibility of the potential.

The *tersoff/mod* potential is fitted to both the elastic constants and melting point by employing the modified Tersoff potential function form in which the angular-dependent term is improved. The model performs extremely well in describing the crystalline, liquid, and amorphous phases (Schelling).

Only a single pair_coeff command is used with the *tersoff/mod* style which specifies a Tersoff/MOD potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of Tersoff/MOD elements to atom types

As an example, imagine the Si.tersoff_mod file has Tersoff values for Si. If your LAMMPS simulation has 3 Si atoms types, you would use the following pair_coeff command:

```
pair_coeff * * Si.tersoff_mod Si Si Si
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the Tersoff/MOD file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *tersoff/mod* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Tersoff/MOD file in the *potentials* directory of the LAMMPS distribution have a ".tersoff.mod" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to coefficients in the formula above:

- element 1 (the center atom in a 3-body interaction)
- element 2 (the atom bonded to the center atom)
- element 3 (the atom influencing the 1-2 bond in a bond-order sense)
- beta
- alpha
- h
- eta
- beta_ters = 1 (dummy parameter)
- lambda2 (1/distance units)
- B (energy units)
- R (distance units)
- D (distance units)
- lambda1 (1/distance units)
- A (energy units)
- n
- c1
- c2
- c3
- c4
- c5

The n, eta, lambda2, B, lambda1, and A parameters are only used for two-body interactions. The beta, alpha, c1, c2, c3, c4, c5, h parameters are only used for three-body interactions. The R and D parameters are used for both two-body and three-body interactions. The non-annotated parameters are unitless.

The Tersoff/MOD potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries.

For a single-element simulation, only a single entry is required (e.g. SiSiSi). As annotated above, the first element in the entry is the center atom in a three-body interaction and it is bonded to the 2nd atom and the bond is influenced by the 3rd atom. Thus an entry for SiSiSi means Si bonded to a Si with another Si atom influencing the bond.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making

LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

This pair style does not support the pair_modify shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

This pair style requires the newton setting to be "on" for pair interactions.

The Tersoff/MOD potential files provided with LAMMPS (see the potentials directory) are parameterized for metal units. You can use the Tersoff/MOD potential with any LAMMPS units, but you would need to create your own Tersoff/MOD potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

Related commands:

pair_coeff

Default: none

(Kumagai) T. Kumagai, S. Izumi, S. Hara, S. Sakai, Comp. Mat. Science, 39, 457 (2007).

(Tersoff_1) J. Tersoff, Phys Rev B, 37, 6991 (1988).

(Tersoff_2) J. Tersoff, Phys Rev B, 38, 9902 (1988).

(Murty) M.V.R. Murty, H.A. Atwater, Phys Rev B, 51, 4889 (1995).

(Schelling) Patrick K. Schelling, Comp. Mat. Science, 44, 274 (2008).

pair_style tersoff/zbl command

pair_style tersoff/zbl/kk command

pair_style tersoff/zbl/omp command

Syntax:

```
pair_style tersoff/zbl
```

Examples:

```
pair_style tersoff/zbl
pair_coeff * * SiC.tersoff.zbl Si C Si
```

Description:

The *tersoff/zbl* style computes a 3-body Tersoff potential (Tersoff_1) with a close-separation pairwise modification based on a Coulomb potential and the Ziegler-Biersack-Littmark universal screening function (ZBL), giving the energy E of a system of atoms as

$$
\begin{aligned}
E &= \frac{1}{2}\sum_i \sum_{j \neq i} V_{ij} \\
V_{ij} &= (1 - f_F(r_{ij}))V_{ij}^{ZBL} + f_F(r_{ij})V_{ij}^{Tersoff} \\
f_F(r_{ij}) &= \frac{1}{1 + e^{-A_F(r_{ij} - r_C)}}
\end{aligned}
$$

$$
\begin{aligned}
V_{ij}^{ZBL} &= \frac{1}{4\pi\epsilon_0}\frac{Z_1 Z_2\, e^2}{r_{ij}}\phi(r_{ij}/a) \\
a &= \frac{0.8854\, a_0}{Z_1^{0.23} + Z_2^{0.23}} \\
\phi(x) &= 0.1818e^{-3.2x} + 0.5099e^{-0.9423x} + 0.2802e^{-0.4029x} + 0.02817e^{-0.2}
\end{aligned}
$$

$$
\begin{aligned}
V_{ij}^{Tersoff} &= f_C(r_{ij})\left[f_R(r_{ij}) + b_{ij} f_A(r_{ij})\right] \\
f_C(r) &= \begin{cases} 1 & : \quad r < R - D \\ \frac{1}{2} - \frac{1}{2}\sin\left(\frac{\pi}{2}\frac{r-R}{D}\right) & : \quad R - D < r < R + D \\ 0 & : \quad r > R + D \end{cases} \\
f_R(r) &= A\exp(-\lambda_1 r) \\
f_A(r) &= -B\exp(-\lambda_2 r) \\
b_{ij} &= (1 + \beta^n {\zeta_{ij}}^n)^{-\frac{1}{2n}} \\
\zeta_{ij} &= \sum_{k \neq i,j} f_C(r_{ik}) g(\theta_{ijk}) \exp\left[{\lambda_3}^m (r_{ij} - r_{ik})^m\right] \\
g(\theta) &= \gamma_{ijk}\left(1 + \frac{c^2}{d^2} - \frac{c^2}{[d^2 + (\cos\theta - \cos\theta_0)^2]}\right)
\end{aligned}
$$

The f_F term is a fermi-like function used to smoothly connect the ZBL repulsive potential with the Tersoff potential. There are 2 parameters used to adjust it: A_F and r_C. A_F controls how "sharp" the transition is between the two, and r_C is essentially the cutoff for the ZBL potential.

For the ZBL portion, there are two terms. The first is the Coulomb repulsive term, with Z1, Z2 as the number of protons in each nucleus, e as the electron charge (1 for metal and real units) and epsilon0 as the permittivity of vacuum. The second part is the ZBL universal screening function, with a0 being the Bohr radius (typically 0.529 Angstroms), and the remainder of the coefficients provided by the original paper. This screening function should be applicable to most systems. However, it is only accurate for small separations (i.e. less than 1 Angstrom).

For the Tersoff portion, f_R is a two-body term and f_A includes three-body interactions. The summations in the formula are over all neighbors J and K of atom I within a cutoff distance = R + D.

Only a single pair_coeff command is used with the *tersoff/zbl* style which specifies a Tersoff/ZBL potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of Tersoff/ZBL elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file.

As an example, imagine the SiC.tersoff.zbl file has Tersoff/ZBL values for Si and C. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * SiC.tersoff Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the Tersoff/ZBL file. The final C argument maps LAMMPS atom type 4 to the C element in the Tersoff/ZBL file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *tersoff/zbl* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Tersoff/ZBL files in the *potentials* directory of the LAMMPS distribution have a ".tersoff.zbl" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to coefficients in the formula above:

- element 1 (the center atom in a 3-body interaction)
- element 2 (the atom bonded to the center atom)
- element 3 (the atom influencing the 1-2 bond in a bond-order sense)
- m
- gamma
- lambda3 (1/distance units)
- c
- d
- costheta0 (can be a value < -1 or > 1)
- n
- beta
- lambda2 (1/distance units)
- B (energy units)
- R (distance units)
- D (distance units)

- lambda1 (1/distance units)
- A (energy units)
- Z_i
- Z_j
- ZBLcut (distance units)
- ZBLexpscale (1/distance units)

The n, beta, lambda2, B, lambda1, and A parameters are only used for two-body interactions. The m, gamma, lambda3, c, d, and costheta0 parameters are only used for three-body interactions. The R and D parameters are used for both two-body and three-body interactions. The Z_i,Z_j, ZBLcut, ZBLexpscale parameters are used in the ZBL repulsive portion of the potential and in the Fermi-like function. The non-annotated parameters are unitless. The value of m must be 3 or 1.

The Tersoff/ZBL potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries.

For a single-element simulation, only a single entry is required (e.g. SiSiSi). For a two-element simulation, the file must contain 8 entries (for SiSiSi, SiSiC, SiCSi, SiCC, CSiSi, CSiC, CCSi, CCC), that specify Tersoff parameters for all permutations of the two elements interacting in three-body configurations. Thus for 3 elements, 27 entries would be required, etc.

As annotated above, the first element in the entry is the center atom in a three-body interaction and it is bonded to the 2nd atom and the bond is influenced by the 3rd atom. Thus an entry for SiCC means Si bonded to a C with another C atom influencing the bond. Thus three-body parameters for SiCSi and SiSiC entries will not, in general, be the same. The parameters used for the two-body interaction come from the entry where the 2nd element is repeated. Thus the two-body parameters for Si interacting with C, comes from the SiCC entry.

The parameters used for a particular three-body interaction come from the entry with the corresponding three elements. The parameters used only for two-body interactions (n, beta, lambda2, B, lambda1, and A) in entries whose 2nd and 3rd element are different (e.g. SiCSi) are not used for anything and can be set to 0.0 if desired.

Note that the twobody parameters in entries such as SiCC and CSiSi are often the same, due to the common use of symmetric mixing rules, but this is not always the case. For example, the beta and n parameters in Tersoff_2 (Tersoff_2) are not symmetric.

We chose the above form so as to enable users to define all commonly used variants of the Tersoff portion of the potential. In particular, our form reduces to the original Tersoff form when m = 3 and gamma = 1, while it reduces to the form of Albe et al. when beta = 1 and m = 1. Note that in the current Tersoff implementation in LAMMPS, m must be specified as either 3 or 1. Tersoff used a slightly different but equivalent form for alloys, which we will refer to as Tersoff_2 potential (Tersoff_2).

LAMMPS parameter values for Tersoff_2 can be obtained as follows: gamma = omega_ijk, lambda3 = 0 and the value of m has no effect. The parameters for species i and j can be calculated using the Tersoff_2 mixing rules:

$$
\begin{aligned}
\lambda_1^{i,j} &= \frac{1}{2}(\lambda_1^i + \lambda_1^j) \\
\lambda_2^{i,j} &= \frac{1}{2}(\lambda_2^i + \lambda_2^j) \\
A_{i,j} &= (A_i A_j)^{1/2} \\
B_{i,j} &= \chi_{ij}(B_i B_j)^{1/2} \\
R_{i,j} &= (R_i R_j)^{1/2} \\
S_{i,j} &= (S_i S_j)^{1/2}
\end{aligned}
$$

Tersoff_2 parameters R and S must be converted to the LAMMPS parameters R and D (R is different in both forms), using the following relations: R=(R'+S')/2 and D=(S'-R')/2, where the primes indicate the Tersoff_2 parameters.

In the potentials directory, the file SiCGe.tersoff provides the LAMMPS parameters for Tersoff's various versions of Si, as well as his alloy parameters for Si, C, and Ge. This file can be used for pure Si, (three different versions), pure C, pure Ge, binary SiC, and binary SiGe. LAMMPS will generate an error if this file is used with any combination involving C and Ge, since there are no entries for the GeC interactions (Tersoff did not publish parameters for this cross-interaction.) Tersoff files are also provided for the SiC alloy (SiC.tersoff) and the GaN (GaN.tersoff) alloys.

Many thanks to Rutuparna Narulkar, David Farrell, and Xiaowang Zhou for helping clarify how Tersoff parameters for alloys have been defined in various papers. Also thanks to Ram Devanathan for providing the base ZBL implementation.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above from values in the potential file.

This pair style does not support the pair_modify shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

This pair style requires the newton setting to be "on" for pair interactions.

The Tersoff/ZBL potential files provided with LAMMPS (see the potentials directory) are parameterized for metal units. You can use the Tersoff potential with any LAMMPS units, but you would need to create your own Tersoff potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

Related commands:

pair_coeff

Default: none

(Tersoff_1) J. Tersoff, Phys Rev B, 37, 6991 (1988).

(ZBL) J.F. Ziegler, J.P. Biersack, U. Littmark, 'Stopping and Ranges of Ions in Matter' Vol 1, 1985, Pergamon Press.

(Albe) J. Nord, K. Albe, P. Erhart and K. Nordlund, J. Phys.: Condens. Matter, 15, 5649(2003).

(Tersoff_2) J. Tersoff, Phys Rev B, 39, 5566 (1989); errata (PRB 41, 3248)

pair_style thole command

Syntax:

```
pair_style thole damp cutoff
```

- thole = style name
- damp = global damping parameter
- cutoff = global cutoff

Examples:

```
pair_style hybrid/overlay ... thole 2.6 12.0
pair_coeff 1 1 thole 1.0
pair_coeff 1 2 thole 1.0 2.6 10.0
pair_coeff * 2 thole 1.0 2.6
```

Description:

The *thole* pair style is meant to be used with force fields that include explicit polarization through Drude dipoles. This link describes how to use the thermalized Drude oscillator model in LAMMPS and polarizable models in LAMMPS are discussed in this Section.

The *thole* pair style should be used as a sub-style within in the pair_hybrid/overlay command, in conjunction with a main pair style including Coulomb interactions, i.e. any pair style containing *coul/cut* or *coul/long* in its style name.

The *thole* pair style computes the Coulomb interaction damped at short distances by a function

$$T_{ij}(r_{ij}) = 1 - \left(1 + \frac{s_{ij} r_{ij} }{2} \right) \exp \left(- s_{ij} r_{ij} \right)$$

This function results from an adaptation to point charges (Noskov) of the dipole screening scheme originally proposed by Thole. The scaling coefficient s_{ij} is determined by the polarizability of the atoms, α_i, and by a Thole damping parameter a. This Thole damping parameter usually takes a value of 2.6, but in certain force fields the value can depend upon the atom types. The mixing rule for Thole damping parameters is the arithmetic average, and for polarizabilities the geometric average between the atom-specific values.

$$s_{ij} = \frac{ a_{ij} }{ (\alpha_{ij})^{1/3} } = \frac{ (a_i + a_j)/2 }{ [(\alpha_i\alpha_j)^{1/2}]^{1/3} }$$

The damping function is only applied to the interactions between the point charges representing the induced dipoles on polarizable sites, that is, charges on Drude particles, $q_{D,i}$, and opposite charges, $-q_{D,i}$, located on the respective core particles (to which each Drude particle is bonded). Therefore, Thole screening is not applied to the full charge of the core particle q_i, but only to the $-q_{D,i}$ part of it.

The interactions between core charges are subject to the weighting factors set by the special_bonds command. The interactions between Drude particles and core charges or non-polarizable atoms are also subject to these weighting factors. The Drude particles inherit the 1-2, 1-3 and 1-4 neighbor relations from their respective cores.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the example above.

- alpha (distance units^3)
- damp
- cutoff (distance units)

The last two coefficients are optional. If not specified the global Thole damping parameter or global cutoff specified in the pair_style command are used. In order to specify a cutoff (third argument) a damp parameter (second argument) must also be specified.

Mixing:

The *thole* pair style does not support mixing. Thus, coefficients for all I,J pairs must be specified explicitly.

Restrictions:

These pair styles are part of the USER-DRUDE package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This pair_style should currently not be used with the charmm dihedral style if the latter has non-zero 1-4 weighting factors. This is because the *thole* pair style does not know which pairs are 1-4 partners of which dihedrals.

Related commands:

fix drude, fix langevin/drude, fix drude/transform, compute temp/drude

Default: none

(Noskov) Noskov, Lamoureux and Roux, J Phys Chem B, 109, 6705 (2005).

(Thole) Chem Phys, 59, 341 (1981).

pair_style tri/lj command

Syntax:

```
pair_style tri/lj cutoff
```

cutoff = global cutoff for interactions (distance units)

Examples:

```
pair_style tri/lj 3.0
pair_coeff * * 1.0 1.0
pair_coeff 1 1 1.0 1.5 2.5
```

Description:

Style *tri/lj* treats particles which are triangles as a set of small spherical particles that tile the triangle surface as explained below. Interactions between two triangles, each with N1 and N2 spherical particles, are calculated as the pairwise sum of N1*N2 Lennard-Jones interactions. Interactions between a triangle with N spherical particles and a point particle are treated as the pairwise sum of N Lennard-Jones interactions. See the pair_style lj/cut doc page for the definition of Lennard-Jones interactions.

The cutoff distance for an interaction between 2 triangles, or between a triangle and a point particle, is calculated from the position of the triangle (its centroid), not between pairs of individual spheres comprising the triangle. Thus an interaction is either calculated in its entirety or not at all.

The set of non-overlapping spherical particles that represent a triangle, for purposes of this pair style, are generated in the following manner. Assume the triangle is of type I, and sigma_II has been specified. We want a set of spheres with centers in the plane of the triangle, none of them larger in diameter than sigma_II, which completely cover the triangle's area, but with minimial overlap and a minimal total number of spheres. This is done in a recursive manner. Place a sphere at the centroid of the original triangle. Calculate what diameter it must have to just cover all 3 corner points of the triangle. If that diameter is equal to or smaller than sigma_II, then include a sphere of the calculated diameter in the set of covering spheres. It the diameter is larger than sigma_II, then split the triangle into 2 triangles by bisecting its longest side. Repeat the process on each sub-triangle, recursing as far as needed to generate a set of covering spheres. When finished, the original criteria are met, and the set of covering spheres shoule be near minimal in number and overlap, at least for input triangles with a reasonable aspect-ratio.

The LJ interaction between 2 spheres on different triangles of types I,J is computed with an arithmetic mixing of the sigma values of the 2 spheres and using the specified epsilon value for I,J atom types. Note that because the sigma values for triangles spheres is computed using only sigma_II values, specific to the triangles's type, this means that any specified sigma_IJ values (for I != J) are effectively ignored.

For style *tri/lj*, the following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands:

- epsilon (energy units)
- sigma (distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global cutoff is used.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the epsilon and sigma coefficients and cutoff distance for all of this pair style can be mixed. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style does not support the pair_modify shift, table, and tail options.

This pair style does not write its information to binary restart files.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This style is part of the ASPHERE package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Defining particles to be triangles so they participate in tri/tri or tri/particle interactions requires the use the atom_style tri command.

Related commands:

pair_coeff, pair_style line/lj

Default: none

pair_style vashishta command

pair_style vashishta/omp command

Syntax:

```
pair_style vashishta
```

Examples:

```
pair_style vashishta
pair_coeff * * SiC.vashishta Si C
```

Description:

The *vashishta* style computes the combined 2-body and 3-body family of potentials developed in the group of Vashishta and co-workers. By combining repulsive, screened Coulombic, screened charge-dipole, and dispersion interactions with a bond-angle energy based on the Stillinger-Weber potential, this potential has been used to describe a variety of inorganic compounds, including SiO2 Vashishta1990, SiC Vashishta2007, and InP Branicio2009.

The potential for the energy U of a system of atoms is

$$U = \sum_{i}^{N}\sum_{j>i}^{N} U_{ij}^{(2)}(r_{ij}) + \sum_{i}^{N}\sum_{j\neq i}^{N}\sum_{k>j,k\neq i}^{N} U_{ijk}^{(3)}(r_{ij},r_{ik},\theta_{ijk})$$

$$U_{ij}^{(2)}(r) = \frac{H_{ij}}{r^{\eta_{ij}}} + \frac{Z_i Z_j}{r}\exp(-r/\lambda_{1,ij}) - \frac{D_{ij}}{r^4}\exp(-r/\lambda_{4,ij}) - \frac{W_{ij}}{r^6}, r <$$

$$U_{ijk}^{(3)}(r_{ij},r_{ik},\theta_{ijk}) = B_{ijk}\frac{\left[\cos\theta_{ijk}-\cos\theta_{0ijk}\right]^2}{1+C_{ijk}\left[\cos\theta_{ijk}-\cos\theta_{0ijk}\right]^2}\times \exp\left(\frac{\gamma_{ij}}{r_{ij}-r_{0,ij}}\right)\exp\left(\frac{\gamma_{ik}}{r_{ik}-r_{0,ik}}\right), r_{ij} < r_{0,ij}, r_{ik} < r_{0,ik}$$

where we follow the notation used in Branicio2009. U2 is a two-body term and U3 is a three-body term. The summation over two-body terms is over all neighbors J within a cutoff distance = *rc*. The twobody terms are shifted and tilted by a linear function so that the energy and force are both zero at *rc*. The summation over three-body terms is over all neighbors J and K within a cut-off distance = *r0*, where the exponential screening function becomes zero.

Only a single pair_coeff command is used with the *vashishta* style which specifies a Vashishta potential file with parameters for all needed elements. These are mapped to LAMMPS atom types by specifying N additional arguments after the filename in the pair_coeff command, where N is the number of LAMMPS atom types:

- filename
- N element names = mapping of Vashishta elements to atom types

See the pair_coeff doc page for alternate ways to specify the path for the potential file.

As an example, imagine a file SiC.vashishta has parameters for Si and C. If your LAMMPS simulation has 4 atoms types and you want the 1st 3 to be Si, and the 4th to be C, you would use the following pair_coeff command:

```
pair_coeff * * SiC.vashishta Si Si Si C
```

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. The first three Si arguments map LAMMPS atom types 1,2,3 to the Si element in the file. The final C argument maps LAMMPS atom type 4 to the C element in the file. If a mapping value is specified as NULL, the mapping is not performed. This can be used when a *vashishta* potential is used as part of the *hybrid* pair style. The NULL values are placeholders for atom types that will be used with other potentials.

Vashishta files in the *potentials* directory of the LAMMPS distribution have a ".vashishta" suffix. Lines that are not blank or comments (starting with #) define parameters for a triplet of elements. The parameters in a single entry correspond to the two-body and three-body coefficients in the formulae above:

- element 1 (the center atom in a 3-body interaction)
- element 2
- element 3
- H (energy units)
- eta
- Zi (electron charge units)
- Zj (electron charge units)
- lambda1 (distance units)
- D (energy units)
- lambda4 (distance units)
- W (energy units)
- rc (distance units)
- B (energy units)
- gamma
- r0 (distance units)
- C
- costheta0

The non-annotated parameters are unitless. The Vashishta potential file must contain entries for all the elements listed in the pair_coeff command. It can also contain entries for additional elements not being used in a particular simulation; LAMMPS ignores those entries. For a single-element simulation, only a single entry is required (e.g. SiSiSi). For a two-element simulation, the file must contain 8 entries (for SiSiSi, SiSiC, SiCSi, SiCC, CSiSi, CSiC, CCSi, CCC), that specify parameters for all permutations of the two elements interacting in three-body configurations. Thus for 3 elements, 27 entries would be required, etc.

Depending on the particular version of the Vashishta potential, the values of these parameters may be keyed to the identities of zero, one, two, or three elements. In order to make the input file format unambiguous, general, and simple to code, LAMMPS uses a slightly confusing method for specifying parameters. All parameters are divided into two classes: two-body and three-body. Two-body and three-body parameters are handled differently, as described below. The two-body parameters are H, eta, lambda1, D, lambda4, W, rc, gamma, and r0. They appear in the above formulae with two subscripts. The parameters Zi and Zj are also classified as two-body parameters, even though they only have 1 subscript. The three-body parameters are B, C, costheta0. They appear in the above

formulae with three subscripts. Two-body and three-body parameters are handled differently, as described below.

The first element in each entry is the center atom in a three-body interaction, while the second and third elements are two neighbor atoms. Three-body parameters for a central atom I and two neighbors J and K are taken from the IJK entry. Note that even though three-body parameters do not depend on the order of J and K, LAMMPS stores three-body parameters for both IJK and IKJ. The user must ensure that these values are equal. Two-body parameters for an atom I interacting with atom J are taken from the IJJ entry, where the 2nd and 3rd elements are the same. Thus the two-body parameters for Si interacting with C come from the SiCC entry. Note that even though two-body parameters (except possibly gamma and r0 in U3) do not depend on the order of the two elements, LAMMPS will get the Si-C value from the SiCC entry and the C-Si value from the CSiSi entry. The user must ensure that these values are equal. Two-body parameters appearing in entries where the 2nd and 3rd elements are different are stored but never used. It is good practice to enter zero for these values. Note that the three-body function U3 above contains the two-body parameters gamma and r0. So U3 for a central C atom bonded to an Si atom and a second C atom will take three-body parameters from the CSiC entry, but two-body parameters from the CCC and CSiSi entries.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, where types I and J correspond to two different element types, mixing is performed by LAMMPS as described above from values in the potential file.

This pair style does not support the pair_modify shift, table, and tail options.

This pair style does not write its information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This pair style is part of the MANYBODY package. It is only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

This pair style requires the newton setting to be "on" for pair interactions.

The Vashishta potential files provided with LAMMPS (see the potentials directory) are parameterized for metal units. You can use the Vashishta potential with any LAMMPS units, but you would need to create your own Vashishta potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

Related commands:

pair_coeff

Default: none

(Vashishta1990) P. Vashishta, R. K. Kalia, J. P. Rino, Phys. Rev. B 41, 12197 (1990).

(Vashishta2007) P. Vashishta, R. K. Kalia, A. Nakano, J. P. Rino. J. Appl. Phys. 101, 103515 (2007).

(Branicio2009) Branicio, Rino, Gan and Tsuzuki, J. Phys Condensed Matter 21 (2009) 095002

pair_write command

Syntax:

```
pair_write itype jtype N style inner outer file keyword Qi Qj
```

- itype,jtype = 2 atom types
- N = # of values
- style = *r* or *rsq* or *bitmap*
- inner,outer = inner and outer cutoff (distance units)
- file = name of file to write values to
- keyword = section name in file for this set of tabulated values
- Qi,Qj = 2 atom charges (charge units) (optional)

Examples:

```
pair_write 1 3 500 r 1.0 10.0 table.txt LJ
pair_write 1 1 1000 rsq 2.0 8.0 table.txt Yukawa_1_1 -0.5 0.5
```

Description:

Write energy and force values to a file as a function of distance for the currently defined pair potential. This is useful for plotting the potential function or otherwise debugging its values. If the file already exists, the table of values is appended to the end of the file to allow multiple tables of energy and force to be included in one file.

The energy and force values are computed at distances from inner to outer for 2 interacting atoms of type itype and jtype, using the appropriate pair_coeff coefficients. If the style is *r*, then N distances are used, evenly spaced in r; if the style is *rsq*, N distances are used, evenly spaced in r^2.

For example, for N = 7, style = *r*, inner = 1.0, and outer = 4.0, values are computed at r = 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0.

If the style is *bitmap*, then 2^N values are written to the file in a format and order consistent with how they are read in by the pair_coeff command for pair style *table*. For reasonable accuracy in a bitmapped table, choose N >= 12, an *inner* value that is smaller than the distance of closest approach of 2 atoms, and an *outer* value <= cutoff of the potential.

If the pair potential is computed between charged atoms, the charges of the pair of interacting atoms can optionally be specified. If not specified, values of Qi = Qj = 1.0 are used.

The file is written in the format used as input for the pair_style *table* option with *keyword* as the section name. Each line written to the file lists an index number (1-N), a distance (in distance units), an energy (in energy units), and a force (in force units).

Restrictions:

All force field coefficients for pair and other kinds of interactions must be set before this command can be invoked.

Due to how the pairwise force is computed, an inner value > 0.0 must be specified even if the potential has a finite

value at r = 0.0.

For EAM potentials, the pair_write command only tabulates the pairwise portion of the potential, not the embedding portion.

Related commands:

pair_style, pair_coeff

Default: none

pair_style yukawa command

pair_style yukawa/gpu command

pair_style yukawa/omp command

Syntax:

```
pair_style yukawa kappa cutoff
```

- kappa = screening length (inverse distance units)
- cutoff = global cutoff for Yukawa interactions (distance units)

Examples:

```
pair_style yukawa 2.0 2.5
pair_coeff 1 1 100.0 2.3
pair_coeff * * 100.0
```

Description:

Style *yukawa* computes pairwise interactions with the formula

$$E = A \frac{e^{-\kappa r}}{r} \qquad r < r_c$$

Rc is the cutoff.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- A (energy*distance units)
- cutoff (distance units)

The last coefficient is optional. If not specified, the global yukawa cutoff is used.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the A coefficient and cutoff distance for this pair style can be mixed. A is an energy value mixed like a LJ epsilon. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style supports the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions: none

Related commands:

pair_coeff

Default: none

pair_style yukawa/colloid command

pair_style yukawa/colloid/gpu command

pair_style yukawa/colloid/omp command

Syntax:

```
pair_style yukawa/colloid kappa cutoff
```

- kappa = screening length (inverse distance units)
- cutoff = global cutoff for colloidal Yukawa interactions (distance units)

Examples:

```
pair_style yukawa/colloid 2.0 2.5
pair_coeff 1 1 100.0 2.3
pair_coeff * * 100.0
```

Description:

Style *yukawa/colloid* computes pairwise interactions with the formula

$$E = \frac{A}{\kappa} e^{-\kappa(r-(r_i+r_j))} \qquad r < r_c$$

where Ri and Rj are the radii of the two particles and Rc is the cutoff.

In contrast to pair_style yukawa, this functional form arises from the Coulombic interaction between two colloid particles, screened due to the presence of an electrolyte, see the book by Safran for a derivation in the context of DVLO theory. Pair_style yukawa is a screened Coulombic potential between two point-charges and uses no such approximation.

This potential applies to nearby particle pairs for which the Derjagin approximation holds, meaning h << Ri + Rj, where h is the surface-to-surface separation of the two particles.

When used in combination with pair_style colloid, the two terms become the so-called DLVO potential, which combines electrostatic repulsion and van der Waals attraction.

The following coefficients must be defined for each pair of atoms types via the pair_coeff command as in the examples above, or in the data file or restart files read by the read_data or read_restart commands, or by mixing as described below:

- A (energy/distance units)
- cutoff (distance units)

The prefactor A is determined from the relationship between surface charge and surface potential due to the presence of electrolyte. Note that the A for this potential style has different units than the A used in pair_style yukawa. For low surface potentials, i.e. less than about 25 mV, A can be written as:

```
A = 2 * PI * R*eps*eps0 * kappa * psi^2
```

where

- R = colloid radius (distance units)
- eps0 = permittivity of free space (charge^2/energy/distance units)
- eps = relative permittivity of fluid medium (dimensionless)
- kappa = inverse screening length (1/distance units)
- psi = surface potential (energy/charge units)

The last coefficient is optional. If not specified, the global yukawa/colloid cutoff is used.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the A coefficient and cutoff distance for this pair style can be mixed. A is an energy value mixed like a LJ epsilon. The default mix value is *geometric*. See the "pair_modify" command for details.

This pair style supports the pair_modify shift option for the energy of the pair interaction.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

This pair style writes its information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions:

This style is part of the COLLOID package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

This pair style requires that atoms be finite-size spheres with a diameter, as defined by the atom_style sphere command.

Per-particle polydispersity is not yet supported by this pair style; per-type polydispersity is allowed. This means all particles of the same type must have the same diameter. Each type can have a different diameter.

Related commands:

pair_coeff

Default: none

(Safran) Safran, Statistical Thermodynamics of Surfaces, Interfaces, And Membranes, Westview Press, ISBN: 978-0813340791 (2003).

pair_style zbl command

pair_style zbl/gpu command

pair_style zbl/omp command

Syntax:

```
pair_style zbl inner outer
```

- inner = distance where switching function begins
- outer = global cutoff for ZBL interaction

Examples:

```
pair_style zbl 3.0 4.0
pair_coeff * * 73.0 73.0
pair_coeff 1 1 14.0 14.0
```

Description:

Style *zbl* computes the Ziegler-Biersack-Littmark (ZBL) screened nuclear repulsion for describing high-energy collisions between atoms. (Ziegler). It includes an additional switching function that ramps the energy, force, and curvature smoothly to zero between an inner and outer cutoff. The potential energy due to a pair of atoms at a distance r_ij is given by:

$$
\begin{aligned}
E_{ij}^{ZBL} &= \frac{1}{4\pi\epsilon_0}\frac{Z_i Z_j\, e^2}{r_{ij}}\phi(r_{ij}/a) + S(r_{ij}) \\
a &= \frac{0.46850}{Z_i^{0.23} + Z_j^{0.23}} \\
\phi(x) &= 0.18175e^{-3.19980x} + 0.50986e^{-0.94229x} + 0.28022e^{-0.40290x} + 0.02817e^{-0.20162x}
\end{aligned}
$$

where e is the electron charge, epsilon_0 is the electrical permittivity of vacuum, and Z_i and Z_j are the nuclear charges of the two atoms. The switching function S(r) is identical to that used by pair_style lj/gromacs. Here, the inner and outer cutoff are the same for all pairs of atom types.

The following coefficients must be defined for each pair of atom types via the pair_coeff command as in the examples above, or in the LAMMPS data file.

- Z_i (atomic number for first atom type, e.g. 13.0 for aluminum)
- Z_j (ditto for second atom type)

The values of Z_i and Z_j are normally equal to the atomic numbers of the two atom types. Thus, the user may optionally specify only the coefficients for each I==I pair, and rely on the obvious mixing rule for cross

interactions (see below). Note that when I==I it is required that Z_i == Z_j. When used with hybrid/overlay and pairs are assigned to more than one sub-style, the mixing rule is not used and each pair of types interacting with the ZBL sub-style must be included in a pair_coeff command.

NOTE: The numerical values of the exponential decay constants in the screening function depend on the unit of distance. In the above equation they are given for units of angstroms. LAMMPS will automatically convert these values to the distance unit of the specified LAMMPS units setting. The values of Z should always be given as multiples of a proton's charge, e.g. 29.0 for copper.

Styles with a *cuda*, *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the USER-CUDA, GPU, USER-INTEL, KOKKOS, USER-OMP and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Mixing, shift, table, tail correction, restart, rRESPA info:

For atom type pairs I,J and I != J, the Z_i and Z_j coefficients can be mixed by taking Z_i and Z_j from the values specified for I == I and J == J cases. When used with hybrid/overlay and pairs are assigned to more than one sub-style, the mixing rule is not used and each pair of types interacting with the ZBL sub-style must be included in a pair_coeff command. The pair_modify mix option has no effect on the mixing behavior

The ZBL pair style does not support the pair_modify shift option, since the ZBL interaction is already smoothed to 0.0 at the cutoff.

The pair_modify table option is not relevant for this pair style.

This pair style does not support the pair_modify tail option for adding long-range tail corrections to energy and pressure, since there are no corrections for a potential that goes to 0.0 at the cutoff.

This pair style does not write information to binary restart files, so pair_style and pair_coeff commands must be specified in an input script that reads a restart file.

This pair style can only be used via the *pair* keyword of the run_style respa command. It does not support the *inner*, *middle*, *outer* keywords.

Restrictions: none

Related commands:

pair_coeff

Default: none

(Ziegler) J.F. Ziegler, J. P. Biersack and U. Littmark, "The Stopping and Range of Ions in Matter," Volume 1, Pergamon, 1985.

partition command

Syntax:

```
partition style N command ...
```

- style = *yes* or *no*
- N = partition number (see asterisk form below)
- command = any LAMMPS command

Examples:

```
partition yes 1 processors 4 10 6
partition no 5 print "Active partition"
partition yes *5 fix all nve
partition yes 6* fix all nvt temp 1.0 1.0 0.1
```

Description:

This command invokes the specified command on a subset of the partitions of processors you have defined via the -partition command-line switch. See Section_start 6 for an explanation of the switch.

Normally, every input script command in your script is invoked by every partition. This behavior can be modified by defining world- or universe-style variables that have different values for each partition. This mechanism can be used to cause your script to jump to different input script files on different partitions, if such a variable is used in a jump command.

The "partition" command is another mechanism for having as input script operate differently on different partitions. It is basically a prefix on any LAMMPS command. The commmand will only be invoked on the partition(s) specified by the *style* and *N* arguments.

If the *style* is *yes*, the command will be invoked on any partition which matches the *N* argument. If the *style* is *no* the command will be invoked on all the partitions which do not match the Np argument.

Partitions are numbered from 1 to Np, where Np is the number of partitions specified by the -partition command-line switch.

N can be specified in one of two ways. An explicit numeric value can be used, as in the 1st example above. Or a wild-card asterisk can be used to span a range of partition numbers. This takes the form "*" or "*n" or "n*" or "m*n". An asterisk with no numeric values means all partitions from 1 to Np. A leading asterisk means all partitions from 1 to n (inclusive). A trailing asterisk means all partitions from n to Np (inclusive). A middle asterisk means all partitions from m to n (inclusive).

This command can be useful for the "run_style verlet/split" command which imposed requirements on how the processors command lays out a 3d grid of processors in each of 2 partitions.

Restrictions: none

Related commands:

run_style verlet/split

Default: none

prd command

Syntax:

```
prd N t_event n_dephase t_dephase t_correlate compute-ID seed keyword value ...
```

- N = # of timesteps to run (not including dephasing/quenching)
- t_event = timestep interval between event checks
- n_dephase = number of velocity randomizations to perform in each dephase run
- t_dephase = number of timesteps to run dynamics after each velocity randomization during dephase
- t_correlate = number of timesteps within which 2 consecutive events are considered to be correlated
- compute-ID = ID of the compute used for event detection
- random_seed = random # seed (positive integer)
- zero or more keyword/value pairs may be appended
- keyword = *min* or *temp* or *vel*

```
  min values = etol ftol maxiter maxeval
      etol = stopping tolerance for energy, used in quenching
      ftol = stopping tolerance for force, used in quenching
      maxiter = max iterations of minimize, used in quenching
      maxeval = max number of force/energy evaluations, used in quenching
    temp value = Tdephase
      Tdephase = target temperature for velocity randomization, used in dephasing
    vel values = loop dist
      loop = all or local or geom, used in dephasing
      dist = uniform or gaussian, used in dephasing
    time value = steps or clock
      steps = simulation runs for N timesteps on each replica (default)
      clock = simulation runs for N timesteps across all replicas
```

Examples:

```
prd 5000 100 10 10 100 1 54982
prd 5000 100 10 10 100 1 54982 min 0.1 0.1 100 200
```

Description:

Run a parallel replica dynamics (PRD) simulation using multiple replicas of a system. One or more replicas can be used. The total number of steps *N* to run can be interpreted in one of two ways; see discussion of the *time* keyword below.

PRD is described in this paper by Art Voter. It is a method for performing accelerated dynamics that is suitable for infrequent-event systems that obey first-order kinetics. A good overview of accelerated dynamics methods for such systems in given in this review paper from the same group. To quote from the paper: "The dynamical evolution is characterized by vibrational excursions within a potential basin, punctuated by occasional transitions between basins." The transition probability is characterized by p(t) = k*exp(-kt) where k is the rate constant. Running multiple replicas gives an effective enhancement in the timescale spanned by the multiple simulations, while waiting for an event to occur.

Each replica runs on a partition of one or more processors. Processor partitions are defined at run-time using the -partition command-line switch; see Section_start 6 of the manual. Note that if you have MPI installed, you can run a multi-replica simulation with more replicas (partitions) than you have physical processors, e.g you can run a 10-replica simulation on one or two processors. For PRD, this makes little sense, since this offers no effective

parallel speed-up in searching for infrequent events. See Section_howto 5 of the manual for further discussion.

When a PRD simulation is performed, it is assumed that each replica is running the same model, though LAMMPS does not check for this. I.e. the simulation domain, the number of atoms, the interaction potentials, etc should be the same for every replica.

A PRD run has several stages, which are repeated each time an "event" occurs in one of the replicas, as defined below. The logic for a PRD run is as follows:

```
while (time remains):
  dephase for n_dephase*t_dephase steps
  until (event occurs on some replica):
    run dynamics for t_event steps
    quench
    check for uncorrelated event on any replica
  until (no correlated event occurs):
    run dynamics for t_correlate steps
    quench
    check for correlated event on this replica
  event replica shares state with all replicas
```

Before this loop begins, the state of the system on replica 0 is shared with all replicas, so that all replicas begin from the same initial state. The first potential energy basin is identified by quenching (an energy minimization, see below) the initial state and storing the resulting coordinates for reference.

In the first stage, dephasing is performed by each replica independently to eliminate correlations between replicas. This is done by choosing a random set of velocities, based on the *random_seed* that is specified, and running *t_dephase* timesteps of dynamics. This is repeated *n_dephase* times. At each of the *n_dephase* stages, if an event occurs during the *t_dephase* steps of dynamics for a particular replica, the replica repeats the stage until no event occurs.

If the *temp* keyword is not specified, the target temperature for velocity randomization for each replica is the current temperature of that replica. Otherwise, it is the specified *Tdephase* temperature. The style of velocity randomization is controlled using the keyword *vel* with arguments that have the same meaning as their counterparts in the velocity command.

In the second stage, each replica runs dynamics continuously, stopping every *t_event* steps to check if a transition event has occurred. This check is performed by quenching the system and comparing the resulting atom coordinates to the coordinates from the previous basin. The first time through the PRD loop, the "previous basin" is the set of quenched coordinates from the initial state of the system.

A quench is an energy minimization and is performed by whichever algorithm has been defined by the min_style command. Minimization parameters may be set via the min_modify command and by the *min* keyword of the PRD command. The latter are the settings that would be used with the minimize command. Note that typically, you do not need to perform a highly-converged minimization to detect a transition event.

The event check is performed by a compute with the specified *compute-ID*. Currently there is only one compute that works with the PRD commmand, which is the compute event/displace command. Other event-checking computes may be added. Compute event/displace checks whether any atom in the compute group has moved further than a specified threshold distance. If so, an "event" has occurred.

In the third stage, the replica on which the event occurred (event replica) continues to run dynamics to search for correlated events. This is done by running dynamics for *t_correlate* steps, quenching every *t_event* steps, and checking if another event has occurred.

The first time no correlated event occurs, the final state of the event replica is shared with all replicas, the new basin reference coordinates are updated with the quenched state, and the outer loop begins again. While the replica event is searching for correlated events, all the other replicas also run dynamics and event checking with the same schedule, but the final states are always overwritten by the state of the event replica.

The outer loop of the pseudo-code above continues until *N* steps of dynamics have been performed. Note that *N* only includes the dynamics of stages 2 and 3, not the steps taken during dephasing or the minimization iterations of quenching. The specified *N* is interpreted in one of two ways, depending on the *time* keyword. If the *time* value is *steps*, which is the default, then each replica runs for *N* timesteps. If the *time* value is *clock*, then the simulation runs until *N* aggregate timesteps across all replicas have elapsed. This aggregate time is the "clock" time defined below, which typically advances nearly M times faster than the timestepping on a single replica.

Four kinds of output can be generated during a PRD run: event statistics, thermodynamic output by each replica, dump files, and restart files.

When running with multiple partitions (each of which is a replica in this case), the print-out to the screen and master log.lammps file is limited to event statistics. Note that if a PRD run is performed on only a single replica then the event statistics will be intermixed with the usual thermodynamic output discussed below.

The quantities printed each time an event occurs are the timestep, CPU time, clock, event number, a correlation flag, the number of coincident events, and the replica number of the chosen event.

The timestep is the usual LAMMPS timestep, except that time does not advance during dephasing or quenches, but only during dynamics. Note that are two kinds of dynamics in the PRD loop listed above. The first is when all replicas are performing independent dynamics, waiting for an event to occur. The second is when correlated events are being searched for and only one replica is running dynamics.

The CPU time is the total processor time since the start of the PRD run.

The clock is the same as the timestep except that it advances by M steps every timestep during the first kind of dynamics when the M replicas are running independently. The clock advances by only 1 step per timestep during the second kind of dynamics, since only a single replica is checking for a correlated event. Thus "clock" time represents the aggregate time (in steps) that effectively elapses during a PRD simulation on M replicas. If most of the PRD run is spent in the second stage of the loop above, searching for infrequent events, then the clock will advance nearly M times faster than it would if a single replica was running. Note the clock time between events will be drawn from p(t).

The event number is a counter that increments with each event, whether it is uncorrelated or correlated.

The correlation flag will be 0 when an uncorrelated event occurs during the second stage of the loop listed above, i.e. when all replicas are running independently. The correlation flag will be 1 when a correlated event occurs during the third stage of the loop listed above, i.e. when only one replica is running dynamics.

When more than one replica detects an event at the end of the second stage, then one of them is chosen at random. The number of coincident events is the number of replicas that detected an event. Normally, we expect this value to be 1. If it is often greater than 1, then either the number of replicas is too large, or *t_event* is too large.

The replica number is the ID of the replica (from 0 to M-1) that found the event.

When running on multiple partitions, LAMMPS produces additional log files for each partition, e.g. log.lammps.0, log.lammps.1, etc. For the PRD command, these contain the thermodynamic output for each replica. You will see short runs and minimizations corresponding to the dynamics and quench operations of the

loop listed above. The timestep will be reset aprpopriately depending on whether the operation advances time or not.

After the PRD command completes, timing statistics for the PRD run are printed in each replica's log file, giving a breakdown of how much CPU time was spent in each stage (dephasing, dynamics, quenching, etc).

Any dump files defined in the input script, will be written to during a PRD run at timesteps corresponding to both uncorrelated and correlated events. This means the the requested dump frequency in the dump command is ignored. There will be one dump file (per dump command) created for all partitions.

The atom coordinates of the dump snapshot are those of the minimum energy configuration resulting from quenching following a transition event. The timesteps written into the dump files correspond to the timestep at which the event occurred and NOT the clock. A dump snapshot corresponding to the initial minimum state used for event detection is written to the dump file at the beginning of each PRD run.

If the restart command is used, a single restart file for all the partitions is generated, which allows a PRD run to be continued by a new input script in the usual manner.

The restart file is generated at the end of the loop listed above. If no correlated events are found, this means it contains a snapshot of the system at time T + *t_correlate*, where T is the time at which the uncorrelated event occurred. If correlated events were found, then it contains a snapshot of the system at time T + *t_correlate*, where T is the time of the last correlated event.

The restart frequency specified in the restart command is interpreted differently when performing a PRD run. It does not mean the timestep interval between restart files. Instead it means an event interval for uncorrelated events. Thus a frequency of 1 means write a restart file every time an uncorrelated event occurs. A frequency of 10 means write a restart file every 10th uncorrelated event.

When an input script reads a restart file from a previous PRD run, the new script can be run on a different number of replicas or processors. However, it is assumed that *t_correlate* in the new PRD command is the same as it was previously. If not, the calculation of the "clock" value for the first event in the new run will be slightly off.

Restrictions:

This command can only be used if LAMMPS was built with the REPLICA package. See the Making LAMMPS section for more info on packages.

N and *t_correlate* settings must be integer multiples of *t_event*.

Runs restarted from restart file written during a PRD run will not produce identical results due to changes in the random numbers used for dephasing.

This command cannot be used when any fixes are defined that keep track of elapsed time to perform time-dependent operations. Examples include the "ave" fixes such as fix ave/spatial. Also fix dt/reset and fix deposit.

Related commands:

compute event/displace, min_modify, min_style, run_style, minimize, velocity, temper, neb, tad

Default:

The option defaults are min = 0.1 0.1 40 50, no temp setting, vel = geom gaussian, and time = steps.

(Voter) Voter, Phys Rev B, 57, 13985 (1998).

(Voter2) Voter, Montalenti, Germann, Annual Review of Materials Research 32, 321 (2002).

print command

Syntax:

```
print string keyword value
```

- string = text string to print, which may contain variables
- zero or more keyword/value pairs may be appended
- keyword = *file* or *append* or *screen*

```
  file value = filename
    append value = filename
    screen value = yes or no
```

Examples:

```
print "Done with equilibration" file info.dat
print Vol=$v append info.dat screen no
print "The system volume is now $v"
print 'The system volume is now $v'
print """
System volume = $v
System temperature = $t
"""
```

Description:

Print a text string to the screen and logfile. The text string must be a single argument, so if it is one line but more than one word, it should be enclosed in single or double quotes. To generate multiple lines of output, the string can be enclosed in triple quotes, as in the last example above. If the text string contains variables, they will be evaluated and their current values printed.

If the *file* or *append* keyword is used, a filename is specified to which the output will be written. If *file* is used, then the filename is overwritten if it already exists. If *append* is used, then the filename is appended to if it already exists, or created if it does not exist.

If the *screen* keyword is used, output to the screen and logfile can be turned on or off as desired.

If you want the print command to be executed multiple times (with changing variable values), there are 3 options. First, consider using the fix print command, which will print a string periodically during a simulation. Second, the print command can be used as an argument to the *every* option of the run command. Third, the print command could appear in a section of the input script that is looped over (see the jump and next commands).

See the variable command for a description of *equal* style variables which are typically the most useful ones to use with the print command. Equal-style variables can calculate formulas involving mathematical operations, atom properties, group properties, thermodynamic properties, global values calculated by a compute or fix, or references to other variables.

Restrictions: none

Related commands:

fix print, variable

Default:

The option defaults are no file output and screen = yes.

processors command

Syntax:

```
processors Px Py Pz keyword args ...
```

- Px,Py,Pz = # of processors in each dimension of 3d grid overlaying the simulation domain
- zero or more keyword/arg pairs may be appended
- keyword = *grid* or *map* or *part* or *file*

```
grid arg = gstyle params ...
    gstyle = onelevel or twolevel or numa or custom
      onelevel params = none
      twolevel params = Nc Cx Cy Cz
        Nc = number of cores per node
        Cx,Cy,Cz = # of cores in each dimension of 3d sub-grid assigned to each node
      numa params = none
      custom params = infile
        infile = file containing grid layout
  map arg = cart or cart/reorder or xyz or xzy or yxz or yzx or zxy or zyx
     cart = use MPI_Cart() methods to map processors to 3d grid with reorder = 0
     cart/reorder = use MPI_Cart() methods to map processors to 3d grid with reorder = 1
     xyz,xzy,yxz,yzx,zxy,zyx = map procesors to 3d grid in IJK ordering
  numa arg = none
  part args = Psend Precv cstyle
    Psend = partition # (1 to Np) which will send its processor layout
    Precv = partition # (1 to Np) which will recv the processor layout
    cstyle = multiple
      multiple = Psend grid will be multiple of Precv grid in each dimension
  file arg = outfile
    outfile = name of file to write 3d grid of processors to
```

Examples:

```
processors * * 5
processors 2 4 4
processors * * 8 map xyz
processors * * * grid numa
processors * * * grid twolevel 4 * * 1
processors 4 8 16 grid custom myfile
processors * * * part 1 2 multiple
```

Description:

Specify how processors are mapped as a regular 3d grid to the global simulation box. The mapping involves 2 steps. First if there are P processors it means choosing a factorization P = Px by Py by Pz so that there are Px processors in the x dimension, and similarly for the y and z dimensions. Second, the P processors are mapped to the regular 3d grid. The arguments to this command control each of these 2 steps.

The Px, Py, Pz parameters affect the factorization. Any of the 3 parameters can be specified with an asterisk "*", which means LAMMPS will choose the number of processors in that dimension of the grid. It will do this based on the size and shape of the global simulation box so as to minimize the surface-to-volume ratio of each processor's sub-domain.

Choosing explicit values for Px or Py or Pz can be used to override the default manner in which LAMMPS will create the regular 3d grid of processors, if it is known to be sub-optimal for a particular problem. E.g. a problem where the extent of atoms will change dramatically in a particular dimension over the course of the simulation.

The product of Px, Py, Pz must equal P, the total # of processors LAMMPS is running on. For a 2d simulation, Pz must equal 1.

Note that if you run on a prime number of processors P, then a grid such as 1 x P x 1 will be required, which may incur extra communication costs due to the high surface area of each processor's sub-domain.

Also note that if multiple partitions are being used then P is the number of processors in this partition; see this section for an explanation of the -partition command-line switch. Also note that you can prefix the processors command with the partition command to easily specify different Px,Py,Pz values for different partitions.

You can use the partition command to specify different processor grids for different partitions, e.g.

```
partition yes 1 processors 4 4 4
partition yes 2 processors 2 3 2
```

NOTE: This command only affects the initial regular 3d grid created when the simulation box is first specified via a create_box or read_data or read_restart command. Or if the simulation box is re-created via the replicate command. The same regular grid is initially created, regardless of which comm_style command is in effect.

If load-balancing is never invoked via the balance or fix balance commands, then the initial regular grid will persist for all simulations. If balancing is performed, some of the methods invoked by those commands retain the logical toplogy of the initial 3d grid, and the mapping of processors to the grid specified by the processors command. However the grid spacings in different dimensions may change, so that processors own sub-domains of different sizes. If the comm_style tiled command is used, methods invoked by the balancing commands may discard the 3d grid of processors and tile the simulation domain with sub-domains of different sizes and shapes which no longer have a logical 3d connectivity. If that occurs, all the information specified by the processors command is ignored.

The *grid* keyword affects the factorization of P into Px,Py,Pz and it can also affect how the P processor IDs are mapped to the 3d grid of processors.

The *onelevel* style creates a 3d grid that is compatible with the Px,Py,Pz settings, and which minimizes the surface-to-volume ratio of each processor's sub-domain, as described above. The mapping of processors to the grid is determined by the *map* keyword setting.

The *twolevel* style can be used on machines with multicore nodes to minimize off-node communication. It insures that contiguous sub-sections of the 3d grid are assigned to all the cores of a node. For example if *Nc* is 4, then 2x2x1 or 2x1x2 or 1x2x2 sub-sections of the 3d grid will correspond to the cores of each node. This affects both the factorization and mapping steps.

The *Cx*, *Cy*, *Cz* settings are similar to the *Px*, *Py*, *Pz* settings, only their product should equal *Nc*. Any of the 3 parameters can be specified with an asterisk "*", which means LAMMPS will choose the number of cores in that dimension of the node's sub-grid. As with Px,Py,Pz, it will do this based on the size and shape of the global simulation box so as to minimize the surface-to-volume ratio of each processor's sub-domain.

NOTE: For the *twolevel* style to work correctly, it assumes the MPI ranks of processors LAMMPS is running on are ordered by core and then by node. E.g. if you are running on 2 quad-core nodes, for a total of 8 processors, then it assumes processors 0,1,2,3 are on node 1, and processors 4,5,6,7 are on node 2. This is the default rank ordering for most MPI implementations, but some MPIs provide options for this ordering, e.g. via environment

variable settings.

The *numa* style operates similar to the *twolevel* keyword except that it auto-detects which cores are running on which nodes. Currently, it does this in only 2 levels, but it may be extended in the future to account for socket topology and other non-uniform memory access (NUMA) costs. It also uses a different algorithm than the *twolevel* keyword for doing the two-level factorization of the simulation box into a 3d processor grid to minimize off-node communication, and it does its own MPI-based mapping of nodes and cores to the regular 3d grid. Thus it may produce a different layout of the processors than the *twolevel* options.

The *numa* style will give an error if the number of MPI processes is not divisible by the number of cores used per node, or any of the Px or Py of Pz values is greater than 1.

NOTE: Unlike the *twolevel* style, the *numa* style does not require any particular ordering of MPI ranks i norder to work correctly. This is because it auto-detects which processes are running on which nodes.

The *custom* style uses the file *infile* to define both the 3d factorization and the mapping of processors to the grid.

The file should have the following format. Any number of initial blank or comment lines (starting with a "#" character) can be present. The first non-blank, non-comment line should have 3 values:

```
Px Py Py
```

These must be compatible with the total number of processors and the Px, Py, Pz settings of the processors commmand.

This line should be immediately followed by P = Px*Py*Pz lines of the form:

```
ID I J K
```

where ID is a processor ID (from 0 to P-1) and I,J,K are the processors location in the 3d grid. I must be a number from 1 to Px (inclusive) and similarly for J and K. The P lines can be listed in any order, but no processor ID should appear more than once.

The *map* keyword affects how the P processor IDs (from 0 to P-1) are mapped to the 3d grid of processors. It is only used by the *onelevel* and *twolevel* grid settings.

The *cart* style uses the family of MPI Cartesian functions to perform the mapping, namely MPI_Cart_create(), MPI_Cart_get(), MPI_Cart_shift(), and MPI_Cart_rank(). It invokes the MPI_Cart_create() function with its reorder flag = 0, so that MPI is not free to reorder the processors.

The *cart/reorder* style does the same thing as the *cart* style except it sets the reorder flag to 1, so that MPI can reorder processors if it desires.

The *xyz*, *xzy*, *yxz*, *yzx*, *zxy*, and *zyx* styles are all similar. If the style is IJK, then it maps the P processors to the grid so that the processor ID in the I direction varies fastest, the processor ID in the J direction varies next fastest, and the processor ID in the K direction varies slowest. For example, if you select style *xyz* and you have a 2x2x2 grid of 8 processors, the assignments of the 8 octants of the simulation domain will be:

```
proc 0 = lo x, lo y, lo z octant
proc 1 = hi x, lo y, lo z octant
proc 2 = lo x, hi y, lo z octant
proc 3 = hi x, hi y, lo z octant
proc 4 = lo x, lo y, hi z octant
proc 5 = hi x, lo y, hi z octant
```

```
proc 6 = lo x, hi y, hi z octant
proc 7 = hi x, hi y, hi z octant
```

Note that, in principle, an MPI implementation on a particular machine should be aware of both the machine's network topology and the specific subset of processors and nodes that were assigned to your simulation. Thus its MPI_Cart calls can optimize the assignment of MPI processes to the 3d grid to minimize communication costs. In practice, however, few if any MPI implementations actually do this. So it is likely that the *cart* and *cart/reorder* styles simply give the same result as one of the IJK styles.

Also note, that for the *twolevel* grid style, the *map* setting is used to first map the nodes to the 3d grid, then again to the cores within each node. For the latter step, the *cart* and *cart/reorder* styles are not supported, so an *xyz* style is used in their place.

The *part* keyword affects the factorization of P into Px,Py,Pz.

It can be useful when running in multi-partition mode, e.g. with the run_style verlet/split command. It specifies a dependency bewteen a sending partition *Psend* and a receiving partition *Precv* which is enforced when each is setting up their own mapping of their processors to the simulation box. Each of *Psend* and *Precv* must be integers from 1 to Np, where Np is the number of partitions you have defined via the -partition command-line switch.

A "dependency" means that the sending partition will create its regular 3d grid as Px by Py by Pz and after it has done this, it will send the Px,Py,Pz values to the receiving partition. The receiving partition will wait to receive these values before creating its own regular 3d grid and will use the sender's Px,Py,Pz values as a constraint. The nature of the constraint is determined by the *cstyle* argument.

For a *cstyle* of *multiple*, each dimension of the sender's processor grid is required to be an integer multiple of the corresponding dimension in the receiver's processor grid. This is a requirement of the run_style verlet/split command.

For example, assume the sending partition creates a 4x6x10 grid = 240 processor grid. If the receiving partition is running on 80 processors, it could create a 4x2x10 grid, but it will not create a 2x4x10 grid, since in the y-dimension, 6 is not an integer multiple of 4.

NOTE: If you use the partition command to invoke different "processsors" commands on different partitions, and you also use the *part* keyword, then you must insure that both the sending and receiving partitions invoke the "processors" command that connects the 2 partitions via the *part* keyword. LAMMPS cannot easily check for this, but your simulation will likely hang in its setup phase if this error has been made.

The *file* keyword writes the mapping of the factorization of P processors and their mapping to the 3d grid to the specified file *outfile*. This is useful to check that you assigned physical processors in the manner you desired, which can be tricky to figure out, especially when running on multiple partitions or on, a multicore machine or when the processor ranks were reordered by use of the -reorder command-line switch or due to use of MPI-specific launch options such as a config file.

If you have multiple partitions you should insure that each one writes to a different file, e.g. using a world-style variable for the filename. The file has a self-explanatory header, followed by one-line per processor in this format:

world-ID universe-ID original-ID: I J K: name

The IDs are the processor's rank in this simulation (the world), the universe (of multiple simulations), and the original MPI communicator used to instantiate LAMMPS, respectively. The world and universe IDs will only be different if you are running on more than one partition; see the -partition command-line switch. The universe and

original IDs will only be different if you used the -reorder command-line switch to reorder the processors differently than their rank in the original communicator LAMMPS was instantiated with.

I,J,K are the indices of the processor in the regular 3d grid, each from 1 to Nd, where Nd is the number of processors in that dimension of the grid.

The *name* is what is returned by a call to MPI_Get_processor_name() and should represent an identifier relevant to the physical processors in your machine. Note that depending on the MPI implementation, multiple cores can have the same *name*.

Restrictions:

This command cannot be used after the simulation box is defined by a read_data or create_box command. It can be used before a restart file is read to change the 3d processor grid from what is specified in the restart file.

The *grid numa* keyword only currently works with the *map cart* option.

The *part* keyword (for the receiving partition) only works with the *grid onelevel* or *grid twolevel* options.

Related commands:

partition, -reorder command-line switch

Default:

The option defaults are Px Py Pz = * * *, grid = onelevel, and map = cart.

python command

Syntax:

```
python func keyword args ...
```

- func = name of Python function
- one or more keyword/args pairs must be appended

```
keyword = invoke or input or return or format or file or here or exists
  invoke arg = none = invoke the previously defined Python function
  input args = N i1 i2 ... iN
    N = # of inputs to function
    i1,...,iN = value, SELF, or LAMMPS variable name
      value = integer number, floating point number, or string
      SELF = reference to LAMMPS itself which can be accessed by Python function
      variable = v_name, where name = name of LAMMPS variable, e.g. v_abc
  return arg = varReturn
    varReturn = v_name  = LAMMPS variable name which return value of function will be assigned
  format arg = fstring with M characters
    M = N if no return value, where N = # of inputs
    M = N+1 if there is a return value
    fstring = each character (i,f,s,p) corresponds in order to an input or return value
    'i' = integer, 'f' = floating point, 's' = string, 'p' = SELF
  file arg = filename
    filename = file of Python code, which defines func
  here arg = inline
    inline = one or more lines of Python code which defines func
             must be a single argument, typically enclosed between triple quotes
  exists arg = none = Python code has been loaded by previous python command
```

Examples:

```
python pForce input 2 v_x 20.0 return v_f format fff file force.py
python pForce invoke

python factorial input 1 myN return v_fac format ii here """
def factorial(n):
  if n == 1: return n
  return n * factorial(n-1)
 """

python loop input 1 SELF return v_value format -f here """
def loop(lmpptr,N,cut0):
  from lammps import lammps
  lmp = lammps(ptr=lmpptr)

  # loop N times, increasing cutoff each time

  for i in range(N):
    cut = cut0 + i*0.1
    lmp.set_variable("cut",cut)               # set a variable in LAMMPS
    lmp.command("pair_style lj/cut ${cut}")   # LAMMPS commands
    lmp.command("pair_coeff * * 1.0 1.0")
    lmp.command("run 100")
 """
```

Description:

NOTE: It is not currently possible to use the python command described in this section with Python 3, only with Python 2. The C API changed from Python 2 to 3 and the LAMMPS code is not compatible with both.

Define a Python function or execute a previously defined function. Arguments, including LAMMPS variables, can be passed to the function from the LAMMPS input script and a value returned by the Python function to a LAMMPS variable. The Python code for the function can be included directly in the input script or in a separate Python file. The function can be standard Python code or it can make "callbacks" to LAMMPS through its library interface to query or set internal values within LAMMPS. This is a powerful mechanism for performing complex operations in a LAMMPS input script that are not possible with the simple input script and variable syntax which LAMMPS defines. Thus your input script can operate more like a true programming language.

Use of this command requires building LAMMPS with the PYTHON package which links to the Python library so that the Python interpreter is embedded in LAMMPS. More details about this process are given below.

There are two ways to invoke a Python function once it has been defined. One is using the *invoke* keyword. The other is to assign the function to a python-style variable defined in your input script. Whenever the variable is evaluated, it will execute the Python function to assign a value to the variable. Note that variables can be evaluated in many different ways within LAMMPS. They can be substituted for directly in an input script. Or they can be passed to various commands as arguments, so that the variable is evaluated during a simulation run.

A broader overview of how Python can be used with LAMMPS is given in Section python. There is an examples/python directory which illustrates use of the python command.

The *func* setting specifies the name of the Python function. The code for the function is defined using the *file* or *here* keywords as explained below.

If the *invoke* keyword is used, no other keywords can be used, and a previous python command must have defined the Python function referenced by this command. This invokes the Python function with the previously defined arguments and return value processed as explained below. You can invoke the function as many times as you wish in your input script.

The *input* keyword defines how many arguments *N* the Python function expects. If it takes no arguments, then the *input* keyword should not be used. Each argument can be specified directly as a value, e.g. 6 or 3.14159 or abc (a string of characters). The type of each argument is specified by the *format* keyword as explained below, so that Python will know how to interpret the value. If the word SELF is used for an argument it has a special meaning. A pointer is passed to the Python function which it converts into a reference to LAMMPS itself. This enables the function to call back to LAMMPS through its library interface as explained below. This allows the Python function to query or set values internal to LAMMPS which can affect the subsequent execution of the input script. A LAMMPS variable can also be used as an argument, specified as v_name, where "name" is the name of the variable. Any style of LAMMPS variable can be used, as defined by the variable command. Each time the Python function is invoked, the LAMMPS variable is evaluated and its value is passed to the Python function.

The *return* keyword is only needed if the Python function returns a value. The specified *varReturn* must be of the form v_name, where "name" is the name of a python-style LAMMPS variable, defined by the variable command. The Python function can return a numeric or string value, as specified by the *format* keyword.

As explained on the variable doc page, the definition of a python-style variable associates a Python function name with the variable. This must match the *func* setting for this command. For exampe these two commands would be self-consistent:

```
variable foo python myMultiply
```

```
python myMultiply return v_foo format f file funcs.py
```

The two commands can appear in either order in the input script so long as both are specified before the Python function is invoked for the first time.

The *format* keyword must be used if the *input* or *return* keyword is used. It defines an *fstring* with M characters, where M = sum of number of inputs and outputs. The order of characters corresponds to the N inputs, followed by the return value (if it exists). Each character must be one of the following: "i" for integer, "f" for floating point, "s" for string, or "p" for SELF. Each character defines the type of the corresponding input or output value of the Python function and affects the type conversion that is performed internally as data is passed back and forth between LAMMPS and Python. Note that it is permissible to use a python-style variable in a LAMMPS command that allows for an equal-style variable as an argument, but only if the output of the Python function is flagged as a numeric value ("i" or "f") via the *format* keyword.

Either the *file*, *here*, or *exists* keyword must be used, but only one of them. These keywords specify what Python code to load into the Python interpreter. The *file* keyword gives the name of a file, which should end with a ".py" suffix, which contains Python code. The code will be immediately loaded into and run in the "main" module of the Python interpreter. Note that Python code which contains a function definition does not "execute" the function when it is run; it simply defines the function so that it can be invoked later.

The *here* keyword does the same thing, except that the Python code follows as a single argument to the *here* keyword. This can be done using triple quotes as delimiters, as in the examples above. This allows Python code to be listed verbatim in your input script, with proper indentation, blank lines, and comments, as desired. See Section 3.2, for an explanation of how triple quotes can be used as part of input script syntax.

The *exists* keyword takes no argument. It means that Python code containing the required Python function defined by the *func* setting, is assumed to have been previously loaded by another python command.

Note that the Python code that is loaded and run must contain a function with the specified *func* name. To operate properly when later invoked, the the function code must match the *input* and *return* and *format* keywords specified by the python command. Otherwise Python will generate an error.

This section describes how Python code can be written to work with LAMMPS.

Whether you load Python code from a file or directly from your input script, via the *file* and *here* keywords, the code can be identical. It must be indented properly as Python requires. It can contain comments or blank lines. If the code is in your input script, it cannot however contain triple-quoted Python strings, since that will conflict with the triple-quote parsing that the LAMMPS input script performs.

All the Python code you specify via one or more python commands is loaded into the Python "main" module, i.e. __main__. The code can define global variables or statements that are outside of function definitions. It can contain multiple functions, only one of which matches the *func* setting in the python command. This means you can use the *file* keyword once to load several functions, and the *exists* keyword thereafter in subsequent python commands to access the other functions previously loaded.

A Python function you define (or more generally, the code you load) can import other Python modules or classes, it can make calls to other system functions or functions you define, and it can access or modify global variables (in the "main" module) which will persist between successive function calls. The latter can be useful, for example, to prevent a function from being invoke multiple times per timestep by different commands in a LAMMPS input script that access the returned python-style variable associated with the function. For example, consider this function loaded with two global variables defined outside the function:

```
nsteplast = -1
```

```
nvaluelast = 0

def expensive(nstep):
  global nsteplast,nvaluelast
  if nstep == nsteplast: return nvaluelast
  nsteplast = nstep
  # perform complicated calculation
  nvalue = ...
  nvaluelast = nvalue
  return nvalue
```

Nsteplast stores the previous timestep the function was invoked (passed as an argument to the function). Nvaluelast stores the return value computed on the last function invocation. If the function is invoked again on the same timestep, the previous value is simply returned, without re-computing it. The "global" statement inside the Python function allows it to overwrite the global variables.

Note that if you load Python code multiple times (via multiple python commands), you can overwrite previously loaded variables and functions if you are not careful. E.g. if the code above were loaded twice, the global variables would be re-initialized, which might not be what you want. Likewise, if a function with the same name exists in two chunks of Python code you load, the function loaded second will override the function loaded first.

It's important to realize that if you are running LAMMPS in parallel, each MPI task will load the Python interpreter and execute a local copy of the Python function(s) you define. There is no connection between the Python interpreters running on different processors. This implies three important things.

First, if you put a print statement in your Python function, you will see P copies of the output, when running on P processors. If the prints occur at (nearly) the same time, the P copies of the output may be mixed together. Welcome to the world of parallel programming and debugging.

Second, if your Python code loads modules that are not pre-loaded by the Python library, then it will load the module from disk. This may be a bottleneck if 1000s of processors try to load a module at the same time. On some large supercomputers, loading of modules from disk by Python may be disabled. In this case you would need to pre-build a Python library that has the required modules pre-loaded and link LAMMPS with that library.

Third, if your Python code calls back to LAMMPS (discussed in the next section) and causes LAMMPS to perform an MPI operation requires global communication (e.g. via MPI_Allreduce), such as computing the global temperature of the system, then you must insure all your Python functions (running independently on different processors) call back to LAMMPS. Otherwise the code may hang.

Your Python function can "call back" to LAMMPS through its library interface, if you use the SELF input to pass Python a pointer to LAMMPS. The mechanism for doing this in your Python function is as follows:

```
def foo(lmpptr,...):
  from lammps import lammps
  lmp = lammps(ptr=lmpptr)
  lmp.command('print "Hello from inside Python"')
  ...
```

The function definition must include a variable (lmpptr in this case) which corresponds to SELF in the python command. The first line of the function imports the Python module lammps.py in the python dir of the distribution. The second line creates a Python object "lmp" which wraps the instance of LAMMPS that called the function. The "ptr=lmpptr" argument is what makes that happen. The thrid line invokes the command() function in the LAMMPS library interface. It takes a single string argument which is a LAMMPS input script command for LAMMPS to execute, the same as if it appeared in your input script. In this case, LAMMPS should output

```
Hello from inside Python
```

to the screen and log file. Note that since the LAMMPS print command itself takes a string in quotes as its argument, the Python string must be delimited with a different style of quotes.

Section 11.7 describes the syntax for how Python wraps the various functions included in the LAMMPS library interface.

A more interesting example is in the examples/python/in.python script which loads and runs the following function from examples/python/funcs.py:

```
def loop(N,cut0,thresh,lmpptr):
  print "LOOP ARGS",N,cut0,thresh,lmpptr
  from lammps import lammps
  lmp = lammps(ptr=lmpptr)
  natoms = lmp.get_natoms()

  for i in range(N):
    cut = cut0 + i*0.1

    lmp.set_variable("cut",cut)                  # set a variable in LAMMPS
    lmp.command("pair_style lj/cut ${cut}")      # LAMMPS command
    #lmp.command("pair_style lj/cut %d" % cut)   # LAMMPS command option

    lmp.command("pair_coeff * * 1.0 1.0")        # ditto
    lmp.command("run 10")                        # ditto
    pe = lmp.extract_compute("thermo_pe",0,0)    # extract total PE from LAMMPS
    print "PE",pe/natoms,thresh
    if pe/natoms <thresh: return
```

with these input script commands:

```
python          loop input 4 10 1.0 -4.0 SELF format iffp file funcs.py
python          loop invoke
```

This has the effect of looping over a series of 10 short runs (10 timesteps each) where the pair style cutoff is increased from a value of 1.0 in distance units, in increments of 0.1. The looping stops when the per-atom potential energy falls below a threshhold of -4.0 in energy units. More generally, Python can be used to implement a loop with complex logic, much more so than can be created using the LAMMPS jump and if commands.

Several LAMMPS library functions are called from the loop function. Get_natoms() returns the number of atoms in the simulation, so that it can be used to normalize the potential energy that is returned by extract_compute() for the "thermo_pe" compute that is defined by default for LAMMPS thermodynamic output. Set_variable() sets the value of a string variable defined in LAMMPS. This library function is a useful way for a Python function to return multiple values to LAMMPS, more than the single value that can be passed back via a return statement. This cutoff value in the "cut" variable is then substituted (by LAMMPS) in the pair_style command that is executed next. Alternatively, the "LAMMPS command option" line could be used in place of the 2 preceeding lines, to have Python insert the value into the LAMMPS command string.

NOTE: When using the callback mechanism just described, recognize that there are some operations you should not attempt because LAMMPS cannot execute them correctly. If the Python function is invoked between runs in the LAMMPS input script, then it should be OK to invoke any LAMMPS input script command via the library interface command() or file() functions, so long as the command would work if it were executed in the LAMMPS input script directly at the same point.

However, a Python function can also be invoked during a run, whenever an associated LAMMPS variable it is assigned to is evaluted. If the variable is an input argument to another LAMMPS command (e.g. fix setforce), then the Python function will be invoked inside the class for that command, in one of its methods that is invoked in the middle of a timestep. You cannot execute arbitrary input script commands from the Python function (again, via the command() or file() functions) at that point in the run and expect it to work. Other library functions such as those that invoke computes or other variables may have hidden side effects as well. In these cases, LAMMPS has no simple way to check that something illogical is being attempted.

If you run Python code directly on your workstation, either interactively or by using Python to launch a Python script stored in a file, and your code has an error, you will typically see informative error messages. That is not the case when you run Python code from LAMMPS using an embedded Python interpreter. The code will typically fail silently. LAMMPS will catch some errors but cannot tell you where in the Python code the problem occurred. For example, if the Python code cannot be loaded and run because it has syntax or other logic errors, you may get an error from Python pointing to the offending line, or you may get one of these generic errors from LAMMPS:

```
Could not process Python file
Could not process Python string
```

When the Python function is invoked, if it does not return properly, you will typically get this generic error from LAMMPS:

```
Python function evaluation failed
```

Here are three suggestions for debugging your Python code while running it under LAMMPS.

First, don't run it under LAMMPS, at least to start with! Debug it using plain Python. Load and invoke your function, pass it arguments, check return values, etc.

Second, add Python print statements to the function to check how far it gets and intermediate values it calculates. See the discussion above about printing from Python when running in parallel.

Third, use Python exception handling. For example, say this statement in your Python function is failing, because you have not initialized the variable foo:

```
foo += 1
```

If you put one (or more) statements inside a "try" statement, like this:

```
import exceptions
print "Inside simple function"
try:
  foo += 1      # one or more statements here
except Exception, e:
  print "FOO error:",e
```

then you will get this message printed to the screen:

```
FOO error: local variable 'foo' referenced before assignment
```

If there is no error in the try statements, then nothing is printed. Either way the function continues on (unless you put a return or sys.exit() in the except clause).

Restrictions:

This command is part of the PYTHON package. It is only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

Building LAMMPS with the PYTHON package will link LAMMPS with the Python library on your system. Settings to enable this are in the lib/python/Makefile.lammps file. See the lib/python/README file for information on those settings.

If you use Python code which calls back to LAMMPS, via the SELF input argument explained above, there is an extra step required when building LAMMPS. LAMMPS must also be built as a shared library and your Python function must be able to to load the Python module in python/lammps.py that wraps the LAMMPS library interface. These are the same steps required to use Python by itself to wrap LAMMPS. Details on these steps are explained in Section python. Note that it is important that the stand-alone LAMMPS executable and the LAMMPS shared library be consistent (built from the same source code files) in order for this to work. If the two have been built at different times using different source files, problems may occur.

As described above, you can use the python command to invoke a Python function which calls back to LAMMPS through its Python-wrapped library interface. However you cannot do the opposite. I.e. you cannot call LAMMPS from Python and invoke the python command to "callback" to Python and execute a Python function. LAMMPS will generate an error if you try to do that. Note that we think there actually should be a way to do that, but haven't yet been able to figure out how to do it successfully.

Related commands:

shell, variable

Default: none

quit command

Syntax:

```
quit status
```

status = numerical exit status (optional)

Examples:

quit if "$n > 10000" then "quit 1":pre

Description:

This command causes LAMMPS to exit, after shutting down all output cleanly.

It can be used as a debug statement in an input script, to terminate the script at some intermediate point.

It can also be used as an invoked command inside the "then" or "else" portion of an if command.

The optional status argument is an integer which signals the return status to a program calling LAMMPS. A return status of 0 usually indicates success. A status != 0 is failure, where the specified value can be used to distinguish the kind of error, e.g. where in the input script the quit was invoked. If not specified, a status of 0 is returned.

Restrictions: none

Related commands:

if

Default: none

read_data command

Syntax:

```
read_data file keyword args ...
```

- file = name of data file to read in
- zero or more keyword/arg pairs may be appended
- keyword = *add* or *offset* or *shift* or *extra/atom/types* or *extra/bond/types* or *extra/angle/types* or *extra/dihedral/types* or *extra/improper/types* or *group* or *fix*

```
add arg = append or Nstart or merge
    append = add new atoms with IDs appended to current IDs
    Nstart = add new atoms with IDs starting with Nstart
    merge = add new atoms with their IDs unchanged
  offset args = toff boff aoff doff ioff
    toff = offset to add to atom types
    boff = offset to add to bond types
    aoff = offset to add to angle types
    doff = offset to add to dihedral types
    ioff = offset to add to improper types
  shift args = Sx Sy Sz
    Sx,Sy,Sz = distance to shift atoms when adding to system (distance units)
  extra/atom/types arg = # of extra atom types
  extra/bond/types arg = # of extra bond types
  extra/angle/types arg = # of extra angle types
  extra/dihedral/types arg = # of extra dihedral types
  extra/improper/types arg = # of extra improper types
  group args = groupID
    groupID = add atoms in data file to this group
  fix args = fix-ID header-string section-string
    fix-ID = ID of fix to process header lines and sections of data file
    header-string = header lines containing this string will be passed to fix
    section-string = section names with this string will be passed to fix
```

Examples:

```
read_data data.lj
read_data ../run7/data.polymer.gz
read_data data.protein fix mycmap crossterm CMAP
read_data data.water add append offset 3 1 1 1 1 shift 0.0 0.0 50.0
read_data data.water add merge 1 group solvent
```

Description:

Read in a data file containing information LAMMPS needs to run a simulation. The file can be ASCII text or a gzipped text file (detected by a .gz suffix). This is one of 3 ways to specify initial atom coordinates; see the read_restart and create_atoms commands for alternative methods. Also see the explanation of the -restart command-line switch which can convert a restart file to a data file.

This command can be used multiple times to add new atoms and their properties to an existing system by using the *add*, *offset*, and *shift* keywords. See more details below, which includes the use case for the *extra* keywords.

The *group* keyword adds all the atoms in the data file to the specified group-ID. The group will be created if it does not already exist. This is useful if you are reading multiple data files and wish to put sets of atoms into

different groups so they can be operated on later. E.g. a group of added atoms can be moved to new positions via the displace_atoms command. Note that atoms read from the data file are also always added to the "all" group. The group command discusses atom groups, as used in LAMMPS.

The use of the *fix* keyword is discussed below.

Reading multiple data files

The read_data command can be used multiple times with the same or different data files to build up a complex system from components contained in individual data files. For example one data file could contain fluid in a confined domain; a second could contain wall atoms, and the second file could be read a third time to create a wall on the other side of the fluid. The third set of atoms could be rotated to an opposing direction using the displace_atoms command, after the third read_data command is used.

The *add*, *offset*, *shift*, *extra*, and *group* keywords are useful in this context.

If a simulation box does not yet exist, the *add* keyword cannot be used; the read_data command is being used for the first time. If a simulation box does exist, due to using the create_box command, or a previous read_data command, then the *add* keyword must be used.

NOTE: The simulation box size (xlo to xhi, ylo to yhi, zlo to zhi) in the new data file will be merged with the existing simulation box to create a large enough box in each dimension to contain both the existing and new atoms. Each box dimension never shrinks due to this merge operation, it only stays the same or grows. Care must be used if you are growing the existing simulation box in a periodic dimension. If there are existing atoms with bonds that straddle that periodic boundary, then the atoms may become far apart if the box size grows. This will separate the atoms in the bond, which can lead to "lost" bond atoms or bad dynamics.

The three choices for the *add* argument affect how the IDs of atoms in the data file are treated. If *append* is specified, atoms in the data file are added to the current system, with their atom IDs reset so that an atomID = M in the data file becomes atomID = N+M, where N is the largest atom ID in the current system. This rule is applied to all occurrences of atom IDs in the data file, e.g. in the Velocity or Bonds section. If *Nstart* is specified, then *Nstart* is a numeric value is given, e.g. 1000, so that an atomID = M in the data file becomes atomID = 1000+M. If *merge* is specified, the data file atoms are added to the current system without changing their IDs. They are assumed to merge (without duplication) with the currently defined atoms. It is up to you to insure there are no multiply defined atom IDs, as LAMMPS only performs an incomplete check that this is the case by insuring the resulting max atomID >= the number of atoms.

The *offset* and *shift* keywords can only be used if the *add* keyword is also specified.

The *offset* keyword adds the specified offset values to the atom types, bond types, angle types, dihedral types, and improper types as they are read from the data file. E.g. if *toff* = 2, and the file uses atom types 1,2,3, then the added atoms will have atom types 3,4,5. These offsets apply to all occurrences of types in the data file, e.g. for the Atoms or Masses or Pair Coeffs or Bond Coeffs sections. This makes it easy to use atoms and molecules and their attributes from a data file in different simulations, where you want their types (atom, bond, angle, etc) to be different depending on what other types already exist. All five offset values must be specified, but individual values will be ignored if the data file does not use that attribute (e.g. no bonds).

The *shift* keyword can be used to specify an (Sx, Sy, Sz) displacement applied to the coordinates of each atom. Sz must be 0.0 for a 2d simulation. This is a mechanism for adding structured collections of atoms at different locations within the simulation box, to build up a complex geometry. It is up to you to insure atoms do not end up overlapping unphysically which would lead to bad dynamics. Note that the displace_atoms command can be used to move a subset of atoms after they have been read from a data file. Likewise, the delete_atoms command can be

used to remove overlapping atoms. Note that the shift values (Sx, Sy, Sz) are also added to the simulation box information (xlo, xhi, ylo, yhi, zlo, zhi) in the data file to shift its boundaries. E.g. xlo_new = xlo + Sx, xhi_new = xhi + Sx.

The *extra* keywords can only be used the first time the read_data command is used. They are useful if you intend to add new atom, bond, angle, etc types later with additional read_data commands. This is because the maximum number of allowed atom, bond, angle, etc types is set by LAMMPS when the system is first initialized. If you do not use the *extra* keywords, then the number of these types will be limited to what appears in the first data file you read. For example, if the first data file is a solid substrate of Si, it will likely specify a single atom type. If you read a second data file with a different material (water molecules) that sit on top of the substrate, you will want to use different atom types for those atoms. You can only do this if you set the *extra/atom/types* keyword to a sufficiently large value when reading the substrate data file. Note that use of the *extra* keywords also allows each data file to contain sections like Masses or Pair Coeffs or Bond Coeffs which are sized appropriately for the number of types in that data file. If the *offset* keyword is used appropriately when each data file is read, the values in those sections will be stored correctly in the larger data structures allocated by the use of the *extra* keywords. E.g. the substrate file can list mass and pair coefficients for type 1 silicon atoms. The water file can list mass and pair coeffcients for type 1 and type 2 hydrogen and oxygen atoms. Use of the *extra* and *offset* keywords will store those mass and pair coefficient values appropriately in data structures that allow for 3 atom types (Si, H, O). Of course, you would still need to specify coefficients for H/Si and O/Si interactions in your input script to have a complete pairwise interaction model.

An alternative to using the *extra* keywords with the read_data command, is to use the create_box command to initialize the simulation box and all the various type limits you need via its *extra* keywords. Then use the read_data command one or more times to populate the system with atoms, bonds, angles, etc, using the *offset* keyword if desired to alter types used in the various data files you read.

Format of a data file

The structure of the data file is important, though many settings and sections are optional or can come in any order. See the examples directory for sample data files for different problems.

A data file has a header and a body. The header appears first. The first line of the header is always skipped; it typically contains a description of the file. Then lines are read one at a time. Lines can have a trailing comment starting with '#' that is ignored. If the line is blank (only whitespace after comment is deleted), it is skipped. If the line contains a header keyword, the corresponding value(s) is read from the line. If it doesn't contain a header keyword, the line begins the body of the file.

The body of the file contains zero or more sections. The first line of a section has only a keyword. This line can have a trailing comment starting with '#' that is either ignored or can be used to check for a style match, as described below. The next line is skipped. The remaining lines of the section contain values. The number of lines depends on the section keyword as described below. Zero or more blank lines can be used between sections. Sections can appear in any order, with a few exceptions as noted below.

The keyword *fix* can be used one or more times. Each usage specifies a fix that will be used to process a specific portion of the data file. Any header line containing *header-string* and any section with a name containing *section-string* will be passed to the specified fix. See the fix property/atom command for an example of a fix that operates in this manner. The doc page for the fix defines the syntax of the header line(s) and section(s) that it reads from the data file. Note that the *header-string* can be specified as NULL, in which case no header lines are passed to the fix. This means that it can infer the length of its Section from standard header settings, such as the number of atoms.

The formatting of individual lines in the data file (indentation, spacing between words and numbers) is not important except that header and section keywords (e.g. atoms, xlo xhi, Masses, Bond Coeffs) must be capitalized as shown and can't have extra white space between their words - e.g. two spaces or a tab between the 2 words in "xlo xhi" or the 2 words in "Bond Coeffs", is not valid.

Format of the header of a data file

These are the recognized header keywords. Header lines can come in any order. The value(s) are read from the beginning of the line. Thus the keyword *atoms* should be in a line like "1000 atoms"; the keyword *ylo yhi* should be in a line like "-10.0 10.0 ylo yhi"; the keyword *xy xz yz* should be in a line like "0.0 5.0 6.0 xy xz yz". All these settings have a default value of 0, except the lo/hi box size defaults are -0.5 and 0.5. A line need only appear if the value is different than the default.

- *atoms* = # of atoms in system
- *bonds* = # of bonds in system
- *angles* = # of angles in system
- *dihedrals* = # of dihedrals in system
- *impropers* = # of impropers in system
- *atom types* = # of atom types in system
- *bond types* = # of bond types in system
- *angle types* = # of angle types in system
- *dihedral types* = # of dihedral types in system
- *improper types* = # of improper types in system
- *extra bond per atom* = leave space for this many new bonds per atom
- *extra angle per atom* = leave space for this many new angles per atom
- *extra dihedral per atom* = leave space for this many new dihedrals per atom
- *extra improper per atom* = leave space for this many new impropers per atom
- *extra special per atom* = leave space for this many new special bonds per atom
- *ellipsoids* = # of ellipsoids in system
- *lines* = # of line segments in system
- *triangles* = # of triangles in system
- *bodies* = # of bodies in system
- *xlo xhi* = simulation box boundaries in x dimension
- *ylo yhi* = simulation box boundaries in y dimension
- *zlo zhi* = simulation box boundaries in z dimension
- *xy xz yz* = simulation box tilt factors for triclinic system

The initial simulation box size is determined by the lo/hi settings. In any dimension, the system may be periodic or non-periodic; see the boundary command. When the simulation box is created it is also partitioned into a regular 3d grid of rectangular bricks, one per processor, based on the number of processors being used and the settings of the processors command. The partitioning can later be changed by the balance or fix balance commands.

If the *xy xz yz* line does not appear, LAMMPS will set up an axis-aligned (orthogonal) simulation box. If the line does appear, LAMMPS creates a non-orthogonal simulation domain shaped as a parallelepiped with triclinic symmetry. The parallelepiped has its "origin" at (xlo,ylo,zlo) and is defined by 3 edge vectors starting from the origin given by A = (xhi-xlo,0,0); B = (xy,yhi-ylo,0); C = (xz,yz,zhi-zlo). *Xy,xz,yz* can be 0.0 or positive or negative values and are called "tilt factors" because they are the amount of displacement applied to faces of an originally orthogonal box to transform it into the parallelepiped.

By default, the tilt factors (xy,xz,yz) can not skew the box more than half the distance of the corresponding parallel box length. For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be

between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = ..., -15, -5, 5, 15, 25, ... are all geometrically equivalent. If you wish to define a box with tilt factors that exceed these limits, you can use the box tilt command, with a setting of *large*; a setting of *small* is the default.

See Section_howto 12 of the doc pages for a geometric description of triclinic boxes, as defined by LAMMPS, and how to transform these parameters to and from other commonly used triclinic representations.

When a triclinic system is used, the simulation domain should normally be periodic in the dimension that the tilt is applied to, which is given by the second dimension of the tilt factor (e.g. y for xy tilt). This is so that pairs of atoms interacting across that boundary will have one of them shifted by the tilt factor. Periodicity is set by the boundary command. For example, if the xy tilt factor is non-zero, then the y dimension should be periodic. Similarly, the z dimension should be periodic if xz or yz is non-zero. LAMMPS does not require this periodicity, but you may lose atoms if this is not the case.

Also note that if your simulation will tilt the box, e.g. via the fix deform command, the simulation box must be setup to be triclinic, even if the tilt factors are initially 0.0. You can also change an orthogonal box to a triclinic box or vice versa by using the change box command with its *ortho* and *triclinic* options.

For 2d simulations, the *zlo zhi* values should be set to bound the z coords for atoms that appear in the file; the default of -0.5 0.5 is valid if all z coords are 0.0. For 2d triclinic simulations, the xz and yz tilt factors must be 0.0.

If the system is periodic (in a dimension), then atom coordinates can be outside the bounds (in that dimension); they will be remapped (in a periodic sense) back inside the box. Note that if the *add* option is being used to add atoms to a simulation box that already exists, this periodic remapping will be performed using simulation box bounds that are the union of the existing box and the box boundaries in the new data file.

NOTE: If the system is non-periodic (in a dimension), then all atoms in the data file must have coordinates (in that dimension) that are "greater than or equal to" the lo value and "less than or equal to" the hi value. If the non-periodic dimension is of style "fixed" (see the boundary command), then the atom coords must be strictly "less than" the hi value, due to the way LAMMPS assign atoms to processors. Note that you should not make the lo/hi values radically smaller/larger than the extent of the atoms. For example, if your atoms extend from 0 to 50, you should not specify the box bounds as -10000 and 10000. This is because LAMMPS uses the specified box size to layout the 3d grid of processors. A huge (mostly empty) box will be sub-optimal for performance when using "fixed" boundary conditions (see the boundary command). When using "shrink-wrap" boundary conditions (see the boundary command), a huge (mostly empty) box may cause a parallel simulation to lose atoms when LAMMPS shrink-wraps the box around the atoms. The read_data command will generate an error in this case.

The "extra bond per atom" setting (angle, dihedral, improper) is only needed if new bonds (angles, dihedrals, impropers) will be added to the system when a simulation runs, e.g. by using the fix bond/create command. This will pre-allocate space in LAMMPS data structures for storing the new bonds (angles, dihedrals, impropers).

The "extra special per atom" setting is typically only needed if new bonds/angles/etc will be added to the system, e.g. by using the fix bond/create command. Or if entire new molecules will be added to the system, e.g. by using the fix deposit or fix pour commands, which will have more special 1-2,1-3,1-4 neighbors than any other molecules defined in the data file. Using this setting will pre-allocate space in the LAMMPS data structures for storing these neighbors. See the special_bonds and molecule doc pages for more discussion of 1-2,1-3,1-4 neighbors.

NOTE: All of the "extra" settings are only used if they appear in the first data file read; see the description of the *add* keyword above for reading multiple data files. If they appear in later data files, they are ignored.

The "ellipsoids" and "lines" and "triangles" and "bodies" settings are only used with atom_style ellipsoid or line or tri or body and specify how many of the atoms are finite-size ellipsoids or lines or triangles or bodies; the remainder are point particles. See the discussion of ellipsoidflag and the *Ellipsoids* section below. See the discussion of lineflag and the *Lines* section below. See the discussion of triangleflag and the *Triangles* section below. See the discussion of bodyflag and the *Bodies* section below.

NOTE: For atom_style template, the molecular topology (bonds,angles,etc) is contained in the molecule templates read-in by the molecule command. This means you cannot set the *bonds*, *angles*, etc header keywords in the data file, nor can you define *Bonds*, *Angles*, etc sections as discussed below. You can set the *bond types*, *angle types*, etc header keywords, though it is not necessary. If specified, they must match the maximum values defined in any of the template molecules.

Format of the body of a data file

These are the section keywords for the body of the file.

- *Atoms, Velocities, Masses, Ellipsoids, Lines, Triangles, Bodies* = atom-property sections
- *Bonds, Angles, Dihedrals, Impropers* = molecular topology sections
- *Pair Coeffs, PairIJ Coeffs, Bond Coeffs, Angle Coeffs, Dihedral Coeffs, Improper Coeffs* = force field sections
- *BondBond Coeffs, BondAngle Coeffs, MiddleBondTorsion Coeffs, EndBondTorsion Coeffs, AngleTorsion Coeffs, AngleAngleTorsion Coeffs, BondBond13 Coeffs, AngleAngle Coeffs* = class 2 force field sections

These keywords will check an appended comment for a match with the currently defined style:

- *Atoms, Pair Coeffs, PairIJ Coeffs, Bond Coeffs, Angle Coeffs, Dihedral Coeffs, Improper Coeffs*

For example, these lines:

```
Atoms # sphere
Pair Coeffs # lj/cut
```

will check if the currently-defined atom_style is *sphere*, and the current pair_style is *lj/cut*. If not, LAMMPS will issue a warning to indicate that the data file section likely does not contain the correct number or type of parameters expected for the currently-defined style.

Each section is listed below in alphabetic order. The format of each section is described including the number of lines it must contain and rules (if any) for where it can appear in the data file.

Any individual line in the various sections can have a trailing comment starting with "#" for annotation purposes. E.g. in the Atoms section:

```
10 1 17 -1.0 10.0 5.0 6.0   # salt ion
```

Angle Coeffs section:

- one line per angle type
- line syntax: ID coeffs

  ```
  ID = angle type (1-N)
  coeffs = list of coeffs
  ```
- example:

```
6 70 108.5 0 0
```

The number and meaning of the coefficients are specific to the defined angle style. See the angle_style and angle_coeff commands for details. Coefficients can also be set via the angle_coeff command in the input script.

AngleAngle Coeffs section:

- one line per improper type
- line syntax: ID coeffs

```
ID = improper type (1-N)
coeffs = list of coeffs (see improper_coeff)
```

AngleAngleTorsion Coeffs section:

- one line per dihedral type
- line syntax: ID coeffs

```
ID = dihedral type (1-N)
coeffs = list of coeffs (see dihedral_coeff)
```

Angles section:

- one line per angle
- line syntax: ID type atom1 atom2 atom3

```
ID = number of angle (1-Nangles)
type = angle type (1-Nangletype)
atom1,atom2,atom3 = IDs of 1st,2nd,3rd atoms in angle
```

example:

```
2 2 17 29 430
```

The 3 atoms are ordered linearly within the angle. Thus the central atom (around which the angle is computed) is the atom2 in the list. E.g. H,O,H for a water molecule. The *Angles* section must appear after the *Atoms* section. All values in this section must be integers (1, not 1.0).

AngleTorsion Coeffs section:

- one line per dihedral type
- line syntax: ID coeffs

```
ID = dihedral type (1-N)
coeffs = list of coeffs (see dihedral_coeff)
```

Atoms section:

- one line per atom
- line syntax: depends on atom style

An *Atoms* section must appear in the data file if natoms > 0 in the header section. The atoms can be listed in any order. These are the line formats for each atom style in LAMMPS. As discussed below, each line can optionally have 3 flags (nx,ny,nz) appended to it, which indicate which image of a periodic simulation box the atom is in.

These may be important to include for some kinds of analysis.

angle	atom-ID molecule-ID atom-type x y z
atomic	atom-ID atom-type x y z
body	atom-ID atom-type bodyflag mass x y z
bond	atom-ID molecule-ID atom-type x y z
charge	atom-ID atom-type q x y z
dipole	atom-ID atom-type q x y z mux muy muz
dpd	atom-ID atom-type theta x y z
electron	atom-ID atom-type q spin eradius x y z
ellipsoid	atom-ID atom-type ellipsoidflag density x y z
full	atom-ID molecule-ID atom-type q x y z
line	atom-ID molecule-ID atom-type lineflag density x y z
meso	atom-ID atom-type rho e cv x y z
molecular	atom-ID molecule-ID atom-type x y z
peri	atom-ID atom-type volume density x y z
smd	atom-ID atom-type molecule volume mass kernel-radius contact-radius x y z
sphere	atom-ID atom-type diameter density x y z
template	atom-ID molecule-ID template-index template-atom atom-type x y z
tri	atom-ID molecule-ID atom-type triangleflag density x y z
wavepacket	atom-ID atom-type charge spin eradius etag cs_re cs_im x y z
hybrid	atom-ID atom-type x y z sub-style1 sub-style2 ...

The per-atom values have these meanings and units, listed alphabetically:

- atom-ID = integer ID of atom
- atom-type = type of atom (1-Ntype)
- bodyflag = 1 for body particles, 0 for point particles
- contact-radius = ??? (distance units)
- cs_re,cs_im = real/imaginary parts of wavepacket coefficients
- cv = heat capacity (need units) for SPH particles
- density = density of particle (mass/distance^3 or mass/distance^2 or mass/distance units, depending on dimensionality of particle)
- diameter = diameter of spherical atom (distance units)
- e = energy (need units) for SPH particles
- ellipsoidflag = 1 for ellipsoidal particles, 0 for point particles
- eradius = electron radius (or fixed-core radius)
- etag = integer ID of electron that each wavepacket belongs to
- kernel-radius = ??? (distance units)
- lineflag = 1 for line segment particles, 0 for point or spherical particles
- mass = mass of particle (mass units)
- molecule-ID = integer ID of molecule the atom belongs to
- mux,muy,muz = components of dipole moment of atom (dipole units)
- q = charge on atom (charge units)
- rho = density (need units) for SPH particles
- spin = electron spin (+1/-1), 0 = nuclei, 2 = fixed-core, 3 = pseudo-cores (i.e. ECP)
- template-atom = which atom within a template molecule the atom is
- template-index = which molecule within the molecule template the atom is part of
- theta = internal temperature of a DPD particle

- triangleflag = 1 for triangular particles, 0 for point or sperhical particles
- volume = volume of Peridynamic particle (distance^3 units)
- x,y,z = coordinates of atom (distance units)

The units for these quantities depend on the unit style; see the units command for details.

For 2d simulations specify z as 0.0, or a value within the *zlo zhi* setting in the data file header.

The atom-ID is used to identify the atom throughout the simulation and in dump files. Normally, it is a unique value from 1 to Natoms for each atom. Unique values larger than Natoms can be used, but they will cause extra memory to be allocated on each processor, if an atom map array is used, but not if an atom map hash is used; see the atom_modify command for details. If an atom map is not used (e.g. an atomic system with no bonds), and you don't care if unique atom IDs appear in dump files, then the atom-IDs can all be set to 0.

The molecule ID is a 2nd identifier attached to an atom. Normally, it is a number from 1 to N, identifying which molecule the atom belongs to. It can be 0 if it is an unbonded atom or if you don't care to keep track of molecule assignments.

The diameter specifies the size of a finite-size spherical particle. It can be set to 0.0, which means that atom is a point particle.

The ellipsoidflag, lineflag, triangleflag, and bodyflag determine whether the particle is a finite-size ellipsoid or line or triangle or body of finite size, or whether the particle is a point particle. Additional attributes must be defined for each ellipsoid, line, triangle, or body in the corresponding *Ellipsoids*, *Lines*, *Triangles*, or *Bodies* section.

The *template-index* and *template-atom* are only defined used by atom_style template. In this case the molecule command is used to define a molecule template which contains one or more molecules. If an atom belongs to one of those molecules, its *template-index* and *template-atom* are both set to positive integers; if not the values are both 0. The *template-index* is which molecule (1 to Nmols) the atom belongs to. The *template-atom* is which atom (1 to Natoms) within the molecule the atom is.

Some pair styles and fixes and computes that operate on finite-size particles allow for a mixture of finite-size and point particles. See the doc pages of individual commands for details.

For finite-size particles, the density is used in conjunction with the particle volume to set the mass of each particle as mass = density * volume. In this context, volume can be a 3d quantity (for spheres or ellipsoids), a 2d quantity (for triangles), or a 1d quantity (for line segments). If the volume is 0.0, meaning a point particle, then the density value is used as the mass. One exception is for the body atom style, in which case the mass of each particle (body or point particle) is specified explicitly. This is because the volume of the body is unknown.

For atom_style hybrid, following the 5 initial values (ID,type,x,y,z), specific values for each sub-style must be listed. The order of the sub-styles is the same as they were listed in the atom_style command. The sub-style specific values are those that are not the 5 standard ones (ID,type,x,y,z). For example, for the "charge" sub-style, a "q" value would appear. For the "full" sub-style, a "molecule-ID" and "q" would appear. These are listed in the same order they appear as listed above. Thus if

```
atom_style hybrid charge sphere
```

were used in the input script, each atom line would have these fields:

```
atom-ID atom-type x y z q diameter density
```

Note that if a non-standard value is defined by multiple sub-styles, it must appear mutliple times in the atom line. E.g. the atom line for atom_style hybrid dipole full would list "q" twice:

```
atom-ID atom-type x y z q mux muy myz molecule-ID q
```

Atom lines specify the (x,y,z) coordinates of atoms. These can be inside or outside the simulation box. When the data file is read, LAMMPS wraps coordinates outside the box back into the box for dimensions that are periodic. As discussed above, if an atom is outside the box in a non-periodic dimension, it will be lost.

LAMMPS always stores atom coordinates as values which are inside the simulation box. It also stores 3 flags which indicate which image of the simulation box (in each dimension) the atom would be in if its coordinates were unwrapped across periodic boundaries. An image flag of 0 means the atom is still inside the box when unwrapped. A value of 2 means add 2 box lengths to get the unwrapped coordinate. A value of -1 means subtract 1 box length to get the unwrapped coordinate. LAMMPS updates these flags as atoms cross periodic boundaries during the simulation. The dump command can output atom atom coordinates in wrapped or unwrapped form, as well as the 3 image flags.

In the data file, atom lines (all lines or none of them) can optionally list 3 trailing integer values (nx,ny,nz), which are used to initialize the atom's image flags. If nx,ny,nz values are not listed in the data file, LAMMPS initializes them to 0. Note that the image flags are immediately updated if an atom's coordinates need to wrapped back into the simulation box.

It is only important to set image flags correctly in a data file if a simulation model relies on unwrapped coordinates for some calculation; otherwise they can be left unspecified. Examples of LAMMPS commands that use unwrapped coordinates internally are as follows:

- Atoms in a rigid body (see fix rigid, fix rigid/small) must have consistent image flags, so that when the atoms are unwrapped, they are near each other, i.e. as a single body.
- If the replicate command is used to generate a larger system, image flags must be consistent for bonded atoms when the bond crosses a periodic boundary. I.e. the values of the image flags should be different by 1 (in the appropriate dimension) for the two atoms in such a bond.
- If you plan to dump image flags and perform post-analysis that will unwrap atom coordinates, it may be important that a continued run (restarted from a data file) begins with image flags that are consistent with the previous run.

Atom velocities and other atom quantities not defined above are set to 0.0 when the *Atoms* section is read. Velocities can be set later by a *Velocities* section in the data file or by a velocity or set command in the input script.

Bodies section:

- one or more lines per body
- first line syntax: atom-ID Ninteger Ndouble

```
Ninteger = # of integer quantities for this particle
Ndouble = # of floating-point quantities for this particle
```

- 0 or more integer lines with total of Ninteger values
- 0 or more double lines with total of Ndouble values
- example:

```
12 3 6
2 3 2
1.0 2.0 3.0 1.0 2.0 4.0
```

- example:

```
12 0 14
1.0 2.0 3.0 1.0 2.0 4.0 1.0
2.0 3.0 1.0 2.0 4.0 4.0 2.0
```

The *Bodies* section must appear if atom_style body is used and any atoms listed in the *Atoms* section have a bodyflag = 1. The number of bodies should be specified in the header section via the "bodies" keyword.

Each body can have a variable number of integer and/or floating-point values. The number and meaning of the values is defined by the body style, as described in the body doc page. The body style is given as an argument to the atom_style body command.

The Ninteger and Ndouble values determine how many integer and floating-point values are specified for this particle. Ninteger and Ndouble can be as large as needed and can be different for every body. Integer values are then listed next on subsequent lines. Lines are read one at a time until Ninteger values are read. Floating-point values follow on subsequent lines, Again lines are read one at a time until Ndouble values are read. Note that if there are no values of a particular type, no lines appear for that type.

The *Bodies* section must appear after the *Atoms* section.

Bond Coeffs section:

- one line per bond type
- line syntax: ID coeffs

```
ID = bond type (1-N)
coeffs = list of coeffs
```

- example:

```
4 250 1.49
```

The number and meaning of the coefficients are specific to the defined bond style. See the bond_style and bond_coeff commands for details. Coefficients can also be set via the bond_coeff command in the input script.

BondAngle Coeffs section:

- one line per angle type
- line syntax: ID coeffs

```
ID = angle type (1-N)
coeffs = list of coeffs (see class 2 section of angle_coeff)
```

BondBond Coeffs section:

- one line per angle type
- line syntax: ID coeffs

```
ID = angle type (1-N)
coeffs = list of coeffs (see class 2 section of angle_coeff)
```

BondBond13 Coeffs section:

- one line per dihedral type

- line syntax: ID coeffs

```
ID = dihedral type (1-N)
coeffs = list of coeffs (see class 2 section of dihedral_coeff)
```

Bonds section:

- one line per bond
- line syntax: ID type atom1 atom2

```
ID = bond number (1-Nbonds)
type = bond type (1-Nbondtype)
atom1,atom2 = IDs of 1st,2nd atoms in bond
```

- example:

```
12 3 17 29
```

The *Bonds* section must appear after the *Atoms* section. All values in this section must be integers (1, not 1.0).

Dihedral Coeffs section:

- one line per dihedral type
- line syntax: ID coeffs

```
ID = dihedral type (1-N)
coeffs = list of coeffs
```

- example:

```
3 0.6 1 0 1
```

The number and meaning of the coefficients are specific to the defined dihedral style. See the dihedral_style and dihedral_coeff commands for details. Coefficients can also be set via the dihedral_coeff command in the input script.

Dihedrals section:

- one line per dihedral
- line syntax: ID type atom1 atom2 atom3 atom4

```
ID = number of dihedral (1-Ndihedrals)
type = dihedral type (1-Ndihedraltype)
atom1,atom2,atom3,atom4 = IDs of 1st,2nd,3rd,4th atoms in dihedral
```

- example:

```
12 4 17 29 30 21
```

The 4 atoms are ordered linearly within the dihedral. The *Dihedrals* section must appear after the *Atoms* section. All values in this section must be integers (1, not 1.0).

Ellipsoids section:

- one line per ellipsoid
- line syntax: atom-ID shapex shapey shapez quatw quati quatj quatk

```
atom-ID = ID of atom which is an ellipsoid
shapex,shapey,shapez = 3 diameters of ellipsoid (distance units)
quatw,quati,quatj,quatk = quaternion components for orientation of atom
```

- example:

```
12 1 2 1 1 0 0 0
```

The *Ellipsoids* section must appear if atom_style ellipsoid is used and any atoms are listed in the *Atoms* section with an ellipsoidflag = 1. The number of ellipsoids should be specified in the header section via the "ellipsoids" keyword.

The 3 shape values specify the 3 diameters or aspect ratios of a finite-size ellipsoidal particle, when it is oriented along the 3 coordinate axes. They must all be non-zero values.

The values *quatw*, *quati*, *quatj*, and *quatk* set the orientation of the atom as a quaternion (4-vector). Note that the shape attributes specify the aspect ratios of an ellipsoidal particle, which is oriented by default with its x-axis along the simulation box's x-axis, and similarly for y and z. If this body is rotated (via the right-hand rule) by an angle theta around a unit vector (a,b,c), then the quaternion that represents its new orientation is given by (cos(theta/2), a*sin(theta/2), b*sin(theta/2), c*sin(theta/2)). These 4 components are quatw, quati, quatj, and quatk as specified above. LAMMPS normalizes each atom's quaternion in case (a,b,c) is not specified as a unit vector.

The *Ellipsoids* section must appear after the *Atoms* section.

EndBondTorsion Coeffs section:

- one line per dihedral type
- line syntax: ID coeffs

```
ID = dihedral type (1-N)
coeffs = list of coeffs (see class 2 section of dihedral_coeff)
```

Improper Coeffs section:

- one line per improper type
- line syntax: ID coeffs

```
ID = improper type (1-N)
coeffs = list of coeffs
```

- example:

```
2 20 0.0548311
```

The number and meaning of the coefficients are specific to the defined improper style. See the improper_style and improper_coeff commands for details. Coefficients can also be set via the improper_coeff command in the input script.

Impropers section:

- one line per improper
- line syntax: ID type atom1 atom2 atom3 atom4

```
ID = number of improper (1-Nimpropers)
type = improper type (1-Nimpropertype)
atom1,atom2,atom3,atom4 = IDs of 1st,2nd,3rd,4th atoms in improper
```

- example:

```
12 3 17 29 13 100
```

The ordering of the 4 atoms determines the definition of the improper angle used in the formula for each improper style. See the doc pages for individual styles for details.

The *Impropers* section must appear after the *Atoms* section. All values in this section must be integers (1, not 1.0).

Lines section:

- one line per line segment
- line syntax: atom-ID x1 y1 x2 y2

```
atom-ID = ID of atom which is a line segment
x1,y1 = 1st end point
x2,y2 = 2nd end point
```

- example:

```
12 1.0 0.0 2.0 0.0
```

The *Lines* section must appear if atom_style line is used and any atoms are listed in the *Atoms* section with a lineflag = 1. The number of lines should be specified in the header section via the "lines" keyword.

The 2 end points are the end points of the line segment. The ordering of the 2 points should be such that using a right-hand rule to cross the line segment with a unit vector in the +z direction, gives an "outward" normal vector perpendicular to the line segment. I.e. normal = (c2-c1) x (0,0,1). This orientation may be important for defining some interactions.

The *Lines* section must appear after the *Atoms* section.

Masses section:

- one line per atom type
- line syntax: ID mass

```
ID = atom type (1-N)
mass = mass value
```

- example:

```
3 1.01
```

This defines the mass of each atom type. This can also be set via the mass command in the input script. This section cannot be used for atom styles that define a mass for individual atoms - e.g. atom_style sphere.

MiddleBondTorsion Coeffs section:

- one line per dihedral type
- line syntax: ID coeffs

```
ID = dihedral type (1-N)
coeffs = list of coeffs (see class 2 section of dihedral_coeff)
```

Pair Coeffs section:

- one line per atom type
- line syntax: ID coeffs

```
ID = atom type (1-N)
coeffs = list of coeffs
```

- example:

```
3 0.022 2.35197 0.022 2.35197
```

The number and meaning of the coefficients are specific to the defined pair style. See the pair_style and pair_coeff commands for details. Since pair coefficients for types I != J are not specified, these will be generated automatically by the pair style's mixing rule. See the individual pair_style doc pages and the pair_modify mix command for details. Pair coefficients can also be set via the pair_coeff command in the input script.

PairIJ Coeffs section:

- one line per pair of atom types for all I,J with I <= J
- line syntax: ID1 ID2 coeffs

```
ID1 = atom type I = 1-N
ID2 = atom type J = I-N, with I <= J
coeffs = list of coeffs
```

- examples:

```
3 3 0.022 2.35197 0.022 2.35197
3 5 0.022 2.35197 0.022 2.35197
```

This section must have N*(N+1)/2 lines where N = # of atom types. The number and meaning of the coefficients are specific to the defined pair style. See the pair_style and pair_coeff commands for details. Since pair coefficients for types I != J are all specified, these values will turn off the default mixing rule defined by the pair style. See the individual pair_style doc pages and the pair_modify mix command for details. Pair coefficients can also be set via the pair_coeff command in the input script.

Triangles section:

- one line per triangle
- line syntax: atom-ID x1 y1 x2 y2

```
atom-ID = ID of atom which is a line segment
x1,y1,z1 = 1st corner point
x2,y2,z2 = 2nd corner point
x3,y3,z3 = 3rd corner point
```

- example:

```
12 0.0 0.0 0.0 2.0 0.0 1.0 0.0 2.0 1.0
```

The *Triangles* section must appear if atom_style tri is used and any atoms are listed in the *Atoms* section with a triangleflag = 1. The number of lines should be specified in the header section via the "triangles" keyword.

The 3 corner points are the corner points of the triangle. The ordering of the 3 points should be such that using a right-hand rule to go from point1 to point2 to point3 gives an "outward" normal vector to the face of the triangle. I.e. normal = (c2-c1) x (c3-c1). This orientation may be important for defining some interactions.

The *Triangles* section must appear after the *Atoms* section.

Velocities section:

- one line per atom
- line syntax: depends on atom style

all styles except those listed	atom-ID vx vy vz
electron	atom-ID vx vy vz ervel
ellipsoid	atom-ID vx vy vz lx ly lz
sphere	atom-ID vx vy vz wx wy wz
hybrid	atom-ID vx vy vz sub-style1 sub-style2 ...

where the keywords have these meanings:

vx,vy,vz = translational velocity of atom lx,ly,lz = angular momentum of aspherical atom wx,wy,wz = angular velocity of spherical atom ervel = electron radial velocity (0 for fixed-core):ul

The velocity lines can appear in any order. This section can only be used after an *Atoms* section. This is because the *Atoms* section must have assigned a unique atom ID to each atom so that velocities can be assigned to them.

Vx, vy, vz, and ervel are in units of velocity. Lx, ly, lz are in units of angular momentum (distance-velocity-mass). Wx, Wy, Wz are in units of angular velocity (radians/time).

For atom_style hybrid, following the 4 initial values (ID,vx,vy,vz), specific values for each sub-style must be listed. The order of the sub-styles is the same as they were listed in the atom_style command. The sub-style specific values are those that are not the 5 standard ones (ID,vx,vy,vz). For example, for the "sphere" sub-style, "wx", "wy", "wz" values would appear. These are listed in the same order they appear as listed above. Thus if

```
atom_style hybrid electron sphere
```

were used in the input script, each velocity line would have these fields:

```
atom-ID vx vy vz ervel wx wy wz
```

Translational velocities can also be set by the velocity command in the input script.

Restrictions:

To read gzipped data files, you must compile LAMMPS with the -DLAMMPS_GZIP option - see the Making LAMMPS section of the documentation.

Related commands:

read_dump, read_restart, create_atoms, write_data

Default:

The default for all the *extra* keywords is 0.

read_dump command

Syntax:

```
read_dump file Nstep field1 field2 ... keyword values ...
```

- file = name of dump file to read
- Nstep = snapshot timestep to read from file
- one or more fields may be appended

```
field = x or y or z or vx or vy or vz or q or ix or iy or iz
  x,y,z = atom coordinates
  vx,vy,vz = velocity components
  q = charge
  ix,iy,iz = image flags in each dimension
```

- zero or more keyword/value pairs may be appended
- keyword = *box* or *replace* or *purge* or *trim* or *add* or *label* or *scaled* or *wrapped* or *format*

```
box value = yes or no = replace simulation box with dump box
  replace value = yes or no = overwrite atoms with dump atoms
  purge value = yes or no = delete all atoms before adding dump atoms
  trim value = yes or no = trim atoms not in dump snapshot
  add value = yes or no = add new dump atoms to system
  label value = field column
    field = one of the listed fields or id or type
    column = label on corresponding column in dump file
  scaled value = yes or no = coords in dump file are scaled/unscaled
  wrapped value = yes or no = coords in dump file are wrapped/unwrapped
  format values = format of dump file, must be last keyword if used
    native = native LAMMPS dump file
    xyz = XYZ file
    molfile style path = VMD molfile plugin interface
      style = dcd or xyz or others supported by molfile plugins
      path = optional path for location of molfile plugins
```

Examples:

```
read_dump dump.file 5000 x y z
read_dump dump.xyz 5 x y z box no format xyz
read_dump dump.xyz 10 x y z box no format molfile xyz "../plugins"
read_dump dump.dcd 0 x y z box yes format molfile dcd
read_dump dump.file 1000 x y z vx vy vz box yes format molfile lammpstrj /usr/local/lib/vmd/plugins/
read_dump dump.file 5000 x y vx vy trim yes
read_dump ../run7/dump.file.gz 10000 x y z box yes
read_dump dump.xyz 10 x y z box no format molfile xyz ../plugins
read_dump dump.dcd 0 x y z format molfile dcd
read_dump dump.file 1000 x y z vx vy vz format molfile lammpstrj /usr/local/lib/vmd/plugins/LINUXAMD
```

Description:

Read atom information from a dump file to overwrite the current atom coordinates, and optionally the atom velocities and image flags and the simluation box dimensions. This is useful for restarting a run from a particular snapshot in a dump file. See the read_restart and read_data commands for alternative methods to do this. Also see the rerun command for a means of reading multiple snapshots from a dump file.

Note that a simulation box must already be defined before using the read_dump command. This can be done by the create_box, read_data, or read_restart commands. The read_dump command can reset the simulation box dimensions, as explained below.

Also note that reading per-atom information from a dump snapshot is limited to the atom coordinates, velocities and image flags, as explained below. Other atom properties, which may be necessary to run a valid simulation, such as atom charge, or bond topology information for a molecular system, are not read from (or even contained in) dump files. Thus this auxiliary information should be defined in the usual way, e.g. in a data file read in by a read_data command, before using the read_dump command, or by the set command, after the dump snapshot is read.

If the dump filename specified as *file* ends with ".gz", the dump file is read in gzipped format. You cannot (yet) read a dump file that was written in binary format with a ".bin" suffix, or to multiple files via the "%" option in the dump file name. See the dump command for details.

The format of the dump file is selected through the *format* keyword. If specified, it must be the last keyword used, since all remaining arguments are passed on to the dump reader. The *native* format is for native LAMMPS dump files, written with a dump atom or dump custom command. The *xyz* format is for generic XYZ formatted dump files. These formats take no additional values.

The *molfile* format supports reading data through using the VMD molfile plugin interface. This dump reader format is only available, if the USER-MOLFILE package has been installed when compiling LAMMPS.

The *molfile* format takes one or two additional values. The *style* value determines the file format to be used and can be any format that the molfile plugins support, such as DCD or XYZ. Note that DCD dump files can be written by LAMMPS via the dump dcd command. The *path* value specifies a list of directories which LAMMPS will search for the molfile plugins appropriate to the specified *style*. The syntax of the *path* value is like other search paths: it can contain multiple directories separated by a colon (or semi-colon on windows). The *path* keyword is optional and defaults to ".", i.e. the current directory.

Support for other dump format readers may be added in the future.

Global information is first read from the dump file, namely timestep and box information.

The dump file is scanned for a snapshot with a time stamp that matches the specified *Nstep*. This means the LAMMPS timestep the dump file snapshot was written on for the *native* format. Note that the *xyz* and *molfile* formats do not store the timestep. For these formats, timesteps are numbered logically, in a sequential manner, starting from 0. Thus to access the 10th snapshot in an *xyz* or *mofile* formatted dump file, use *Nstep* = 9.

The dimensions of the simulation box for the selected snapshot are also read; see the *box* keyword discussion below. For the *native* format, an error is generated if the snapshot is for a triclinic box and the current simulation box is orthogonal or vice versa. A warning will be generated if the snapshot box boundary conditions (periodic, shrink-wrapped, etc) do not match the current simulation boundary conditions, but the boundary condition information in the snapshot is otherwise ignored. See the "boundary" command for more details.

For the *xyz* format, no information about the box is available, so you must set the *box* flag to *no*. See details below.

For the *molfile* format, reading simulation box information is typically supported, but the location of the simulation box origin is lost and no explicit information about periodicity or orthogonal/triclinic box shape is available. The USER-MOLFILE package makes a best effort to guess based on heuristics, but this may not always work perfectly.

Per-atom information from the dump file snapshot is then read from the dump file snapshot. This corresponds to the specified *fields* listed in the read_dump command. It is an error to specify a z-dimension field, namely *z*, *vz*, or *iz*, for a 2d simulation.

For dump files in *native* format, each column of per-atom data has a text label listed in the file. A matching label for each field must appear, e.g. the label "vy" for the field *vy*. For the *x*, *y*, *z* fields any of the following labels are considered a match:

```
x, xs, xu, xsu for field x
y, ys, yu, ysu for field y
z, zs, zu, zsu for field z
```

The meaning of xs (scaled), xu (unwrapped), and xsu (scaled and unwrapped) is explained on the dump command doc page. These labels are searched for in the list of column labels in the dump file, in order, until a match is found.

The dump file must also contain atom IDs, with a column label of "id".

If the *add* keyword is specified with a value of *yes*, as discussed below, the dump file must contain atom types, with a column label of "type".

If a column label you want to read from the dump file is not a match to a specified field, the *label* keyword can be used to specify the specific column label from the dump file to associate with that field. An example is if a time-averaged coordinate is written to the dump file via the fix ave/atom command. The column will then have a label corresponding to the fix-ID rather than "x" or "xs". The *label* keyword can also be used to specify new column labels for fields *id* and *type*.

For dump files in *xyz* format, only the *x*, *y*, and *z* fields are supported. The dump file does not store atom IDs, so these are assigned consecutively to the atoms as they appear in the dump file, starting from 1. Thus you should insure that order of atoms is consistent from snapshot to snapshot in the the XYZ dump file. See the dump_modify sort command if the XYZ dump file was written by LAMMPS.

For dump files in *molfile* format, the *x*, *y*, *z*, *vx*, *vy*, and *vz* fields can be specified. However, not all molfile formats store velocities, or their respective plugins may not support reading of velocities. The molfile dump files do not store atom IDs, so these are assigned consecutively to the atoms as they appear in the dump file, starting from 1. Thus you should insure that order of atoms are consistent from snapshot to snapshot in the the molfile dump file. See the dump_modify sort command if the dump file was written by LAMMPS.

Information from the dump file snapshot is used to overwrite or replace properties of the current system. There are various options for how this is done, determined by the specified fields and optional keywords.

The timestep of the snapshot becomes the current timestep for the simulation. See the reset_timestep command if you wish to change this after the dump snapshot is read.

If the *box* keyword is specified with a *yes* value, then the current simulation box dimensions are replaced by the dump snapshot box dimensions. If the *box* keyword is specified with a *no* value, the current simulatoin box is unchanged.

If the *purge* keyword is specified with a *yes* value, then all current atoms in the system are deleted before any of the operations invoked by the *replace*, *trim*, or *add* keywords take place.

If the *replace* keyword is specified with a *yes* value, then atoms with IDs that are in both the current system and the dump snapshot have their properties overwritten by field values. If the *replace* keyword is specified with a *no* value, atoms with IDs that are in both the current system and the dump snapshot are not modified.

If the *trim* keyword is specified with a *yes* value, then atoms with IDs that are in the current system but not in the dump snapshot are deleted. These atoms are unaffected if the *trim* keyword is specified with a *no* value.

If the *add* keyword is specified with a *yes* value, then atoms with IDs that are in the dump snapshot, but not in the current system are added to the system. These dump atoms are ignored if the *add* keyword is specified with a *no* value.

Note that atoms added via the *add* keyword will have only the attributes read from the dump file due to the *field* arguments. If *x* or *y* or *z* is not specified as a field, a value of 0.0 is used for added atoms. Added atoms must have an atom type, so this value must appear in the dump file.

Any other attributes (e.g. charge or particle diameter for spherical particles) will be set to default values, the same as if the create_atoms command were used.

Note that atom IDs are not preserved for new dump snapshot atoms added via the *add* keyword. The procedure for assigning new atom IDS to added atoms is the same as is described for the create_atoms command.

Atom coordinates read from the dump file are first converted into unscaled coordinates, relative to the box dimensions of the snapshot. These coordinates are then be assigned to an existing or new atom in the current simulation. The coordinates will then be remapped to the simulation box, whether it is the original box or the dump snapshot box. If periodic boundary conditions apply, this means the atom will be remapped back into the simulation box if necessary. If shrink-wrap boundary conditions apply, the new coordinates may change the simulation box dimensions. If fixed boundary conditions apply, the atom will be lost if it is outside the simulation box.

For *native* format dump files, the 3 xyz image flags for an atom in the dump file are set to the corresponding values appearing in the dump file if the *ix*, *iy*, *iz* fields are specified. If not specified, the image flags for replaced atoms are not changed and image flags for new atoms are set to default values. If coordinates read from the dump file are in unwrapped format (e.g. *xu*) then the image flags for read-in atoms are also set to default values. The remapping procedure described in the previous paragraph will then change images flags for all atoms (old and new) if periodic boundary conditions are applied to remap an atom back into the simulation box.

NOTE: If you get a warning about inconsistent image flags after reading in a dump snapshot, it means one or more pairs of bonded atoms now have inconsistent image flags. As discussed in Section errors this may or may not cause problems for subsequent simulations, One way this can happen is if you read image flag fields from the dump file but do not also use the dump file box parameters.

LAMMPS knows how to compute unscaled and remapped coordinates for the snapshot column labels discussed above, e.g. *x*, *xs*, *xu*, *xsu*. If another column label is assigned to the *x* or *y* or *z* field via the *label* keyword, e.g. for coordinates output by the fix ave/atom command, then LAMMPS needs to know whether the coordinate information in the dump file is scaled and/or wrapped. This can be set via the *scaled* and *wrapped* keywords. Note that the value of the *scaled* and *wrapped* keywords is ignored for fields *x* or *y* or *z* if the *label* keyword is not used to assign a column label to that field.

The scaled/unscaled and wrapped/unwrapped setting must be identical for any of the *x*, *y*, *z* fields that are specified. Thus you cannot read *xs* and *yu* from the dump file. Also, if the dump file coordinates are scaled and the simulation box is triclinic, then all 3 of the *x*, *y*, *z* fields must be specified, since they are all needed to generate absolute, unscaled coordinates.

Restrictions:

To read gzipped dump files, you must compile LAMMPS with the -DLAMMPS_GZIP option - see the Making LAMMPS section of the documentation.

The *molfile* dump file formats are part of the USER-MOLFILE package. They are only enabled if LAMMPS was built with that packages. See the Making LAMMPS section for more info.

Related commands:

dump, dump molfile, read_data, read_restart, rerun

Default:

The option defaults are box = yes, replace = yes, purge = no, trim = no, add = no, scaled = no, wrapped = yes, and format = native.

read_restart command

Syntax:

```
read_restart file flag
```

- file = name of binary restart file to read in
- flag = remap (optional)

Examples:

```
read_restart save.10000
read_restart save.10000 remap
read_restart restart.*
read_restart restart.*.mpiio
read_restart poly.*.% remap
```

Description:

Read in a previously saved system configuration from a restart file. This allows continuation of a previous run. Details about what information is stored (and not stored) in a restart file is given below. Basically this operation will re-create the simulation box with all its atoms and their attributes as well as some related global settings, at the point in time it was written to the restart file by a previous simluation. The simulation box will be partitioned into a regular 3d grid of rectangular bricks, one per processor, based on the number of processors in the current simulation and the settings of the processors command. The partitioning can later be changed by the balance or fix balance commands.

NOTE: Normally, restart files are written by the restart or write_restart commands so that all atoms in the restart file are inside the simulation box. If this is not the case, the read_restart command will print an error that atoms were "lost" when the file is read. This error should be reported to the LAMMPS developers so the invalid writing of the restart file can be fixed. If you still wish to use the restart file, the optional *remap* flag can be appended to the read_restart command. This should avoid the error, by explicitly remapping each atom back into the simulation box, updating image flags for the atom appropriately.

Restart files are saved in binary format to enable exact restarts, meaning that the trajectories of a restarted run will precisely match those produced by the original run had it continued on.

Several things can prevent exact restarts due to round-off effects, in which case the trajectories in the 2 runs will slowly diverge. These include running on a different number of processors or changing certain settings such as those set by the newton or processors commands. LAMMPS will issue a warning in these cases.

Certain fixes will not restart exactly, though they should provide statistically similar results. These include fix shake and fix langevin.

Certain pair styles will not restart exactly, though they should provide statistically similar results. This is because the forces they compute depend on atom velocities, which are used at half-step values every timestep when forces are computed. When a run restarts, forces are initially evaluated with a full-step velocity, which is different than if the run had continued. These pair styles include granular pair styles, pair dpd, and pair lubricate.

If a restarted run is immediately different than the run which produced the restart file, it could be a LAMMPS bug, so consider reporting it if you think the behavior is wrong.

Because restart files are binary, they may not be portable to other machines. In this case, you can use the -restart command-line switch to convert a restart file to a data file.

Similar to how restart files are written (see the write_restart and restart commands), the restart filename can contain two wild-card characters. If a "*" appears in the filename, the directory is searched for all filenames that match the pattern where "*" is replaced with a timestep value. The file with the largest timestep value is read in. Thus, this effectively means, read the latest restart file. It's useful if you want your script to continue a run from where it left off. See the run command and its "upto" option for how to specify the run command so it doesn't need to be changed either.

If a "%" character appears in the restart filename, LAMMPS expects a set of multiple files to exist. The restart and write_restart commands explain how such sets are created. Read_restart will first read a filename where "%" is replaced by "base". This file tells LAMMPS how many processors created the set and how many files are in it. Read_restart then reads the additional files. For example, if the restart file was specified as save.% when it was written, then read_restart reads the files save.base, save.0, save.1, ... save.P-1, where P is the number of processors that created the restart file.

Note that P could be the total number of processors in the previous simulation, or some subset of those processors, if the *fileper* or *nfile* options were used when the restart file was written; see the restart and write_restart commands for details. The processors in the current LAMMPS simulation share the work of reading these files; each reads a roughly equal subset of the files. The number of processors which created the set can be different the number of processors in the current LAMMPS simulation. This can be a fast mode of input on parallel machines that support parallel I/O.

A restart file can also be read in parallel as one large binary file via the MPI-IO library, assuming it was also written with MPI-IO. MPI-IO is part of the MPI standard for versions 2.0 and above. Using MPI-IO requires two steps. First, build LAMMPS with its MPIIO package installed, e.g.

```
make yes-mpiio    # installs the MPIIO package
make g++          # build LAMMPS for your platform
```

Second, use a restart filename which contains ".mpiio". Note that it does not have to end in ".mpiio", just contain those characters. Unlike MPI-IO dump files, a particular restart file must be both written and read using MPI-IO.

Here is the list of information included in a restart file, which means these quantities do not need to be re-specified in the input script that reads the restart file, though you can redefine many of these settings after the restart file is read.

- units
- atom style and atom_modify settings id, map, sort
- comm style and comm_modify settings mode, cutoff, vel
- timestep
- simulation box size and shape and boundary settings
- atom group definitions
- per-type atom settings such as mass
- per-atom attributes including their group assignments and molecular topology attributes (bonds, angles, etc)
- force field styles (pair, bond, angle, etc)
- force field coefficients (pair, bond, angle, etc) in some cases (see below)
- pair_modify settings, except the compute option

- special_bonds settings

Here is a list of information not stored in a restart file, which means you must re-issue these commands in your input script, after reading the restart file.

- fix commands (see below)
- compute commands (see below)
- variable commands
- region commands
- neighbor list criteria including neigh_modify settings
- kspace_style and kspace_modify settings
- info for thermodynamic, dump, or restart output

Note that some force field styles (pair, bond, angle, etc) do not store their coefficient info in restart files. Typically these are many-body or tabulated potentials which read their parameters from separate files. In these cases you will need to re-specify the "pair pair_coeff, bond_coeff, etc commands in your restart input script. The doc pages for individual force field styles mention if this is the case. This is also true of pair_style hybrid (bond hybrid, angle hybrid, etc) commands; they do not store coefficient info.

As indicated in the above list, the fixes used for a simulation are not stored in the restart file. This means the new input script should specify all fixes it will use. However, note that some fixes store an internal "state" which is written to the restart file. This allows the fix to continue on with its calculations in a restarted simulation. To re-enable such a fix, the fix command in the new input script must use the same fix-ID and group-ID as was used in the input script that wrote the restart file. If a match is found, LAMMPS prints a message indicating that the fix is being re-enabled. If no match is found before the first run or minimization is performed by the new script, the "state" information for the saved fix is discarded. See the doc pages for individual fixes for info on which ones can be restarted in this manner.

Likewise, the computes used for a simulation are not stored in the restart file. This means the new input script should specify all computes it will use. However, some computes create a fix internally to store "state" information that persists from timestep to timestep. An example is the compute msd command which uses a fix to store a reference coordinate for each atom, so that a displacement can be calculated at any later time. If the compute command in the new input script uses the same compute-ID and group-ID as was used in the input script that wrote the restart file, then it will create the same fix in the restarted run. This means the re-created fix will be re-enabled with the stored state information as described in the previous paragraph, so that the compute can continue its calculations in a consistent manner.

Some pair styles, like the granular pair styles, also use a fix to store "state" information that persists from timestep to timestep. In the case of granular potentials, it is contact information between pairs of touching particles. This info will also be re-enabled in the restart script, assuming you re-use the same granular pair style.

LAMMPS allows bond interactions (angle, etc) to be turned off or deleted in various ways, which can affect how their info is stored in a restart file.

If bonds (angles, etc) have been turned off by the fix shake or delete_bonds command, their info will be written to a restart file as if they are turned on. This means they will need to be turned off again in a new run after the restart file is read.

Bonds that are broken (e.g. by a bond-breaking potential) are written to the restart file as broken bonds with a type of 0. Thus these bonds will still be broken when the restart file is read.

Bonds that have been broken by the fix bond/break command have disappeared from the system. No information

about these bonds is written to the restart file.

Restrictions:

To write and read restart files in parallel with MPI-IO, the MPIIO package must be installed.

Related commands:

read_data, read_dump, write_restart, restart

Default: none

region command

Syntax:

```
region ID style args keyword arg ...
```

- ID = user-assigned name for the region
- style = *delete* or *block* or *cone* or *cylinder* or *plane* or *prism* or *sphere* or *union* or *intersect*

```
  delete = no args
    block args = xlo xhi ylo yhi zlo zhi
      xlo,xhi,ylo,yhi,zlo,zhi = bounds of block in all dimensions (distance units)
    cone args = dim c1 c2 radlo radhi lo hi
      dim = x or y or z = axis of cone
      c1,c2 = coords of cone axis in other 2 dimensions (distance units)
      radlo,radhi = cone radii at lo and hi end (distance units)
      lo,hi = bounds of cone in dim (distance units)
    cylinder args = dim c1 c2 radius lo hi
      dim = x or y or z = axis of cylinder
      c1,c2 = coords of cylinder axis in other 2 dimensions (distance units)
      radius = cylinder radius (distance units)
        radius can be a variable (see below)
      lo,hi = bounds of cylinder in dim (distance units)
    plane args = px py pz nx ny nz
      px,py,pz = point on the plane (distance units)
      nx,ny,nz = direction normal to plane (distance units)
    prism args = xlo xhi ylo yhi zlo zhi xy xz yz
      xlo,xhi,ylo,yhi,zlo,zhi = bounds of untilted prism (distance units)
      xy = distance to tilt y in x direction (distance units)
      xz = distance to tilt z in x direction (distance units)
      yz = distance to tilt z in y direction (distance units)
    sphere args = x y z radius
      x,y,z = center of sphere (distance units)
      radius = radius of sphere (distance units)
        radius can be a variable (see below)
    union args = N reg-ID1 reg-ID2 ...
      N = # of regions to follow, must be 2 or greater
      reg-ID1,reg-ID2, ... = IDs of regions to join together
    intersect args = N reg-ID1 reg-ID2 ...
      N = # of regions to follow, must be 2 or greater
      reg-ID1,reg-ID2, ... = IDs of regions to intersect
```

- zero or more keyword/arg pairs may be appended
- keyword = *side* or *units* or *move* or *rotate*

```
  side value = in or out
      in = the region is inside the specified geometry
      out = the region is outside the specified geometry
    units value = lattice or box
      lattice = the geometry is defined in lattice units
      box = the geometry is defined in simulation box units
    move args = v_x v_y v_z
      v_x,v_y,v_z = equal-style variables for x,y,z displacement of region over time
    rotate args = v_theta Px Py Pz Rx Ry Rz
      v_theta = equal-style variable for rotaton of region over time (in radians)
      Px,Py,Pz = origin for axis of rotation (distance units)
      Rx,Ry,Rz = axis of rotation vector
```

- accelerated styles (with same args) = *block/kk*

Examples:

```
region 1 block -3.0 5.0 INF 10.0 INF INF
region 2 sphere 0.0 0.0 0.0 5 side out
region void cylinder y 2 3 5 -5.0 EDGE units box
region 1 prism 0 10 0 10 0 10 2 0 0
region outside union 4 side1 side2 side3 side4
region 2 sphere 0.0 0.0 0.0 5 side out move v_left v_up NULL
```

Description:

This command defines a geometric region of space. Various other commands use regions. For example, the region can be filled with atoms via the create_atoms command. Or a bounding box around the region, can be used to define the simulation box via the create_box command. Or the atoms in the region can be identified as a group via the group command, or deleted via the delete_atoms command. Or the surface of the region can be used as a boundary wall via the fix wall/region command.

Commands which use regions typically test whether an atom's position is contained in the region or not. For this purpose, coordinates exactly on the region boundary are considered to be interior to the region. This means, for example, for a spherical region, an atom on the sphere surface would be part of the region if the sphere were defined with the *side in* keyword, but would not be part of the region if it were defined using the *side out* keyword. See more details on the *side* keyword below.

Normally, regions in LAMMPS are "static", meaning their geometric extent does not change with time. If the *move* or *rotate* keyword is used, as described below, the region becomes "dynamic", meaning it's location or orientation changes with time. This may be useful, for example, when thermostatting a region, via the compute temp/region command, or when the fix wall/region command uses a region surface as a bounding wall on particle motion, i.e. a rotating container.

The *delete* style removes the named region. Since there is little overhead to defining extra regions, there is normally no need to do this, unless you are defining and discarding large numbers of regions in your input script.

The lo/hi values for *block* or *cone* or *cylinder* or *prism* styles can be specified as EDGE or INF. EDGE means they extend all the way to the global simulation box boundary. Note that this is the current box boundary; if the box changes size during a simulation, the region does not. INF means a large negative or positive number (1.0e20), so it should encompass the simulation box even if it changes size. If a region is defined before the simulation box has been created (via create_box or read_data or read_restart commands), then an EDGE or INF parameter cannot be used. For a *prism* region, a non-zero tilt factor in any pair of dimensions cannot be used if both the lo/hi values in either of those dimensions are INF. E.g. if the xy tilt is non-zero, then xlo and xhi cannot both be INF, nor can ylo and yhi.

NOTE: Regions in LAMMPS do not get wrapped across periodic boundaries, as specified by the boundary command. For example, a spherical region that is defined so that it overlaps a periodic boundary is not treated as 2 half-spheres, one on either side of the simulation box.

NOTE: Regions in LAMMPS are always 3d geometric objects, regardless of whether the dimension of a simulation is 2d or 3d. Thus when using regions in a 2d simulation, you should be careful to define the region so that its intersection with the 2d x-y plane of the simulation has the 2d geometric extent you want.

For style *cone*, an axis-aligned cone is defined which is like a *cylinder* except that two different radii (one at each end) can be defined. Either of the radii (but not both) can be 0.0.

For style *cone* and *cylinder*, the c1,c2 params are coordinates in the 2 other dimensions besides the cylinder axis

dimension. For dim = x, c1/c2 = y/z; for dim = y, c1/c2 = x/z; for dim = z, c1/c2 = x/y. Thus the third example above specifies a cylinder with its axis in the y-direction located at x = 2.0 and z = 3.0, with a radius of 5.0, and extending in the y-direction from -5.0 to the upper box boundary.

For style *plane*, a plane is defined which contain the point (px,py,pz) and has a normal vector (nx,ny,nz). The normal vector does not have to be of unit length. The "inside" of the plane is the half-space in the direction of the normal vector; see the discussion of the *side* option below.

For style *prism*, a parallelepiped is defined (it's too hard to spell parallelepiped in an input script!). The parallelepiped has its "origin" at (xlo,ylo,zlo) and is defined by 3 edge vectors starting from the origin given by A = (xhi-xlo,0,0); B = (xy,yhi-ylo,0); C = (xz,yz,zhi-zlo). *Xy,xz,yz* can be 0.0 or positive or negative values and are called "tilt factors" because they are the amount of displacement applied to faces of an originally orthogonal box to transform it into the parallelepiped.

A prism region that will be used with the create_box command to define a triclinic simulation box must have tilt factors (xy,xz,yz) that do not skew the box more than half the distance of corresponding the parallel box length. For example, if xlo = 2 and xhi = 12, then the x box length is 10 and the xy tilt factor must be between -5 and 5. Similarly, both xz and yz must be between -(xhi-xlo)/2 and +(yhi-ylo)/2. Note that this is not a limitation, since if the maximum tilt factor is 5 (as in this example), then configurations with tilt = ..., -15, -5, 5, 15, 25, ... are all geometrically equivalent.

The *radius* value for style *sphere* and *cylinder* can be specified as an equal-style variable. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated each timestep, and its value used to determine the radius of the region.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a time-dependent radius.

See Section_howto 12 of the doc pages for a geometric description of triclinic boxes, as defined by LAMMPS, and how to transform these parameters to and from other commonly used triclinic representations.

The *union* style creates a region consisting of the volume of all the listed regions combined. The *intersect* style creates a region consisting of the volume that is common to all the listed regions.

NOTE: The *union* and *intersect* regions operate by invoking methods from their list of sub-regions. Thus you cannot delete the sub-regions after defining the *union* or *intersection* region.

The *side* keyword determines whether the region is considered to be inside or outside of the specified geometry. Using this keyword in conjunction with *union* and *intersect* regions, complex geometries can be built up. For example, if the interior of two spheres were each defined as regions, and a *union* style with *side* = out was constructed listing the region-IDs of the 2 spheres, the resulting region would be all the volume in the simulation box that was outside both of the spheres.

The *units* keyword determines the meaning of the distance units used to define the region for any argument above listed as having distance units. It also affects the scaling of the velocity vector specfied with the *vel* keyword, the amplitude vector specified with the *wiggle* keyword, and the rotation point specified with the *rotate* keyword, since they each involve a distance metric.

A *box* value selects standard distance units as defined by the units command, e.g. Angstroms for units = real or metal. A *lattice* value means the distance units are in lattice spacings. The lattice command must have been previously used to define the lattice spacings which are used as follows:

- For style *block*, the lattice spacing in dimension x is applied to xlo and xhi, similarly the spacings in dimensions y,z are applied to ylo/yhi and zlo/zhi.
- For style *cone*, the lattice spacing in argument *dim* is applied to lo and hi. The spacings in the two radial dimensions are applied to c1 and c2. The two cone radii are scaled by the lattice spacing in the dimension corresponding to c1.
- For style *cylinder*, the lattice spacing in argument *dim* is applied to lo and hi. The spacings in the two radial dimensions are applied to c1 and c2. The cylinder radius is scaled by the lattice spacing in the dimension corresponding to c1.
- For style *plane*, the lattice spacing in dimension x is applied to px and nx, similarly the spacings in dimensions y,z are applied to py/ny and pz/nz.
- For style *prism*, the lattice spacing in dimension x is applied to xlo and xhi, similarly for ylo/yhi and zlo/zhi. The lattice spacing in dimension x is applied to xy and xz, and the spacing in dimension y to yz.
- For style *sphere*, the lattice spacing in dimensions x,y,z are applied to the sphere center x,y,z. The spacing in dimension x is applied to the sphere radius.

If the *move* or *rotate* keywords are used, the region is "dynamic", meaning its location or orientation changes with time. These keywords cannot be used with a *union* or *intersect* style region. Instead, the keywords should be used to make the individual sub-regions of the *union* or *intersect* region dynamic. Normally, each sub-region should be "dynamic" in the same manner (e.g. rotate around the same point), though this is not a requirement.

The *move* keyword allows one or more equal-style variables to be used to specify the x,y,z displacement of the region, typically as a function of time. A variable is specified as v_name, where name is the variable name. Any of the three variables can be specified as NULL, in which case no displacement is calculated in that dimension.

Note that equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. Thus it is easy to specify a region displacement that change as a function of time or spans consecutive runs in a continuous fashion. For the latter, see the *start* and *stop* keywords of the run command and the *elaplong* keyword of thermo_style custom for details.

For example, these commands would displace a region from its initial position, in the positive x direction, effectively at a constant velocity:

```
variable dx equal ramp(0,10)
region 2 sphere 10.0 10.0 0.0 5 move v_dx NULL NULL
```

Note that the initial displacemet is 0.0, though that is not required.

Either of these varaibles would "wiggle" the region back and forth in the y direction:

```
variable dy equal swiggle(0,5,100)
variable dysame equal 5*sin(2*PI*elaplong*dt/100)
region 2 sphere 10.0 10.0 0.0 5 move NULL v_dy NULL
```

The *rotate* keyword rotates the region around a rotation axis R = (Rx,Ry,Rz) that goes thru a point P = (Px,Py,Pz). The rotation angle is calculated, presumably as a function of time, by a variable specified as v_theta, where theta is the variable name. The variable should generate its result in radians. The direction of rotation for the region around the rotation axis is consistent with the right-hand rule: if your right-hand thumb points along R, then your fingers wrap around the axis in the direction of rotation.

The *move* and *rotate* keywords can be used together. In this case, the displacement specified by the *move* keyword is applied to the P point of the *rotate* keyword.

Styles with a *kk* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed in Section_accelerate of the manual. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

The code using the region (such as a fix or compute) must also be supported by Kokkos or no acceleration will occur. Currently, only *block* style regions are supported by Kokkos.

These accelerated styles are part of the Kokkos package. They are only enabled if LAMMPS was built with that package. See the Making LAMMPS section for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

A prism cannot be of 0.0 thickness in any dimension; use a small z thickness for 2d simulations. For 2d simulations, the xz and yz parameters must be 0.0.

Related commands:

lattice, create_atoms, delete_atoms, group

Default:

The option defaults are side = in, units = lattice, and no move or rotation.

replicate command

Syntax:

```
replicate nx ny nz
```

- nx,ny,nz = replication factors in each dimension

Examples:

```
replicate 2 3 2
```

Description:

Replicate the current simulation one or more times in each dimension. For example, replication factors of 2,2,2 will create a simulation with 8x as many atoms by doubling the simulation domain in each dimension. A replication factor of 1 in a dimension leaves the simulation domain unchanged. When the new simulation box is created it is also partitioned into a regular 3d grid of rectangular bricks, one per processor, based on the number of processors being used and the settings of the processors command. The partitioning can later be changed by the balance or fix balance commands.

All properties of the atoms are replicated, including their velocities, which may or may not be desirable. New atom IDs are assigned to new atoms, as are molecule IDs. Bonds and other topology interactions are created between pairs of new atoms as well as between old and new atoms. This is done by using the image flag for each atom to "unwrap" it out of the periodic box before replicating it.

This means that any molecular bond you specify in the original data file that crosses a periodic boundary should be between two atoms with image flags that differ by 1. This will allow the bond to be unwrapped appropriately.

Restrictions:

A 2d simulation cannot be replicated in the z dimension.

If a simulation is non-periodic in a dimension, care should be used when replicating it in that dimension, as it may put atoms nearly on top of each other.

NOTE: You cannot use the replicate command on a system which has a molecule that spans the box and is bonded to itself across a periodic boundary, so that the molecule is efffectively a loop. A simple example would be a linear polymer chain that spans the simulation box and bonds back to itself across the periodic boundary. More realistic examples would be a CNT (meant to be an infinitely long CNT) or a graphene sheet or a bulk periodic crystal where there are explicit bonds specified between near neighbors. (Note that this only applies to systems that have permanent bonds as specified in the data file. A CNT that is just atoms modeled with the AIREBO potential has no such permanent bonds, so it can be replicated.) The reason replication does not work with those systems is that the image flag settings described above cannot be made consistent. I.e. it is not possible to define images flags so that when every pair of bonded atoms is unwrapped (using the image flags), they will be close to each other. The only way the replicate command could work in this scenario is for it to break a bond, insert more atoms, and re-connect the loop for the larger simulation box. But it is not clever enough to do this. So you will have to construct a larger version of your molecule as a pre-processing step and input a new data file to LAMMPS.

If the current simulation was read in from a restart file (before a run is performed), there can have been no fix information stored in the file for individual atoms. Similarly, no fixes can be defined at the time the replicate command is used that require vectors of atom information to be stored. This is because the replicate command does not know how to replicate that information for new atoms it creates.

Replicating a system that has rigid bodies (defined via the fix rigid command), either currently defined or that created the restart file which was read in before replicating, can cause problems if there is a bond between a pair of rigid bodies that straddle a periodic boundary. This is because the periodic image information for particles in the rigid bodies are set differently than for a non-rigid system and can result in a new bond being created that spans the periodic box. Thus you cannot use the replicate command in this scenario.

Related commands: none

Default: none

rerun command

Syntax:

```
rerun file1 file2 ... keyword args ...
```

- file1,file2,... = dump file(s) to read
- one or more keywords may be appended, keyword *dump* must appear and be last

```
keyword = first or last or every or skip or start or stop or dump
 first args = Nfirts
   Nfirst = dump timestep to start on
 last args = Nlast
   Nlast = dumptimestep to stop on
 every args = Nevery
   Nevery = read snapshots matching every this many timesteps
 skip args = Nskip
   Nskip = read one out of every Nskip snapshots
 start args = Nstart
   Nstart = timestep on which pseudo run will start
 stop args = Nstop
   Nstop = timestep to which pseudo run will end
 dump args = same as read_dump command starting with its field arguments
```

Examples:

```
rerun dump.file dump x y z vx vy vz
rerun dump1.txt dump2.txt first 10000 every 1000 dump x y z
rerun dump.vels dump x y z vx vy vz box yes format molfile lammpstrj
rerun dump.dcd dump x y z box no format molfile dcd
rerun ../run7/dump.file.gz skip 2 dump x y z box yes
```

Description:

Perform a psuedo simulation run where atom information is read one snapshot at a time from a dump file(s), and energies and forces are computed on the shapshot to produce thermodynamic or other output.

This can be useful in the following kinds of scenarios, after an initial simulation produced the dump file:

- Compute the energy and forces of snaphots using a different potential.
- Calculate one or more diagnostic quantities on the snapshots that weren't computed in the initial run. These can also be computed with settings not used in the initial run, e.g. computing an RDF via the compute rdf command with a longer cutoff than was used initially.
- Calculate the portion of per-atom forces resulting from a subset of the potential. E.g. compute only Coulombic forces. This can be done by only defining only a Coulombic pair style in the rerun script. Doing this in the original script would result in different (bad) dynamics.

Conceptually, using the rerun command is like running an input script that has a loop in it (see the next and jump commands). Each iteration of the loop reads one snapshot from the dump file via the read_dump command, sets the timestep to the appropriate value, and then invokes a run command for zero timesteps to simply compute energy and forces, and any other thermodynamic output or diagnostic info you have defined. This computation also invokes any fixes you have defined that apply constraints to the system, such as fix shake or fix indent.

Note that a simulation box must already be defined before using the rerun command. This can be done by the create_box, read_data, or read_restart commands.

Also note that reading per-atom information from dump snapshots is limited to the atom coordinates, velocities and image flags as explained in the read_dump command. Other atom properties, which may be necessary to compute energies and forces, such as atom charge, or bond topology information for a molecular system, are not read from (or even contained in) dump files. Thus this auxiliary information should be defined in the usual way, e.g. in a data file read in by a read_data command, before using the rerun command.

If more than one dump file is specified, the dump files are read one after the other. It is assumed that snapshot timesteps will be in ascending order. If a snapshot is encountered that is not in ascending order, it will cause the rerun command to complete.

The *first*, *last*, *every*, *skip* keywords determine which snapshots are read from the dump file(s). Snapshots are skipped until they have a timestamp >= *Nfirst*. When a snapshot with a timestamp > *Nlast* is encountered, the rerun command finishes. Note below that the defaults for *first* and *last* are to read all snapshots. If the *every* keyword is set to a value > 0, then only snapshots with timestamps that are a multiple of *Nevery* are read (the first snapshot is always read). If *Nevery* = 0, then this criterion is ignored, i.e. every snapshot is read that meets the other criteria. If the *skip* keyword is used, then after the first snapshot is read, every Nth snapshot is read, where N = *Nskip*. E.g. if *Nskip* = 3, then only 1 out of every 3 snapshots is read, assuming the snapshot timestamp is also consistent with the other criteria.

The *start* and *stop* keywords do not affect which snapshots are read from the dump file(s). Rather, they have the same meaning that they do for the run command. They only need to be defined if (a) you are using a fix command that changes some value over time, and (b) you want the reference point for elapsed time (from start to stop) to be different than the *first* and *last* settings. See the doc page for individual fixes to see which ones can be used with the *start/stop* keywords. Note that if you define neither of the *start*/*stop* or *first*/*last* keywords, then LAMMPS treats the pseudo run as going from 0 to a huge value (effectively infinity). This means that any quantity that a fix scales as a fraction of elapsed time in the run, will essentially remain at its intiial value. Also note that an error will occur if you read a snapshot from the dump file with a timestep value larger than the *stop* setting you have specified.

The *dump* keyword is required and must be the last keyword specified. Its arguments are passed internally to the read_dump command. The first argument following the *dump* keyword should be the *field1* argument of the read_dump command. See the read_dump doc page for details on the various options it allows for extracting information from the dump file snapshots, and for using that information to alter the LAMMPS simulation.

In general, a LAMMPS input script that uses a rerun command can include and perform all the usual operations of an input script that uses the run command. There are a few exceptions and points to consider, as discussed here.

Fixes that perform time integration, such as fix nve or fix npt are not invoked, since no time integration is performed. Fixes that perturb or constrain the forces on atoms will be invoked, just as they would during a normal run. Examples are fix indent and fix langevin. So you should think carefully as to whether that makes sense for the manner in which you are reprocessing the dump snapshots.

If you only want the rerun script to perform analyses that do not involve pair interactions, such as use compute msd to calculated displacements over time, you do not need to define a pair style, which may also mean neighbor lists will not need to be calculated which saves time. The comm_modify cutoff command can also be used to insure ghost atoms are acquired from far enough away for operations like bond and angle evaluations, if no pair style is being used.

Every time a snapshot is read, the timestep for the simulation is reset, as if the reset_timestep command were used. This command has some restrictions as to what fixes can be defined. See its doc page for details. For example, the fix deposit and fix dt/reset fixes are in this category. They also make no sense to use with a rerun command.

If time-averaging fixes like fix ave/time are used, they are invoked on timesteps that are a function of their *Nevery*, *Nrepeat*, and *Nfreq* settings. As an example, see the fix ave/time doc page for details. You must insure those settings are consistent with the snapshot timestamps that are read from the dump file(s). If an averaging fix is not invoked on a timestep it expects to be, LAMMPS will flag an error.

The various forms of LAMMPS output, as defined by the thermo_style, thermo, dump, and restart commands occur on specific timesteps. If successvive dump snapshots skip those timesteps, then no output will be produced. E.g. if you request thermodynamic output every 100 steps, but the dump file snapshots are every 1000 steps, then you will only see thermodynamic output every 1000 steps.

Restrictions:

To read gzipped dump files, you must compile LAMMPS with the -DLAMMPS_GZIP option - see the Making LAMMPS section of the documentation.

Related commands:

read_dump

Default:

The option defaults are first = 0, last = a huge value (effectively infinity), start = same as first, stop = same as last, every = 0, skip = 1;

reset_timestep command

Syntax:

```
reset_timestep N
```

- N = timestep number

Examples:

```
reset_timestep 0
reset_timestep 4000000
```

Description:

Set the timestep counter to the specified value. This command normally comes after the timestep has been set by reading a restart file via the read_restart command, or a previous simulation advanced the timestep.

The read_data and create_box commands set the timestep to 0; the read_restart command sets the timestep to the value it had when the restart file was written.

Restrictions: none

This command cannot be used when any fixes are defined that keep track of elapsed time to perform certain kinds of time-dependent operations. Examples are the fix deposit and fix dt/reset commands. The former adds atoms on specific timesteps. The latter keeps track of accumulated time.

Various fixes use the current timestep to calculate related quantities. If the timestep is reset, this may produce unexpected behavior, but LAMMPS allows the fixes to be defined even if the timestep is reset. For example, commands which thermostat the system, e.g. fix nvt, allow you to specify a target temperature which ramps from Tstart to Tstop which may persist over several runs. If you change the timestep, you may induce an instantaneous change in the target temperature.

Resetting the timestep clears flags for computes that may have calculated some quantity from a previous run. This means these quantity cannot be accessed by a variable in between runs until a new run is performed. See the variable command for more details.

Related commands:

rerun

Default: none

restart command

Syntax:

```
restart 0
restart N root keyword value ...
restart N file1 file2 keyword value ...
```

- N = write a restart file every this many timesteps
- N can be a variable (see below)
- root = filename to which timestep # is appended
- file1,file2 = two full filenames, toggle between them when writing file
- zero or more keyword/value pairs may be appended
- keyword = *fileper* or *nfile*

```
fileper arg = Np
    Np = write one file for every this many processors
  nfile arg = Nf
    Nf = write this many files, one from each of Nf processors
```

Examples:

```
restart 0
restart 1000 poly.restart
restart 1000 poly.restart.mpiio
restart 1000 restart.*.equil
restart 10000 poly.%.1 poly.%.2 nfile 10
restart v_mystep poly.restart
```

Description:

Write out a binary restart file with the current state of the simulation every so many timesteps, in either or both of two modes, as a run proceeds. A value of 0 means do not write out any restart files. The two modes are as follows. If one filename is specified, a series of filenames will be created which include the timestep in the filename. If two filenames are specified, only 2 restart files will be created, with those names. LAMMPS will toggle between the 2 names as it writes successive restart files.

Note that you can specify the restart command twice, once with a single filename and once with two filenames. This would allow you, for example, to write out archival restart files every 100000 steps using a single filenname, and more frequent temporary restart files every 1000 steps, using two filenames. Using restart 0 will turn off both modes of output.

Similar to dump files, the restart filename(s) can contain two wild-card characters.

If a "*" appears in the single filename, it is replaced with the current timestep value. This is only recognized when a single filename is used (not when toggling back and forth). Thus, the 3rd example above creates restart files as follows: restart.1000.equil, restart.2000.equil, etc. If a single filename is used with no "*", then the timestep value is appended. E.g. the 2nd example above creates restart files as follows: poly.restart.1000, poly.restart.2000, etc.

If a "%" character appears in the restart filename(s), then one file is written for each processor and the "%" character is replaced with the processor ID from 0 to P-1. An additional file with the "%" replaced by "base" is also written, which contains global information. For example, the files written on step 1000 for filename restart.%

would be restart.base.1000, restart.0.1000, restart.1.1000, ..., restart.P-1.1000. This creates smaller files and can be a fast mode of output and subsequent input on parallel machines that support parallel I/O. The optional *fileper* and *nfile* keywords discussed below can alter the number of files written.

The restart file can also be written in parallel as one large binary file via the MPI-IO library, which is part of the MPI standard for versions 2.0 and above. Using MPI-IO requires two steps. First, build LAMMPS with its MPIIO package installed, e.g.

```
make yes-mpiio    # installs the MPIIO package
make g++          # build LAMMPS for your platform
```

Second, use a restart filename which contains ".mpiio". Note that it does not have to end in ".mpiio", just contain those characters. Unlike MPI-IO dump files, a particular restart file must be both written and read using MPI-IO.

Restart files are written on timesteps that are a multiple of N but not on the first timestep of a run or minimization. You can use the write_restart command to write a restart file before a run begins. A restart file is not written on the last timestep of a run unless it is a multiple of N. A restart file is written on the last timestep of a minimization if N > 0 and the minimization converges.

Instead of a numeric value, N can be specifed as an equal-style variable, which should be specified as v_name, where name is the variable name. In this case, the variable is evaluated at the beginning of a run to determine the next timestep at which a restart file will be written out. On that timestep, the variable will be evaluated again to determine the next timestep, etc. Thus the variable should return timestep values. See the stagger() and logfreq() and stride() math functions for equal-style variables, as examples of useful functions to use in this context. Other similar math functions could easily be added as options for equal-style variables.

For example, the following commands will write restart files every step from 1100 to 1200, and could be useful for debugging a simulation where something goes wrong at step 1163:

```
variable        s equal stride(1100,1200,1)
restart         v_s tmp.restart
```

See the read_restart command for information about what is stored in a restart file.

Restart files can be read by a read_restart command to restart a simulation from a particular state. Because the file is binary (to enable exact restarts), it may not be readable on another machine. In this case, you can use the -r command-line switch to convert a restart file to a data file.

NOTE: Although the purpose of restart files is to enable restarting a simulation from where it left off, not all information about a simulation is stored in the file. For example, the list of fixes that were specified during the initial run is not stored, which means the new input script must specify any fixes you want to use. Even when restart information is stored in the file, as it is for some fixes, commands may need to be re-specified in the new input script, in order to re-use that information. See the read_restart command for information about what is stored in a restart file.

The optional *nfile* or *fileper* keywords can be used in conjunction with the "%" wildcard character in the specified restart file name(s). As explained above, the "%" character causes the restart file to be written in pieces, one piece for each of P processors. By default P = the number of processors the simulation is running on. The *nfile* or *fileper* keyword can be used to set P to a smaller value, which can be more efficient when running on a large number of processors.

The *nfile* keyword sets P to the specified Nf value. For example, if Nf = 4, and the simulation is running on 100 processors, 4 files will be written, by processors 0,25,50,75. Each will collect information from itself and the next

24 processors and write it to a restart file.

For the *fileper* keyword, the specified value of Np means write one file for every Np processors. For example, if Np = 4, every 4th processor (0,4,8,12,etc) will collect information from itself and the next 3 processors and write it to a restart file.

Restrictions:

To write and read restart files in parallel with MPI-IO, the MPIIO package must be installed.

Related commands:

write_restart, read_restart

Default:

```
restart 0
```

run command

Syntax:

```
run N keyword values ...
```

- N = # of timesteps
- zero or more keyword/value pairs may be appended
- keyword = *upto* or *start* or *stop* or *pre* or *post* or *every*

```
  upto value = none
    start value = N1
      N1 = timestep at which 1st run started
    stop value = N2
      N2 = timestep at which last run will end
    pre value = no or yes
    post value = no or yes
    every values = M c1 c2 ...
      M = break the run into M-timestep segments and invoke one or more commands between each se
      c1,c2,...,cN = one or more LAMMPS commands, each enclosed in quotes
      c1 = NULL means no command will be invoked
```

Examples:

```
run 10000
run 1000000 upto
run 100 start 0 stop 1000
run 1000 pre no post yes
run 100000 start 0 stop 1000000 every 1000 "print 'Protein Rg = $r'"
run 100000 every 1000 NULL
```

Description:

Run or continue dynamics for a specified number of timesteps.

When the run style is *respa*, N refers to outer loop (largest) timesteps.

A value of N = 0 is acceptable; only the thermodynamics of the system are computed and printed without taking a timestep.

The *upto* keyword means to perform a run starting at the current timestep up to the specified timestep. E.g. if the current timestep is 10,000 and "run 100000 upto" is used, then an additional 90,000 timesteps will be run. This can be useful for very long runs on a machine that allocates chunks of time and terminate your job when time is exceeded. If you need to restart your script multiple times (reading in the last restart file), you can keep restarting your script with the same run command until the simulation finally completes.

The *start* or *stop* keywords can be used if multiple runs are being performed and you want a fix command that changes some value over time (e.g. temperature) to make the change across the entire set of runs and not just a single run. See the doc page for individual fixes to see which ones can be used with the *start/stop* keywords.

For example, consider this fix followed by 10 run commands:

```
fix          1 all nvt 200.0 300.0 1.0
run          1000 start 0 stop 10000
```

```
run          1000 start 0 stop 10000
...
run          1000 start 0 stop 10000
```

The NVT fix ramps the target temperature from 200.0 to 300.0 during a run. If the run commands did not have the start/stop keywords (just "run 1000"), then the temperature would ramp from 200.0 to 300.0 during the 1000 steps of each run. With the start/stop keywords, the ramping takes place over the 10000 steps of all runs together.

The *pre* and *post* keywords can be used to streamline the setup, clean-up, and associated output to the screen that happens before and after a run. This can be useful if you wish to do many short runs in succession (e.g. LAMMPS is being called as a library which is doing other computations between successive short LAMMPS runs).

By default (pre and post = yes), LAMMPS creates neighbor lists, computes forces, and imposes fix constraints before every run. And after every run it gathers and prints timings statistics. If a run is just a continuation of a previous run (i.e. no settings are changed), the initial computation is not necessary; the old neighbor list is still valid as are the forces. So if *pre* is specified as "no" then the initial setup is skipped, except for printing thermodynamic info. Note that if *pre* is set to "no" for the very 1st run LAMMPS performs, then it is overridden, since the initial setup computations must be done.

NOTE: If your input script changes the system between 2 runs, then the initial setup must be performed to insure the change is recognized by all parts of the code that are affected. Examples are adding a fix or dump or compute, changing a neighbor list parameter, or writing restart file which can migrate atoms between processors. LAMMPS has no easy way to check if this has happened, but it is an error to use the *pre no* option in this case.

If *post* is specified as "no", the full timing summary is skipped; only a one-line summary timing is printed.

The *every* keyword provides a means of breaking a LAMMPS run into a series of shorter runs. Optionally, one or more LAMMPS commands (c1, c2, ..., cN) will be executed in between the short runs. If used, the *every* keyword must be the last keyword, since it has a variable number of arguments. Each of the trailing arguments is a single LAMMPS command, and each command should be enclosed in quotes, so that the entire command will be treated as a single argument. This will also prevent any variables in the command from being evaluated until it is executed multiple times during the run. Note that if a command itself needs one of its arguments quoted (e.g. the print command), then you can use a combination of single and double quotes, as in the example above or below.

The *every* keyword is a means to avoid listing a long series of runs and interleaving commands in your input script. For example, a print command could be invoked or a fix could be redefined, e.g. to reset a thermostat temperature. Or this could be useful for invoking a command you have added to LAMMPS that wraps some other code (e.g. as a library) to perform a computation periodically during a long LAMMPS run. See this section of the documentation for info about how to add new commands to LAMMPS. See this section of the documentation for ideas about how to couple LAMMPS to other codes.

With the *every* option, N total steps are simulated, in shorter runs of M steps each. After each M-length run, the specified commands are invoked. If only a single command is specified as NULL, then no command is invoked. Thus these lines:

```
variable q equal x[100]
run 6000 every 2000 "print 'Coord = $q'"
```

are the equivalent of:

```
variable q equal x[100]
run 2000
print "Coord = $q"
run 2000
```

```
print "Coord = $q"
run 2000
print "Coord = $q"
```

which does 3 runs of 2000 steps and prints the x-coordinate of a particular atom between runs. Note that the variable "$q" will be evaluated afresh each time the print command is executed.

Note that by using the line continuation character "&", the run every command can be spread across many lines, though it is still a single command:

```
run 100000 every 1000 &
  "print 'Minimum value = $a'" &
  "print 'Maximum value = $b'" &
  "print 'Temp = $c'" &
  "print 'Press = $d'"
```

If the *pre* and *post* options are set to "no" when used with the *every* keyword, then the 1st run will do the full setup and the last run will print the full timing summary, but these operations will be skipped for intermediate runs.

NOTE: You might hope to specify a command that exits the run by jumping out of the loop, e.g.

```
variable t equal temp
run 10000 every 100 "if '$t <300.0' then 'jump SELF afterrun'"
```

Unfortunately this will not currently work. The run command simply executes each command one at a time each time it pauses, then continues the run. You can replace the jump command with a simple quit command and cause LAMMPS to exit during the middle of a run when the condition is met.

Restrictions:

When not using the *upto* keyword, the number of specified timesteps N must fit in a signed 32-bit integer, so you are limited to slightly more than 2 billion steps (2^31) in a single run. When using *upto*, N can be larger than a signed 32-bit integer, however the difference between N and the current timestep must still be no larger than 2^31 steps.

However, with or without the *upto* keyword, you can perform successive runs to run a simulation for any number of steps (ok, up to 2^63 total steps). I.e. the timestep counter within LAMMPS is a 64-bit signed integer.

Related commands:

minimize, run_style, temper

Default:

The option defaults are start = the current timestep, stop = current timestep + N, pre = yes, and post = yes.

run_style command

Syntax:

```
run_style style args
```

- style = *verlet* or *verlet/split* or *respa* or *respa/omp*

```
  verlet args = none
    verlet/split args = none
    respa args = N n1 n2 ... keyword values ...
      N = # of levels of rRESPA
      n1, n2, ... = loop factor between rRESPA levels (N-1 values)
      zero or more keyword/value pairings may be appended to the loop factors
      keyword = bond or angle or dihedral or improper or
        pair or inner or middle or outer or hybrid or kspace
        bond value = M
          M = which level (1-N) to compute bond forces in
        angle value = M
          M = which level (1-N) to compute angle forces in
        dihedral value = M
          M = which level (1-N) to compute dihedral forces in
        improper value = M
          M = which level (1-N) to compute improper forces in
        pair value = M
          M = which level (1-N) to compute pair forces in
        inner values = M cut1 cut2
          M = which level (1-N) to compute pair inner forces in
          cut1 = inner cutoff between pair inner and
                 pair middle or outer  (distance units)
          cut2 = outer cutoff between pair inner and
                 pair middle or outer  (distance units)
        middle values = M cut1 cut2
          M = which level (1-N) to compute pair middle forces in
          cut1 = inner cutoff between pair middle and pair outer (distance units)
          cut2 = outer cutoff between pair middle and pair outer (distance units)
        outer value = M
          M = which level (1-N) to compute pair outer forces in
        hybrid values = M1 M2 ... (as many values as there are hybrid sub-styles
          M1 = which level (1-N) to compute the first pair_style hybrid sub-style in
          M2 = which level (1-N) to compute the second pair_style hybrid sub-style in
          M3,etc
        kspace value = M
          M = which level (1-N) to compute kspace forces in
```

Examples:

```
run_style verlet
run_style respa 4 2 2 2 bond 1 dihedral 2 pair 3 kspace 4
run_style respa 4 2 2 2 bond 1 dihedral 2 inner 3 5.0 6.0 outer 4 kspace 4

run_style respa 3 4 2 bond 1 hybrid 2 2 1 kspace 3
```

Description:

Choose the style of time integrator used for molecular dynamics simulations performed by LAMMPS.

The *verlet* style is a standard velocity-Verlet integrator.

The *verlet/split* style is also a velocity-Verlet integrator, but it splits the force calculation within each timestep over 2 partitions of processors. See Section_start 6 for an explanation of the -partition command-line switch.

Specifically, this style performs all computation except the kspace_style portion of the force field on the 1st partition. This include the pair style, bond style, neighbor list building, fixes including time intergration, and output. The kspace_style portion of the calculation is performed on the 2nd partition.

This is most useful for the PPPM kspace_style when its performance on a large number of processors degrades due to the cost of communication in its 3d FFTs. In this scenario, splitting your P total processors into 2 subsets of processors, P1 in the 1st partition and P2 in the 2nd partition, can enable your simulation to run faster. This is because the long-range forces in PPPM can be calculated at the same time as pair-wise and bonded forces are being calculated, and the FFTs can actually speed up when running on fewer processors.

To use this style, you must define 2 partitions where P1 is a multiple of P2. Typically having P1 be 3x larger than P2 is a good choice. The 3d processor layouts in each partition must overlay in the following sense. If P1 is a Px1 by Py1 by Pz1 grid, and P2 = Px2 by Py2 by Pz2, then Px1 must be an integer multiple of Px2, and similarly for Py1 a multiple of Py2, and Pz1 a multiple of Pz2.

Typically the best way to do this is to let the 1st partition choose its onn optimal layout, then require the 2nd partition's layout to match the integer multiple constraint. See the processors command with its *part* keyword for a way to control this, e.g.

```
procssors * * * part 1 2 multiple
```

You can also use the partition command to explicitly specity the processor layout on each partition. E.g. for 2 partitions of 60 and 15 processors each:

```
partition yes 1 processors 3 4 5
partition yes 2 processors 3 1 5
```

When you run in 2-partition mode with the *verlet/split* style, the thermodyanmic data for the entire simulation will be output to the log and screen file of the 1st partition, which are log.lammps.0 and screen.0 by default; see the "-plog and -pscreen command-line switches"Section_start.html#start_7 to change this. The log and screen file for the 2nd partition will not contain thermodynamic output beyone the 1st timestep of the run.

See Section_accelerate of the manual for performance details of the speed-up offered by the *verlet/split* style. One important performance consideration is the assignemnt of logical processors in the 2 partitions to the physical cores of a parallel machine. The processors command has options to support this, and strategies are discussed in Section_accelerate of the manual.

The *respa* style implements the rRESPA multi-timescale integrator (Tuckerman) with N hierarchical levels, where level 1 is the innermost loop (shortest timestep) and level N is the outermost loop (largest timestep). The loop factor arguments specify what the looping factor is between levels. N1 specifies the number of iterations of level 1 for a single iteration of level 2, N2 is the iterations of level 2 per iteration of level 3, etc. N-1 looping parameters must be specified.

The timestep command sets the timestep for the outermost rRESPA level. Thus if the example command above for a 4-level rRESPA had an outer timestep of 4.0 fmsec, the inner timestep would be 8x smaller or 0.5 fmsec. All other LAMMPS commands that specify number of timesteps (e.g. neigh_modify parameters, dump every N timesteps, etc) refer to the outermost timesteps.

The rRESPA keywords enable you to specify at what level of the hierarchy various forces will be computed. If not specified, the defaults are that bond forces are computed at level 1 (innermost loop), angle forces are computed where bond forces are, dihedral forces are computed where angle forces are, improper forces are computed where dihedral forces are, pair forces are computed at the outermost level, and kspace forces are computed where pair forces are. The inner, middle, outer forces have no defaults.

The *inner* and *middle* keywords take additional arguments for cutoffs that are used by the pairwise force computations. If the 2 cutoffs for *inner* are 5.0 and 6.0, this means that all pairs up to 6.0 apart are computed by the inner force. Those between 5.0 and 6.0 have their force go ramped to 0.0 so the overlap with the next regime (middle or outer) is smooth. The next regime (middle or outer) will compute forces for all pairs from 5.0 outward, with those from 5.0 to 6.0 having their value ramped in an inverse manner.

Only some pair potentials support the use of the *inner* and *middle* and *outer* keywords. If not, only the *pair* keyword can be used with that pair style, meaning all pairwise forces are computed at the same rRESPA level. See the doc pages for individual pair styles for details.i

Another option for using pair potentials with rRESPA is with the *hybrid* keyword, which requires the use of the pair_style hybrid or hybrid/overlay command. In this scenario, different sub-styles of the hybrid pair style are evaluated at different rRESPA levels. This can be useful, for example, to set different timesteps for hybrid coarse-grained/all-atom models. The *hybrid* keyword requires as many level assignments as there are hybrid substyles, which assigns each sub-style to a rRESPA level, following their order of definition in the pair_style command. Since the *hybrid* keyword operates on pair style computations, it is mututally exclusive with either the *pair* or the *inner*/*middle*/*outer* keywords.

When using rRESPA (or for any MD simulation) care must be taken to choose a timestep size(s) that insures the Hamiltonian for the chosen ensemble is conserved. For the constant NVE ensemble, total energy must be conserved. Unfortunately, it is difficult to know *a priori* how well energy will be conserved, and a fairly long test simulation (~10 ps) is usually necessary in order to verify that no long-term drift in energy occurs with the trial set of parameters.

With that caveat, a few rules-of-thumb may be useful in selecting *respa* settings. The following applies mostly to biomolecular simulations using the CHARMM or a similar all-atom force field, but the concepts are adaptable to other problems. Without SHAKE, bonds involving hydrogen atoms exhibit high-frequency vibrations and require a timestep on the order of 0.5 fmsec in order to conserve energy. The relatively inexpensive force computations for the bonds, angles, impropers, and dihedrals can be computed on this innermost 0.5 fmsec step. The outermost timestep cannot be greater than 4.0 fmsec without risking energy drift. Smooth switching of forces between the levels of the rRESPA hierarchy is also necessary to avoid drift, and a 1-2 angstrom "healing distance" (the distance between the outer and inner cutoffs) works reasonably well. We thus recommend the following settings for use of the *respa* style without SHAKE in biomolecular simulations:

```
timestep  4.0
run_style respa 4 2 2 2 inner 2 4.5 6.0 middle 3 8.0 10.0 outer 4
```

With these settings, users can expect good energy conservation and roughly a 2.5 fold speedup over the *verlet* style with a 0.5 fmsec timestep.

If SHAKE is used with the *respa* style, time reversibility is lost, but substantially longer time steps can be achieved. For biomolecular simulations using the CHARMM or similar all-atom force field, bonds involving hydrogen atoms exhibit high frequency vibrations and require a time step on the order of 0.5 fmsec in order to conserve energy. These high frequency modes also limit the outer time step sizes since the modes are coupled. It is therefore desirable to use SHAKE with respa in order to freeze out these high frequency motions and increase the size of the time steps in the respa hierarchy. The following settings can be used for biomolecular simulations with SHAKE and rRESPA:

```
fix             2 all shake 0.000001 500 0 m 1.0 a 1
timestep        4.0
run_style       respa 2 2 inner 1 4.0 5.0 outer 2
```

With these settings, users can expect good energy conservation and roughly a 1.5 fold speedup over the *verlet* style with SHAKE and a 2.0 fmsec timestep.

For non-biomolecular simulations, the *respa* style can be advantageous if there is a clear separation of time scales - fast and slow modes in the simulation. Even a LJ system can benefit from rRESPA if the interactions are divided by the inner, middle and outer keywords. A 2-fold or more speedup can be obtained while maintaining good energy conservation. In real units, for a pure LJ fluid at liquid density, with a sigma of 3.0 angstroms, and epsilon of 0.1 Kcal/mol, the following settings seem to work well:

```
timestep  36.0
run_style respa 3 3 4 inner 1 3.0 4.0 middle 2 6.0 7.0 outer 3
```

The *respa/omp* styles is a variant of *respa* adapted for use with pair, bond, angle, dihedral, improper, or kspace styles with an *omp* suffix. It is functionally equivalent to *respa* but performs additional operations required for managing *omp* styles. For more on *omp* styles see the Section_accelerate of the manual. Accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

You can specify *respa/omp* explicitly in your input script, or you can use the -suffix command-line switch when you invoke LAMMPS, or you can use the suffix command in your input script.

See Section_accelerate of the manual for more instructions on how to use the accelerated styles effectively.

Restrictions:

The *verlet/split* style can only be used if LAMMPS was built with the REPLICA package. Correspondingly the *respa/omp* style is available only if the USER-OMP package was included. See the Making LAMMPS section for more info on packages.

Whenever using rRESPA, the user should experiment with trade-offs in speed and accuracy for their system, and verify that they are conserving energy to adequate precision.

Related commands:

timestep, run

Default:

```
run_style verlet
```

(Tuckerman) Tuckerman, Berne and Martyna, J Chem Phys, 97, p 1990 (1992).

set command

Syntax:

```
set style ID keyword values ...
```

- style = *atom* or *type* or *mol* or *group* or *region*
- ID = atom ID range or type range or mol ID range or group ID or region ID
- one or more keyword/value pairs may be appended
- keyword = *type* or *type/fraction* or *mol* or *x* or *y* or *z* or *charge* or *dipole* or *dipole/random* or *quat* or *quat/random* or *diameter* or *shape* or *length* or *tri* or *theta* or *theta/random* or *angmom* or *omega* or *mass* or *density* or *volume* or *image* or *bond* or *angle* or *dihedral* or *improper* or *meso/e* or *meso/cv* or *meso/rho* or *smd/contact/radius* or *smd/mass/density* or *dpd/theta* or *i_name* or *d_name*

```
  type value = atom type
      value can be an atom-style variable (see below)
    type/fraction values = type fraction seed
      type = new atom type
      fraction = fraction of selected atoms to set to new atom type
      seed = random # seed (positive integer)
    mol value = molecule ID
      value can be an atom-style variable (see below)
    x,y,z value = atom coordinate (distance units)
      value can be an atom-style variable (see below)
    charge value = atomic charge (charge units)
      value can be an atom-style variable (see below)
    dipole values = x y z
      x,y,z = orientation of dipole moment vector
      any of x,y,z can be an atom-style variable (see below)
    dipole/random value = seed Dlen
      seed = random # seed (positive integer) for dipole moment orientations
      Dlen = magnitude of dipole moment (dipole units)
    quat values = a b c theta
      a,b,c = unit vector to rotate particle around via right-hand rule
      theta = rotation angle (degrees)
      any of a,b,c,theta can be an atom-style variable (see below)
    quat/random value = seed
      seed = random # seed (positive integer) for quaternion orientations
    diameter value = diameter of spherical particle (distance units)
      value can be an atom-style variable (see below)
    shape value = Sx Sy Sz
      Sx,Sy,Sz = 3 diameters of ellipsoid (distance units)
    length value = len
      len = length of line segment (distance units)
      len can be an atom-style variable (see below)
    tri value = side
      side = side length of equilateral triangle (distance units)
      side can be an atom-style variable (see below)
    theta value = angle (degrees)
      angle = orientation of line segment with respect to x-axis
      angle can be an atom-style variable (see below)
    theta/random value = seed
      seed = random # seed (positive integer) for line segment orienations
    angmom values = Lx Ly Lz
      Lx,Ly,Lz = components of angular momentum vector (distance-mass-velocity units)
      any of Lx,Ly,Lz can be an atom-style variable (see below)
    omega values = Wx Wy Wz
      Wx,Wy,Wz = components of angular velocity vector (radians/time units)
```

```
  any of wx,wy,wz can be an atom-style variable (see below)
mass value = per-atom mass (mass units)
  value can be an atom-style variable (see below)
density value = particle density for sphere or ellipsoid (mass/distance^3 or mass/distance^2
  value can be an atom-style variable (see below)
volume value = particle volume for Peridynamic particle (distance^3 units)
  value can be an atom-style variable (see below)
image nx ny nz
  nx,ny,nz = which periodic image of the simulation box the atom is in
bond value = bond type for all bonds between selected atoms
angle value = angle type for all angles between selected atoms
dihedral value = dihedral type for all dihedrals between selected atoms
improper value = improper type for all impropers between selected atoms
meso/e value = energy of SPH particles (need units)
  value can be an atom-style variable (see below)
meso/cv value = heat capacity of SPH particles (need units)
  value can be an atom-style variable (see below)
meso/rho value = density of SPH particles (need units)
  value can be an atom-style variable (see below)
smd/contact/radius = radius for short range interactions, i.e. contact and friction
  value can be an atom-style variable (see below)
smd/mass/density = set particle mass based on volume by providing a mass density
  value can be an atom-style variable (see below)
dpd/theta value = internal temperature of DPD particles (temperature units)
i_name value = value for custom integer vector with name
d_name value = value for custom floating-point vector with name
```

Examples:

```
set group solvent type 2
set group solvent type/fraction 2 0.5 12393
set group edge bond 4
set region half charge 0.5
set type 3 charge 0.5
set type 1*3 charge 0.5
set atom * charge v_atomfile
set atom 100*200 x 0.5 y 1.0
set atom 1492 type 3
```

Description:

Set one or more properties of one or more atoms. Since atom properties are initially assigned by the read_data, read_restart or create_atoms commands, this command changes those assignments. This can be useful for overriding the default values assigned by the create_atoms command (e.g. charge = 0.0). It can be useful for altering pairwise and molecular force interactions, since force-field coefficients are defined in terms of types. It can be used to change the labeling of atoms by atom type or molecule ID when they are output in dump files. It can also be useful for debugging purposes; i.e. positioning an atom at a precise location to compute subsequent forces or energy.

Note that the *style* and *ID* arguments determine which atoms have their properties reset. The remaining keywords specify which properties to reset and what the new values are. Some strings like *type* or *mol* can be used as a style and/or a keyword.

This section describes how to select which atoms to change the properties of, via the *style* and *ID* arguments.

The style *atom* selects all the atoms in a range of atom IDs. The style *type* selects all the atoms in a range of types. The style *mol* selects all the atoms in a range of molecule IDs.

In each of the range cases, the range can be specified as a single numeric value, or a wildcard asterisk can be used to specify a range of values. This takes the form "*" or "*n" or "n*" or "m*n". For example, for the style *type*, if N = the number of atom types, then an asterisk with no numeric values means all types from 1 to N. A leading asterisk means all types from 1 to n (inclusive). A trailing asterisk means all types from n to N (inclusive). A middle asterisk means all types from m to n (inclusive). For all the styles except *mol*, the lowest value for the wildcard is 1; for *mol* it is 0.

The style *group* selects all the atoms in the specified group. The style *region* selects all the atoms in the specified geometric region. See the group and region commands for details of how to specify a group or region.

This section describes the keyword options for which properties to change, for the selected atoms.

Note that except where explicitly prohibited below, all of the keywords allow an atom-style or atomfile-style variable to be used as the specified value(s). If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated, and its resulting per-atom value used to determine the value assigned to each selected atom. Note that the per-atom value from the variable will be ignored for atoms that are not selected via the *style* and *ID* settings explained above. A simple way to use per-atom values from the variable to reset a property for all atoms is to use style *atom* with *ID* = "*"; this selects all atom IDs.

Atom-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters and timestep and elapsed time. They can also include per-atom values, such as atom coordinates. Thus it is easy to specify a time-dependent or spatially-dependent set of per-atom values. As explained on the variable doc page, atomfile-style variables can be used in place of atom-style variables, and thus as arguments to the set command. Atomfile-style variables read their per-atoms values from a file.

NOTE: Atom-style and atomfile-style variables return floating point per-atom values. If the values are assigned to an integer variable, such as the molecule ID, then the floating point value is truncated to its integer portion, e.g. a value of 2.6 would become 2.

Keyword *type* sets the atom type for all selected atoms. The specified value must be from 1 to ntypes, where ntypes was set by the create_box command or the *atom types* field in the header of the data file read by the read_data command.

Keyword *type/fraction* sets the atom type for a fraction of the selected atoms. The actual number of atoms changed is not guaranteed to be exactly the requested fraction, but should be statistically close. Random numbers are used in such a way that a particular atom is changed or not changed, regardless of how many processors are being used. This keyword does not allow use of an atom-style variable.

Keyword *mol* sets the molecule ID for all selected atoms. The atom style being used must support the use of molecule IDs.

Keywords *x*, *y*, *z*, and *charge* set the coordinates or charge of all selected atoms. For *charge*, the atom style being used must support the use of atomic charge.

Keyword *dipole* uses the specified x,y,z values as components of a vector to set as the orientation of the dipole moment vectors of the selected atoms. The magnitude of the dipole moment is set by the length of this orientation vector.

Keyword *dipole/random* randomizes the orientation of the dipole moment vectors for the selected atoms and sets the magnitude of each to the specified *Dlen* value. For 2d systems, the z component of the orientation is set to 0.0. Random numbers are used in such a way that the orientation of a particular atom is the same, regardless of how

many processors are being used. This keyword does not allow use of an atom-style variable.

Keyword *quat* uses the specified values to create a quaternion (4-vector) that represents the orientation of the selected atoms. The particles must define a quaternion for their orientation (e.g. ellipsoids, triangles, body particles) as defined by the atom_style command. Note that particles defined by atom_style ellipsoid have 3 shape parameters. The 3 values must be non-zero for each particle set by this command. They are used to specify the aspect ratios of an ellipsoidal particle, which is oriented by default with its x-axis along the simulation box's x-axis, and similarly for y and z. If this body is rotated (via the right-hand rule) by an angle theta around a unit rotation vector (a,b,c), then the quaternion that represents its new orientation is given by (cos(theta/2), a*sin(theta/2), b*sin(theta/2), c*sin(theta/2)). The theta and a,b,c values are the arguments to the *quat* keyword. LAMMPS normalizes the quaternion in case (a,b,c) was not specified as a unit vector. For 2d systems, the a,b,c values are ignored, since a rotation vector of (0,0,1) is the only valid choice.

Keyword *quat/random* randomizes the orientation of the quaternion for the selected atoms. The particles must define a quaternion for their orientation (e.g. ellipsoids, triangles, body particles) as defined by the atom_style command. Random numbers are used in such a way that the orientation of a particular atom is the same, regardless of how many processors are being used. For 2d systems, only orientations in the xy plane are generated. As with keyword *quat*, for ellipsoidal particles, the 3 shape values must be non-zero for each particle set by this command. This keyword does not allow use of an atom-style variable.

Keyword *diameter* sets the size of the selected atoms. The particles must be finite-size spheres as defined by the atom_style sphere command. The diameter of a particle can be set to 0.0, which means they will be treated as point particles. Note that this command does not adjust the particle mass, even if it was defined with a density, e.g. via the read_data command.

Keyword *shape* sets the size and shape of the selected atoms. The particles must be ellipsoids as defined by the atom_style ellipsoid command. The *Sx*, *Sy*, *Sz* settings are the 3 diameters of the ellipsoid in each direction. All 3 can be set to the same value, which means the ellipsoid is effectively a sphere. They can also all be set to 0.0 which means the particle will be treated as a point particle. Note that this command does not adjust the particle mass, even if it was defined with a density, e.g. via the read_data command.

Keyword *length* sets the length of selected atoms. The particles must be line segments as defined by the atom_style line command. If the specified value is non-zero the line segment is (re)set to a length = the specified value, centered around the particle position, with an orientation along the x-axis. If the specified value is 0.0, the particle will become a point particle. Note that this command does not adjust the particle mass, even if it was defined with a density, e.g. via the read_data command.

Keyword *tri* sets the size of selected atoms. The particles must be triangles as defined by the atom_style tri command. If the specified value is non-zero the triangle is (re)set to be an equilateral triangle in the xy plane with side length = the specified value, with a centroid at the particle position, with its base parallel to the x axis, and the y-axis running from the center of the base to the top point of the triangle. If the specified value is 0.0, the particle will become a point particle. Note that this command does not adjust the particle mass, even if it was defined with a density, e.g. via the read_data command.

Keyword *theta* sets the orientation of selected atoms. The particles must be line segments as defined by the atom_style line command. The specified value is used to set the orientation angle of the line segments with respect to the x axis.

Keyword *theta/random* randomizes the orientation of theta for the selected atoms. The particles must be line segments as defined by the atom_style line command. Random numbers are used in such a way that the orientation of a particular atom is the same, regardless of how many processors are being used. This keyword does not allow use of an atom-style variable.

Keyword *angmom* sets the angular momentum of selected atoms. The particles must be ellipsoids as defined by the atom_style ellipsoid command or triangles as defined by the atom_style tri command. The angular momentum vector of the particles is set to the 3 specified components.

Keyword *omega* sets the angular velocity of selected atoms. The particles must be spheres as defined by the atom_style sphere atom_style.html command. The angular velocity vector of the particles is set to the 3 specified components.

Keyword *mass* sets the mass of all selected particles. The particles must have a per-atom mass attribute, as defined by the atom_style command. See the "mass" command for how to set mass values on a per-type basis.

Keyword *density* also sets the mass of all selected particles, but in a different way. The particles must have a per-atom mass attribute, as defined by the atom_style command. If the atom has a radius attribute (see atom_style sphere) and its radius is non-zero, its mass is set from the density and particle volume. If the atom has a shape attribute (see atom_style ellipsoid) and its 3 shape parameters are non-zero, then its mass is set from the density and particle volume. If the atom has a length attribute (see atom_style line) and its length is non-zero, then its mass is set from the density and line segment length (the input density is assumed to be in mass/distance units). If the atom has an area attribute (see atom_style tri) and its area is non-zero, then its mass is set from the density and triangle area (the input density is assumed to be in mass/distance^2 units). If none of these cases are valid, then the mass is set to the density value directly (the input density is assumed to be in mass units).

Keyword *volume* sets the volume of all selected particles. Currently, only the atom_style peri command defines particles with a volume attribute. Note that this command does not adjust the particle mass.

Keyword *image* sets which image of the simulation box the atom is considered to be in. An image of 0 means it is inside the box as defined. A value of 2 means add 2 box lengths to get the true value. A value of -1 means subtract 1 box length to get the true value. LAMMPS updates these flags as atoms cross periodic boundaries during the simulation. The flags can be output with atom snapshots via the dump command. If a value of NULL is specified for any of nx,ny,nz, then the current image value for that dimension is unchanged. For non-periodic dimensions only a value of 0 can be specified. This keyword does not allow use of atom-style variables. This command can be useful after a system has been equilibrated and atoms have diffused one or more box lengths in various directions. This command can then reset the image values for atoms so that they are effectively inside the simulation box, e.g if a diffusion coefficient is about to be measured via the compute msd command. Care should be taken not to reset the image flags of two atoms in a bond to the same value if the bond straddles a periodic boundary (rather they should be different by +/- 1). This will not affect the dynamics of a simulation, but may mess up analysis of the trajectories if a LAMMPS diagnostic or your own analysis relies on the image flags to unwrap a molecule which straddles the periodic box.

Keywords *bond*, *angle*, *dihedral*, and *improper*, set the bond type (angle type, etc) of all bonds (angles, etc) of selected atoms to the specified value from 1 to nbondtypes (nangletypes, etc). All atoms in a particular bond (angle, etc) must be selected atoms in order for the change to be made. The value of nbondtype (nangletypes, etc) was set by the *bond types* (*angle types*, etc) field in the header of the data file read by the read_data command. These keywords do not allow use of an atom-style variable.

Keywords *meso/e*, *meso/cv*, and *meso/rho* set the energy, heat capacity, and density of smmothed particle hydrodynamics (SPH) particles. See this PDF guide to using SPH in LAMMPS.

Keyword *smd/mass/density* sets the mass of all selected particles, but it is only applicable to the Smooth Mach Dynamics package USER-SMD. It assumes that the particle volume has already been correctly set and calculates particle mass from the provided mass density value.

Keyword *smd/contact/radius* only applies to simulations with the Smooth Mach Dynamics package USER-SMD.

Itsets an interaction radius for computing short-range interactions, e.g. repulsive forces to prevent different individual physical bodies from penetrating each other. Note that the SPH smoothing kernel diameter used for computing long range, nonlocal interactions, is set using the *diameter* keyword.

Keyword *dpd/theta* sets the internal temperature of a DPD particle as defined by the USER-DPD package.

Keywords *i_name* and *d_name* refer to custom integer and floating-point properties that have been added to each atom via the fix property/atom command. When that command is used specific names are given to each attribute which are what is specified as the "name" portion of *i_name* or *d_name*.

Restrictions:

You cannot set an atom attribute (e.g. *mol* or *q* or *volume*) if the atom_style does not have that attribute.

This command requires inter-processor communication to coordinate the setting of bond types (angle types, etc). This means that your system must be ready to perform a simulation before using one of these keywords (force fields set, atom mass set, etc). This is not necessary for other keywords.

Using the *region* style with the bond (angle, etc) keywords can give unpredictable results if there are bonds (angles, etc) that straddle periodic boundaries. This is because the region may only extend up to the boundary and partner atoms in the bond (angle, etc) may have coordinates outside the simulation box if they are ghost atoms.

Related commands:

create_box, create_atoms, read_data

Default: none

shell command

Syntax:

```
shell cmd args
```

- cmd = *cd* or *mkdir* or *mv* or *rm* or *rmdir* or *putenv* or arbitrary command

```
cd arg = dir
    dir = directory to change to
  mkdir args = dir1 dir2 ...
    dir1,dir2 = one or more directories to create
  mv args = old new
    old = old filename
    new = new filename
  rm args = file1 file2 ...
    file1,file2 = one or more filenames to delete
  rmdir args = dir1 dir2 ...
    dir1,dir2 = one or more directories to delete
  putenv args = var1=value1 var2=value2
    var=value = one of more definitions of environment variables
  anything else is passed as a command to the shell for direct execution
```

Examples:

```
shell cd sub1
shell cd ..
shell mkdir tmp1 tmp2 tmp3
shell rmdir tmp1
shell mv log.lammps hold/log.1
shell rm TMP/file1 TMP/file2
shell putenv LAMMPS_POTENTIALS=../../potentials
shell my_setup file1 10 file2
shell my_post_process 100 dump.out
```

Description:

Execute a shell command. A few simple file-based shell commands are supported directly, in Unix-style syntax. Any command not listed above is passed as-is to the C-library system() call, which invokes the command in a shell.

This is means to invoke other commands from your input script. For example, you can move files around in preparation for the next section of the input script. Or you can run a program that pre-processes data for input into LAMMPS. Or you can run a program that post-processes LAMMPS output data.

With the exception of *cd*, all commands, including ones invoked via a system() call, are executed by only a single processor, so that files/directories are not being manipulated by multiple processors.

The *cd* cmd executes the Unix "cd" command to change the working directory. All subsequent LAMMPS commands that read/write files will use the new directory. All processors execute this command.

The *mkdir* cmd executes the Unix "mkdir" command to create one or more directories.

The *mv* cmd executes the Unix "mv" command to rename a file and/or move it to a new directory.

The *rm* cmd executes the Unix "rm" command to remove one or more files.

The *rmdir* cmd executes the Unix "rmdir" command to remove one or more directories. A directory must be empty to be successfully removed.

The *putenv* cmd defines or updates an environment variable directly. Since this command does not pass through the shell, no shell variable expansion or globbing is performed, only the usual substitution for LAMMPS variables defined with the variable command is performed. The resulting string is then used literally.

Any other cmd is passed as-is to the shell along with its arguments as one string, invoked by the C-library system() call. For example, these lines in your input script:

```
variable n equal 10
variable foo string file2
shell my_setup file1 $n ${foo}
```

would be the same as invoking

```
% my_setup file1 10 file2
```

from a command-line prompt. The executable program "my_setup" is run with 3 arguments: file1 10 file2.

Restrictions:

LAMMPS does not detect errors or print warnings when any of these commands execute. E.g. if the specified directory does not exist, executing the *cd* command will silently do nothing.

Related commands: none

Default: none

special_bonds command

Syntax:

```
special_bonds keyword values ...
```

- one or more keyword/value pairs may be appended
- keyword = *amber* or *charmm* or *dreiding* or *fene* or *lj/coul* or *lj* or *coul* or *angle* or *dihedral* or *extra*

```
amber values = none
  charmm values = none
  dreiding values = none
  fene values = none
  lj/coul values = w1,w2,w3
    w1,w2,w3 = weights (0.0 to 1.0) on pairwise Lennard-Jones and Coulombic interactions
  lj values = w1,w2,w3
    w1,w2,w3 = weights (0.0 to 1.0) on pairwise Lennard-Jones interactions
  coul values = w1,w2,w3
    w1,w2,w3 = weights (0.0 to 1.0) on pairwise Coulombic interactions
  angle value = yes or no
  dihedral value = yes or no
  extra value = N
    N = number of extra 1-2,1-3,1-4 interactions to save space for
```

Examples:

```
special_bonds amber
special_bonds charmm
special_bonds fene dihedral no
special_bonds lj/coul 0.0 0.0 0.5 angle yes dihedral yes
special_bonds lj 0.0 0.0 0.5 coul 0.0 0.0 0.0 dihedral yes
special_bonds lj/coul 0 1 1 extra 2
```

Description:

Set weighting coefficients for pairwise energy and force contributions between pairs of atoms that are also permanently bonded to each other, either directly or via one or two intermediate bonds. These weighting factors are used by nearly all pair styles in LAMMPS that compute simple pairwise interactions. Permanent bonds between atoms are specified by defining the bond topology in the data file read by the read_data command. Typically a bond_style command is also used to define a bond potential. The rationale for using these weighting factors is that the interaction between a pair of bonded atoms is all (or mostly) specified by the bond, angle, dihedral potentials, and thus the non-bonded Lennard-Jones or Coulombic interaction between the pair of atoms should be excluded (or reduced by a weighting factor).

NOTE: These weighting factors are NOT used by pair styles that compute many-body interactions, since the "bonds" that result from such interactions are not permanent, but are created and broken dynamically as atom conformations change. Examples of pair styles in this category are EAM, MEAM, Stillinger-Weber, Tersoff, COMB, AIREBO, and ReaxFF. In fact, it generally makes no sense to define permanent bonds between atoms that interact via these potentials, though such bonds may exist elsewhere in your system, e.g. when using the pair_style hybrid command. Thus LAMMPS ignores special_bonds settings when manybody potentials are calculated.

NOTE: Unlike some commands in LAMMPS, you cannot use this command multiple times in an incremental fashion: e.g. to first set the LJ settings and then the Coulombic ones. Each time you use this command it sets all

the coefficients to default values and only overrides the one you specify, so you should set all the options you need each time you use it. See more details at the bottom of this page.

The Coulomb factors are applied to any Coulomb (charge interaction) term that the potential calculates. The LJ factors are applied to the remaining terms that the potential calculates, whether they represent LJ interactions or not. The weighting factors are a scaling pre-factor on the energy and force between the pair of atoms. A value of 1.0 means include the full interaction; a value of 0.0 means exclude it completely.

The 1st of the 3 coefficients (LJ or Coulombic) is the weighting factor on 1-2 atom pairs, which are pairs of atoms directly bonded to each other. The 2nd coefficient is the weighting factor on 1-3 atom pairs which are those separated by 2 bonds (e.g. the two H atoms in a water molecule). The 3rd coefficient is the weighting factor on 1-4 atom pairs which are those separated by 3 bonds (e.g. the 1st and 4th atoms in a dihedral interaction). Thus if the 1-2 coefficient is set to 0.0, then the pairwise interaction is effectively turned off for all pairs of atoms bonded to each other. If it is set to 1.0, then that interaction will be at full strength.

NOTE: For purposes of computing weighted pairwise interactions, 1-3 and 1-4 interactions are not defined from the list of angles or dihedrals used by the simulation. Rather, they are inferred topologically from the set of bonds specified when the simulation is defined from a data or restart file (see read_data or read_restart commands). Thus the set of 1-2,1-3,1-4 interactions that the weights apply to is the same whether angle and dihedral potentials are computed or not, and remains the same even if bonds are constrained, or turned off, or removed during a simulation.

The two exceptions to this rule are (a) if the *angle* or *dihedral* keywords are set to *yes* (see below), or (b) if the delete_bonds command is used with the *special* option that recomputes the 1-2,1-3,1-4 topologies after bonds are deleted; see the delete_bonds command for more details.

The *amber* keyword sets the 3 coefficients to 0.0, 0.0, 0.5 for LJ interactions and to 0.0, 0.0, 0.8333 for Coulombic interactions, which is the default for a commonly used version of the AMBER force field, where the last value is really 5/6. See (Cornell) for a description of the AMBER force field.

The *charmm* keyword sets the 3 coefficients to 0.0, 0.0, 0.0 for both LJ and Coulombic interactions, which is the default for a commonly used version of the CHARMM force field. Note that in pair styles *lj/charmm/coul/charmm* and *lj/charmm/coul/long* the 1-4 coefficients are defined explicitly, and these pairwise contributions are computed as part of the charmm dihedral style - see the pair_coeff and dihedral_style commands for more information. See (MacKerell) for a description of the CHARMM force field.

The *dreiding* keyword sets the 3 coefficients to 0.0, 0.0, 1.0 for both LJ and Coulombic interactions, which is the default for the Dreiding force field, as discussed in (Mayo).

The *fene* keyword sets the 3 coefficients to 0.0, 1.0, 1.0 for both LJ and Coulombic interactions, which is consistent with a coarse-grained polymer model with FENE bonds. See (Kremer) for a description of FENE bonds.

The *lj/coul*, *lj*, and *coul* keywords allow the 3 coefficients to be set explicitly. The *lj/coul* keyword sets both the LJ and Coulombic coefficients to the same 3 values. The *lj* and *coul* keywords only set either the LJ or Coulombic coefficients. Use both of them if you wish to set the LJ coefficients to different values than the Coulombic coefficients.

The *angle* keyword allows the 1-3 weighting factor to be ignored for individual atom pairs if they are not listed as the first and last atoms in any angle defined in the simulation or as 1,3 or 2,4 atoms in any dihedral defined in the simulation. For example, imagine the 1-3 weighting factor is set to 0.5 and you have a linear molecule with 4 atoms and bonds as follows: 1-2-3-4. If your data file defines 1-2-3 as an angle, but does not define 2-3-4 as an

angle or 1-2-3-4 as a dihedral, then the pairwise interaction between atoms 1 and 3 will always be weighted by 0.5, but different force fields use different rules for weighting the pairwise interaction between atoms 2 and 4. If the *angle* keyword is specified as *yes*, then the pairwise interaction between atoms 2 and 4 will be unaffected (full weighting of 1.0). If the *angle* keyword is specified as *no* which is the default, then the 2,4 interaction will also be weighted by 0.5.

The *dihedral* keyword allows the 1-4 weighting factor to be ignored for individual atom pairs if they are not listed as the first and last atoms in any dihedral defined in the simulation. For example, imagine the 1-4 weighting factor is set to 0.5 and you have a linear molecule with 5 atoms and bonds as follows: 1-2-3-4-5. If your data file defines 1-2-3-4 as a dihedral, but does not define 2-3-4-5 as a dihedral, then the pairwise interaction between atoms 1 and 4 will always be weighted by 0.5, but different force fields use different rules for weighting the pairwise interaction between atoms 2 and 5. If the *dihedral* keyword is specified as *yes*, then the pairwise interaction between atoms 2 and 5 will be unaffected (full weighting of 1.0). If the *dihedral* keyword is specified as *no* which is the default, then the 2,5 interaction will also be weighted by 0.5.

The *extra* keyword can be used when additional bonds will be created during a simulation run, e.g. by the fix bond/create command. It can also be used if molecules will be added to the system, e.g. via the fix deposit, or fix pour commands, which will have atoms with more special neighbors than any atom in the current system has.

NOTE: LAMMPS stores and maintains a data structure with a list of the 1st, 2nd, and 3rd neighbors of each atom (within the bond topology of the system). If new bonds are created (or molecules added containing atoms with more special neighbors), the size of this list needs to grow. Note that adding a single bond always adds a new 1st neighbor but may also induce *many* new 2nd and 3rd neighbors, depending on the molecular topology of your system. Using the *extra* keyword leaves empty space in the list for this N additional 1st, 2nd, or 3rd neighbors to be added. If you do not do this, you may get an error when bonds (or molecules) are added.

NOTE: If you reuse this command in an input script, you should set all the options you need each time. This command cannot be used a 2nd time incrementally, e.g. to add some extra storage locations via the *extra* keyword. E.g. these two commands:

special_bonds lj 0.0 1.0 1.0 special_bonds coul 0.0 0.0 1.0

are not the same as

special_bonds lj 0.0 1.0 1.0 coul 0.0 0.0 1.0

In the first case you end up with (after the 2nd command):

LJ: 0.0 0.0 0.0 Coul: coul 0.0 0.0 1.0

because the LJ settings are reset to their default values each time the command is issued.

Likewise

```
special_bonds amber
special_bonds extra 2
```

is not the same as this single command:

```
special_bonds amber extra 2
```

since in the former case, the 2nd command will reset all the LJ and Coulombic weights to 0.0 (the default).

One exception to this rule is the *extra* option itself. It is not reset to its default value of 0 each time the special_bonds command is invoked. This is because it can also be set by the read_data and create_box commands, so this command will not override those settings unless you explicitly use *extra* as an option.

Restrictions: none

Related commands:

delete_bonds, fix bond/create

Default:

All 3 Lennard-Jones and 3 Coulombic weighting coefficients = 0.0, angle = no, dihedral = no, and extra = 0.

(Cornell) Cornell, Cieplak, Bayly, Gould, Merz, Ferguson, Spellmeyer, Fox, Caldwell, Kollman, JACS 117, 5179-5197 (1995).

(Kremer) Kremer, Grest, J Chem Phys, 92, 5057 (1990).

(MacKerell) MacKerell, Bashford, Bellott, Dunbrack, Evanseck, Field, Fischer, Gao, Guo, Ha, et al, J Phys Chem, 102, 3586 (1998).

(Mayo) Mayo, Olfason, Goddard III, J Phys Chem, 94, 8897-8909 (1990).

suffix command

Syntax:

```
suffix style args
```

- style = *off* or *on* or *cuda* or *gpu* or *intel* or *kk* or *omp* or *opt* or *hybrid*
- args = for hybrid style, default suffix to be used and alternative suffix

Examples:

```
suffix off
suffix on
suffix gpu
suffix intel
suffix hybrid intel omp
suffix kk
```

Description:

This command allows you to use variants of various styles if they exist. In that respect it operates the same as the -suffix command-line switch. It also has options to turn off or back on any suffix setting made via the command line.

The specified style can be *cuda*, *gpu*, *intel*, *kk*, *omp*, *opt* or *hybrid*. These refer to optional packages that LAMMPS can be built with, as described in this section of the manual. The "cuda" style corresponds to the USER-CUDA package, the "gpu" style to the GPU package, the "intel" style to the USER-INTEL package, the "kk" style to the KOKKOS package, the "omp" style to the USER-OMP package, and the "opt" style to the OPT package.

These are the variants these packages provide:

- USER-CUDA = a collection of atom, pair, fix, compute, and intergrate styles, optimized to run on one or more NVIDIA GPUs
- GPU = a handful of pair styles and the PPPM kspace_style, optimized to run on one or more GPUs or multicore CPU/GPU nodes
- USER-INTEL = a collection of pair styles and neighbor routines optimized to run in single, mixed, or double precision on CPUs and Intel(R) Xeon Phi(TM) coprocessors.
- KOKKOS = a collection of atom, pair, and fix styles optimized to run using the Kokkos library on various kinds of hardware, including GPUs via Cuda and many-core chips via OpenMP or threading.
- USER-OMP = a collection of pair, bond, angle, dihedral, improper, kspace, compute, and fix styles with support for OpenMP multi-threading
- OPT = a handful of pair styles, cache-optimized for faster CPU performance
- HYBRID = a combination of two packages can be specified (see below)

As an example, all of the packages provide a pair_style lj/cut variant, with style names lj/cut/opt, lj/cut/omp, lj/cut/gpu, lj/cut/intel, lj/cut/cuda, or lj/cut/kk. A variant styles can be specified explicitly in your input script, e.g. pair_style lj/cut/gpu. If the suffix command is used with the appropriate style, you do not need to modify your input script. The specified suffix (opt,omp,gpu,intel,cuda,kk) is automatically appended whenever your input script command creates a new atom, pair, bond, angle, dihedral, improper, kspace, fix, compute, or run style. If the variant version does not exist, the standard version is created.

For "hybrid", two packages are specified. The first is used whenever available. If a style with the first suffix is not available, the style with the suffix for the second package will be used if available. For example, "hybrid intel omp" will use styles from the USER-INTEL package as a first choice and styles from the USER-OMP package as a second choice if no USER-INTEL variant is available.

If the specified style is *off*, then any previously specified suffix is temporarily disabled, whether it was specified by a command-line switch or a previous suffix command. If the specified style is *on*, a disabled suffix is turned back on. The use of these 2 commands lets your input script use a standard LAMMPS style (i.e. a non-accelerated variant), which can be useful for testing or benchmarking purposes. Of course this is also possible by not using any suffix commands, and explictly appending or not appending the suffix to the relevant commands in your input script.

Restrictions: none

Related commands:

Command-line switch -suffix

Default: none

tad command

Syntax:

```
tad N t_event T_lo T_hi delta tmax compute-ID keyword value ...
```

- N = # of timesteps to run (not including dephasing/quenching)
- t_event = timestep interval between event checks
- T_lo = temperature at which event times are desired
- T_hi = temperature at which MD simulation is performed
- delta = desired confidence level for stopping criterion
- tmax = reciprocal of lowest expected preexponential factor (time units)
- compute-ID = ID of the compute used for event detection
- zero or more keyword/value pairs may be appended
- keyword = *min* or *neb* or *min_style* or *neb_style* or *neb_log*

```
  min values = etol ftol maxiter maxeval
      etol = stopping tolerance for energy (energy units)
      ftol = stopping tolerance for force (force units)
      maxiter = max iterations of minimize
      maxeval = max number of force/energy evaluations
    neb values = ftol N1 N2 Nevery
      etol = stopping tolerance for energy (energy units)
      ftol = stopping tolerance for force (force units)
      N1 = max # of iterations (timesteps) to run initial NEB
      N2 = max # of iterations (timesteps) to run barrier-climbing NEB
      Nevery = print NEB statistics every this many timesteps
    neb_style value = quickmin or fire
    neb_step value = dtneb
      dtneb = timestep for NEB damped dynamics minimization
    neb_log value = file where NEB statistics are printed
```

Examples:

```
tad 2000 50 1800 2300 0.01 0.01 event
tad 2000 50 1800 2300 0.01 0.01 event &
    min 1e-05 1e-05 100 100 &
    neb 0.0 0.01 200 200 20 &
    min_style cg &
    neb_style fire &
    neb_log log.neb
```

Description:

Run a temperature accelerated dynamics (TAD) simulation. This method requires two or more partitions to perform NEB transition state searches.

TAD is described in this paper by Art Voter. It is a method that uses accelerated dynamics at an elevated temperature to generate results at a specified lower temperature. A good overview of accelerated dynamics methods for such systems is given in this review paper from the same group. In general, these methods assume that the long-time dynamics is dominated by infrequent events i.e. the system is is confined to low energy basins for long periods, punctuated by brief, randomly-occurring transitions to adjacent basins. TAD is suitable for infrequent-event systems, where in addition, the transition kinetics are well-approximated by harmonic transition state theory (hTST). In hTST, the temperature dependence of transition rates follows the Arrhenius relation. As a

consequence a set of event times generated in a high-temperature simulation can be mapped to a set of much longer estimated times in the low-temperature system. However, because this mapping involves the energy barrier of the transition event, which is different for each event, the first event at the high temperature may not be the earliest event at the low temperature. TAD handles this by first generating a set of possible events from the current basin. After each event, the simulation is reflected backwards into the current basin. This is repeated until the stopping criterion is satisfied, at which point the event with the earliest low-temperature occurrence time is selected. The stopping criterion is that the confidence measure be greater than 1-*delta*. The confidence measure is the probability that no earlier low-temperature event will occur at some later time in the high-temperature simulation. hTST provides an lower bound for this probability, based on the user-specified minimum pre-exponential factor (reciprocal of *tmax*).

In order to estimate the energy barrier for each event, the TAD method invokes the NEB method. Each NEB replica runs on a partition of processors. The current NEB implementation in LAMMPS restricts you to having exactly one processor per replica. For more information, see the documentation for the neb command. In the current LAMMPS implementation of TAD, all the non-NEB TAD operations are performed on the first partition, while the other partitions remain idle. See Section_howto 5 of the manual for further discussion of multi-replica simulations.

A TAD run has several stages, which are repeated each time an event is performed. The logic for a TAD run is as follows:

```
while (time remains):
  while (time <tstop):
    until (event occurs):
      run dynamics for t_event steps
      quench
    run neb calculation using all replicas
    compute tlo from energy barrier
    update earliest event
    update tstop
    reflect back into current basin
  execute earliest event
```

Before this outer loop begins, the initial potential energy basin is identified by quenching (an energy minimization, see below) the initial state and storing the resulting coordinates for reference.

Inside the inner loop, dynamics is run continuously according to whatever integrator has been specified by the user, stopping every *t_event* steps to check if a transition event has occurred. This check is performed by quenching the system and comparing the resulting atom coordinates to the coordinates from the previous basin.

A quench is an energy minimization and is performed by whichever algorithm has been defined by the min_style command; its default is the CG minimizer. The tolerances and limits for each quench can be set by the *min* keyword. Note that typically, you do not need to perform a highly-converged minimization to detect a transition event.

The event check is performed by a compute with the specified *compute-ID*. Currently there is only one compute that works with the TAD commmand, which is the compute event/displace command. Other event-checking computes may be added. Compute event/displace checks whether any atom in the compute group has moved further than a specified threshold distance. If so, an "event" has occurred.

The NEB calculation is similar to that invoked by the neb command, except that the final state is generated internally, instead of being read in from a file. The style of minimization performed by NEB is determined by the *neb_style* keyword and must be a damped dynamics minimizer. The tolerances and limits for each NEB calculation can be set by the *neb* keyword. As discussed on the neb, it is often advantageous to use a larger

timestep for NEB than for normal dyanmics. Since the size of the timestep set by the timestep command is used by TAD for performing dynamics, there is a *neb_step* keyword which can be used to set a larger timestep for each NEB calculation if desired.

A key aspect of the TAD method is setting the stopping criterion appropriately. If this criterion is too conservative, then many events must be generated before one is finally executed. Conversely, if this criterion is too aggressive, high-entropy high-barrier events will be over-sampled, while low-entropy low-barrier events will be under-sampled. If the lowest pre-exponential factor is known fairly accurately, then it can be used to estimate *tmax*, and the value of *delta* can be set to the desired confidence level e.g. *delta* = 0.05 corresponds to 95% confidence. However, for systems where the dynamics are not well characterized (the most common case), it will be necessary to experiment with the values of *delta* and *tmax* to get a good trade-off between accuracy and performance.

A second key aspect is the choice of *t_hi*. A larger value greatly increases the rate at which new events are generated. However, too large a value introduces errors due to anharmonicity (not accounted for within hTST). Once again, for any given system, experimentation is necessary to determine the best value of *t_hi*.

Five kinds of output can be generated during a TAD run: event statistics, NEB statistics, thermodynamic output by each replica, dump files, and restart files.

Event statistics are printed to the screen and master log.lammps file each time an event is executed. The quantities are the timestep, CPU time, global event number *N*, local event number *M*, event status, energy barrier, time margin, *t_lo* and *delt_lo*. The timestep is the usual LAMMPS timestep, which corresponds to the high-temperature time at which the event was detected, in units of timestep. The CPU time is the total processor time since the start of the TAD run. The global event number *N* is a counter that increments with each executed event. The local event number *M* is a counter that resets to zero upon entering each new basin. The event status is *E* when an event is executed, and is *D* for an event that is detected, while *DF* is for a detected event that is also the earliest (first) event at the low temperature.

The time margin is the ratio of the high temperature time in the current basin to the stopping time. This last number can be used to judge whether the stopping time is too short or too long (see above).

t_lo is the low-temperature event time when the current basin was entered, in units of timestep. del*t_lo* is the time of each detected event, measured relative to *t_lo*. *delt_lo* is equal to the high-temperature time since entering the current basin, scaled by an exponential factor that depends on the hi/lo temperature ratio and the energy barrier for that event.

On lines for executed events, with status *E*, the global event number is incremented by one, the local event number and time margin are reset to zero, while the global event number, energy barrier, and *delt_lo* match the last event with status *DF* in the immediately preceding block of detected events. The low-temperature event time *t_lo* is incremented by *delt_lo*.

NEB statistics are written to the file specified by the *neb_log* keyword. If the keyword value is "none", then no NEB statistics are printed out. The statistics are written every *Nevery* timesteps. See the neb command for a full description of the NEB statistics. When invoked from TAD, NEB statistics are never printed to the screen.

Because the NEB calculation must run on multiple partitions, LAMMPS produces additional screen and log files for each partition, e.g. log.lammps.0, log.lammps.1, etc. For the TAD command, these contain the thermodynamic output of each NEB replica. In addition, the log file for the first partition, log.lammps.0, will contain thermodynamic output from short runs and minimizations corresponding to the dynamics and quench operations, as well as a line for each new detected event, as described above.

After the TAD command completes, timing statistics for the TAD run are printed in each replica's log file, giving a breakdown of how much CPU time was spent in each stage (NEB, dynamics, quenching, etc).

Any dump files defined in the input script will be written to during a TAD run at timesteps when an event is executed. This means the the requested dump frequency in the dump command is ignored. There will be one dump file (per dump command) created for all partitions. The atom coordinates of the dump snapshot are those of the minimum energy configuration resulting from quenching following the executed event. The timesteps written into the dump files correspond to the timestep at which the event occurred and NOT the clock. A dump snapshot corresponding to the initial minimum state used for event detection is written to the dump file at the beginning of each TAD run.

If the restart command is used, a single restart file for all the partitions is generated, which allows a TAD run to be continued by a new input script in the usual manner. The restart file is generated after an event is executed. The restart file contains a snapshot of the system in the new quenched state, including the event number and the low-temperature time. The restart frequency specified in the restart command is interpreted differently when performing a TAD run. It does not mean the timestep interval between restart files. Instead it means an event interval for executed events. Thus a frequency of 1 means write a restart file every time an event is executed. A frequency of 10 means write a restart file every 10th executed event. When an input script reads a restart file from a previous TAD run, the new script can be run on a different number of replicas or processors.

Note that within a single state, the dynamics will typically temporarily continue beyond the event that is ultimately chosen, until the stopping criterionis satisfied. When the event is eventually executed, the timestep counter is reset to the value when the event was detected. Similarly, after each quench and NEB minimization, the timestep counter is reset to the value at the start of the minimization. This means that the timesteps listed in the replica log files do not always increase monotonically. However, the timestep values printed to the master log file, dump files, and restart files are always monotonically increasing.

Restrictions:

This command can only be used if LAMMPS was built with the REPLICA package. See the Making LAMMPS section for more info on packages.

N setting must be integer multiple of *t_event*.

Runs restarted from restart files written during a TAD run will only produce identical results if the user-specified integrator supports exact restarts. So fix nvt will produce an exact restart, but fix langevin will not.

This command cannot be used when any fixes are defined that keep track of elapsed time to perform time-dependent operations. Examples include the "ave" fixes such as fix ave/spatial. Also fix dt/reset and fix deposit.

Related commands:

compute event/displace, min_modify, min_style, run_style, minimize, temper, neb, prd

Default:

The option defaults are *min* = 0.1 0.1 40 50, *neb* = 0.01 100 100 10, *neb_style* = *quickmin*, *neb_step* = the same timestep set by the timestep command, and *neb_log* = "none".

(Voter) Sorensen and Voter, J Chem Phys, 112, 9599 (2000)

(Voter2) Voter, Montalenti, Germann, Annual Review of Materials Research 32, 321 (2002).

temper command

Syntax:

```
temper N M temp fix-ID seed1 seed2 index
```

- N = total # of timesteps to run
- M = attempt a tempering swap every this many steps
- temp = initial temperature for this ensemble
- fix-ID = ID of the fix that will control temperature during the run
- seed1 = random # seed used to decide on adjacent temperature to partner with
- seed2 = random # seed for Boltzmann factor in Metropolis swap
- index = which temperature (0 to N-1) I am simulating (optional)

Examples:

```
temper 100000 100 $t tempfix 0 58728
temper 40000 100 $t tempfix 0 32285 $w
```

Description:

Run a parallel tempering or replica exchange simulation using multiple replicas (ensembles) of a system. Two or more replicas must be used.

Each replica runs on a partition of one or more processors. Processor partitions are defined at run-time using the -partition command-line switch; see Section_start 6 of the manual. Note that if you have MPI installed, you can run a multi-replica simulation with more replicas (partitions) than you have physical processors, e.g you can run a 10-replica simulation on one or two processors. You will simply not get the performance speed-up you would see with one or more physical processors per replica. See this section of the manual for further discussion.

Each replica's temperature is controlled at a different value by a fix with *fix-ID* that controls temperature. Possible fix styles are nvt, temp/berendsen, langevin and temp/rescale. The desired temperature is specified by *temp*, which is typically a variable previously set in the input script, so that each partition is assigned a different temperature. See the variable command for more details. For example:

```
variable t world 300.0 310.0 320.0 330.0
fix myfix all nvt temp $t $t 100.0
temper 100000 100 $t myfix 3847 58382
```

would define 4 temperatures, and assign one of them to the thermostat used by each replica, and to the temper command.

As the tempering simulation runs for *N* timesteps, a temperature swap between adjacent ensembles will be attempted every *M* timesteps. If *seed1* is 0, then the swap attempts will alternate between odd and even pairings. If *seed1* is non-zero then it is used as a seed in a random number generator to randomly choose an odd or even pairing each time. Each attempted swap of temperatures is either accepted or rejected based on a Boltzmann-weighted Metropolis criterion which uses *seed2* in the random number generator.

As a tempering run proceeds, multiple log files and screen output files are created, one per replica. By default these files are named log.lammps.M and screen.M where M is the replica number from 0 to N-1, with N = # of replicas. See the section on command-line switches for info on how to change these names.

The main screen and log file (log.lammps) will list information about which temperature is assigned to each replica at each thermodynamic output timestep. E.g. for a simulation with 16 replicas:

```
Running on 16 partitions of processors
Step T0 T1 T2 T3 T4 T5 T6 T7 T8 T9 T10 T11 T12 T13 T14 T15
0    0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
500  1 0 3 2 5 4 6 7 8 9 10 11 12 13 14 15
1000 2 0 4 1 5 3 6 7 8 9 10 11 12 14 13 15
1500 2 1 4 0 5 3 6 7 9 8 10 11 12 14 13 15
2000 2 1 3 0 6 4 5 7 10 8 9 11 12 14 13 15
2500 2 1 3 0 6 4 5 7 11 8 9 10 12 14 13 15
...
```

The column headings T0 to TN-1 mean which temperature is currently assigned to the replica 0 to N-1. Thus the columns represent replicas and the value in each column is its temperature (also numbered 0 to N-1). For example, a 0 in the 4th column (column T3, step 2500) means that the 4th replica is assigned temperature 0, i.e. the lowest temperature. You can verify this time sequence of temperature assignments for the Nth replica by comparing the Nth column of screen output to the thermodynamic data in the corresponding log.lammps.N or screen.N files as time proceeds.

You can have each replica create its own dump file in the following manner:

```
variable rep world 0 1 2 3 4 5 6 7
dump 1 all atom 1000 dump.temper.$rep
```

NOTE: Each replica's dump file will contain a continuous trajectory for its atoms where the temperature varies over time as swaps take place involving that replica. If you want a series of dump files, each with snapshots (from all replicas) that are all at a single temperature, then you will need to post-process the dump files using the information from the log.lammps file. E.g. you could produce one dump file with snapshots at 300K (from all replicas), another with snapshots at 310K, etc. Note that these new dump files will not contain "continuous trajectories" for individual atoms, because two successive snapshots (in time) may be from different replicas.

The last argument *index* in the temper command is optional and is used when restarting a tempering run from a set of restart files (one for each replica) which had previously swapped to new temperatures. The *index* value (from 0 to N-1, where N is the # of replicas) identifies which temperature the replica was simulating on the timestep the restart files were written. Obviously, this argument must be a variable so that each partition has the correct value. Set the variable to the *N* values listed in the log file for the previous run for the replica temperatures at that timestep. For example if the log file listed the following for a simulation with 5 replicas:

```
500000 2 4 0 1 3
```

then a setting of

```
variable w world 2 4 0 1 3
```

would be used to restart the run with a tempering command like the example above with $w as the last argument.

Restrictions:

This command can only be used if LAMMPS was built with the REPLICA package. See the Making LAMMPS section for more info on packages.

Related commands:

variable, prd, neb

Default: none

thermo command

Syntax:

```
thermo N
```

- N = output thermodynamics every N timesteps
- N can be a variable (see below)

Examples:

```
thermo 100
```

Description:

Compute and print thermodynamic info (e.g. temperature, energy, pressure) on timesteps that are a multiple of N and at the beginning and end of a simulation. A value of 0 will only print thermodynamics at the beginning and end.

The content and format of what is printed is controlled by the thermo_style and thermo_modify commands.

Instead of a numeric value, N can be specifed as an equal-style variable, which should be specified as v_name, where name is the variable name. In this case, the variable is evaluated at the beginning of a run to determine the next timestep at which thermodynamic info will be written out. On that timestep, the variable will be evaluated again to determine the next timestep, etc. Thus the variable should return timestep values. See the stagger() and logfreq() and stride() math functions for equal-style variables, as examples of useful functions to use in this context. Other similar math functions could easily be added as options for equal-style variables.

For example, the following commands will output thermodynamic info at timesteps 0,10,20,30,100,200,300,1000,2000,etc:

```
variable        s equal logfreq(10,3,10)
thermo          v_s
```

Restrictions: none

Related commands:

thermo_style, thermo_modify

Default:

```
thermo 0
```

thermo_modify command

Syntax:

```
thermo_modify keyword value ...
```

- one or more keyword/value pairs may be listed

```
keyword = lost or lost/bond or norm or flush or line or format or temp or press:l
  lost value = error or warn or ignore
  lost/bond value = error or warn or ignore
  norm value = yes or no
  flush value = yes or no
  line value = one or multi
  format values = int string or float string or M string
    M = integer from 1 to N, where N = # of quantities being printed
    string = C-style format string
  temp value = compute ID that calculates a temperature
  press value = compute ID that calculates a pressure
```

Examples:

```
thermo_modify lost ignore flush yes
thermo_modify temp myTemp format 3 %15.8g
thermo_modify line multi format float %g
```

Description:

Set options for how thermodynamic information is computed and printed by LAMMPS.

NOTE: These options apply to the currently defined thermo style. When you specify a thermo_style command, all thermodynamic settings are restored to their default values, including those previously reset by a thermo_modify command. Thus if your input script specifies a thermo_style command, you should use the thermo_modify command after it.

The *lost* keyword determines whether LAMMPS checks for lost atoms each time it computes thermodynamics and what it does if atoms are lost. An atom can be "lost" if it moves across a non-periodic simulation box boundary or if it moves more than a box length outside the simulation domain (or more than a processor sub-domain length) before reneighboring occurs. The latter case is typically due to bad dynamics, e.g. too large a timestep or huge forces and velocities. If the value is *ignore*, LAMMPS does not check for lost atoms. If the value is *error* or *warn*, LAMMPS checks and either issues an error or warning. The code will exit with an error and continue with a warning. A warning will only be issued once, the first time an atom is lost. This can be a useful debugging option.

The *lost/bond* keyword determines whether LAMMPS throws an error or not if an atom in a bonded interaction (bond, angle, etc) cannot be found when it creates bonded neighbor lists. By default this is a fatal error. However in some scenarios it may be desirable to only issue a warning or ignore it and skip the computation of the missing bond, angle, etc. An example would be when gas molecules in a vapor are drifting out of the box through a fixed boundary condition (see the boundary command). In this case one atom may be deleted before the rest of the molecule is, on a later timestep.

The *norm* keyword determines whether various thermodynamic output values are normalized by the number of atoms or not, depending on whether it is set to *yes* or *no*. Different unit styles have different defaults for this

setting (see below). Even if *norm* is set to *yes*, a value is only normalized if it is an "extensive" quantity, meaning that it scales with the number of atoms in the system. For the thermo keywords described by the doc page for the thermo_style command, all energy-related keywords are extensive, such as *pe* or *ebond* or *enthalpy*. Other keywords such as *temp* or *press* are "intensive" meaning their value is independent (in a statistical sense) of the number of atoms in the system and thus are never normalized. For thermodynamic output values extracted from fixes and computes in a thermo_style custom command, the doc page for the individual fix or compute lists whether the value is "extensive" or "intensive" and thus whether it is normalized. Thermodynamic output values calculated by a variable formula are assumed to be "intensive" and thus are never normalized. You can always include a divide by the number of atoms in the variable formula if this is not the case.

The *flush* keyword invokes a flush operation after thermodynamic info is written to the log file. This insures the output in that file is current (no buffering by the OS), even if LAMMPS halts before the simulation completes.

The *line* keyword determines whether thermodynamics will be printed as a series of numeric values on one line or in a multi-line format with 3 quantities with text strings per line and a dashed-line header containing the timestep and CPU time. This modify option overrides the *one* and *multi* thermo_style settings.

The *format* keyword sets the numeric format of individual printed quantities. The *int* and *float* keywords set the format for all integer or floating-point quantities printed. The setting with a numeric value M (e.g. format 5 %10.4g) sets the format of the Mth value printed in each output line, e.g. the 5th column of output in this case. If the format for a specific column has been set, it will take precedent over the *int* or *float* setting.

NOTE: The thermo output values *step* and *atoms* are stored internally as 8-byte signed integers, rather than the usual 4-byte signed integers. When specifying the "format int" keyword you can use a "%d"-style format identifier in the format string and LAMMPS will convert this to the corresponding "%lu" form when it is applied to those keywords. However, when specifying the "format M string" keyword for *step* and *natoms*, you should specify a string appropriate for an 8-byte signed integer, e.g. one with "%ld".

The *temp* keyword is used to determine how thermodynamic temperature is calculated, which is used by all thermo quantities that require a temperature ("temp", "press", "ke", "etotal", "enthalpy", "pxx", etc). The specified compute ID must have been previously defined by the user via the compute command and it must be a style of compute that calculates a temperature. As described in the thermo_style command, thermo output uses a default compute for temperature with ID = *thermo_temp*. This option allows the user to override the default.

The *press* keyword is used to determine how thermodynamic pressure is calculated, which is used by all thermo quantities that require a pressure ("press", "enthalpy", "pxx", etc). The specified compute ID must have been previously defined by the user via the compute command and it must be a style of compute that calculates a pressure. As described in the thermo_style command, thermo output uses a default compute for pressure with ID = *thermo_press*. This option allows the user to override the default.

NOTE: If both the *temp* and *press* keywords are used in a single thermo_modify command (or in two separate commands), then the order in which the keywords are specified is important. Note that a pressure compute defines its own temperature compute as an argument when it is specified. The *temp* keyword will override this (for the pressure compute being used by thermodynamics), but only if the *temp* keyword comes after the *press* keyword. If the *temp* keyword comes before the *press* keyword, then the new pressure compute specified by the *press* keyword will be unaffected by the *temp* setting.

Restrictions: none

Related commands:

thermo, thermo_style

Default:

The option defaults are lost = error, norm = yes for unit style of *lj*, norm = no for unit style of *real* and *metal*, flush = no, and temp/press = compute IDs defined by thermo_style.

The defaults for the line and format options depend on the thermo style. For styles "one" and "custom", the line and format defaults are "one", "%8d", and "%12.8g". For style "multi", the line and format defaults are "multi", "%8d", and "%14.4f".

thermo_style command

Syntax:

```
thermo_style style args
```

- style = *one* or *multi* or *custom*
- args = list of arguments for a particular style

```
one args = none
  multi args = none
  custom args = list of keywords
    possible keywords = step, elapsed, elaplong, dt, time,
                        cpu, tpcpu, spcpu, cpuremain, part,
                        atoms, temp, press, pe, ke, etotal, enthalpy,
                        evdwl, ecoul, epair, ebond, eangle, edihed, eimp,
                        emol, elong, etail,
                        vol, density, lx, ly, lz, xlo, xhi, ylo, yhi, zlo, zhi,
                        xy, xz, yz, xlat, ylat, zlat,
                        bonds, angles, dihedrals, impropers,
                        pxx, pyy, pzz, pxy, pxz, pyz,
                        fmax, fnorm, nbuild, ndanger,
                        cella, cellb, cellc, cellalpha, cellbeta, cellgamma,
                        c_ID, c_ID[I], c_ID[I][J],
                        f_ID, f_ID[I], f_ID[I][J],
                        v_name
      step = timestep
      elapsed = timesteps since start of this run
      elaplong = timesteps since start of initial run in a series of runs
      dt = timestep size
      time = simulation time
      cpu = elapsed CPU time in seconds
      tpcpu = time per CPU second
      spcpu = timesteps per CPU second
      cpuremain = estimated CPU time remaining in run
      part = which partition (0 to Npartition-1) this is
      atoms = # of atoms
      temp = temperature
      press = pressure
      pe = total potential energy
      ke = kinetic energy
      etotal = total energy (pe + ke)
      enthalpy = enthalpy (etotal + press*vol)
      evdwl = VanderWaal pairwise energy (includes etail)
      ecoul = Coulombic pairwise energy
      epair = pairwise energy (evdwl + ecoul + elong)
      ebond = bond energy
      eangle = angle energy
      edihed = dihedral energy
      eimp = improper energy
      emol = molecular energy (ebond + eangle + edihed + eimp)
      elong = long-range kspace energy
      etail = VanderWaal energy long-range tail correction
      vol = volume
      density = mass density of system
      lx,ly,lz = box lengths in x,y,z
      xlo,xhi,ylo,yhi,zlo,zhi = box boundaries
      xy,xz,yz = box tilt for triclinic (non-orthogonal) simulation boxes
      xlat,ylat,zlat = lattice spacings as calculated by lattice command
      bonds,angles,dihedrals,impropers = # of these interactions defined
```

```
pxx,pyy,pzz,pxy,pxz,pyz = 6 components of pressure tensor
fmax = max component of force on any atom in any dimension
fnorm = length of force vector for all atoms
nbuild = # of neighbor list builds
ndanger = # of dangerous neighbor list builds
cella,cellb,cellc = periodic cell lattice constants a,b,c
cellalpha, cellbeta, cellgamma = periodic cell angles alpha,beta,gamma
c_ID = global scalar value calculated by a compute with ID
c_ID[I] = Ith component of global vector calculated by a compute with ID
c_ID[I][J] = I,J component of global array calculated by a compute with ID
f_ID = global scalar value calculated by a fix with ID
f_ID[I] = Ith component of global vector calculated by a fix with ID
f_ID[I][J] = I,J component of global array calculated by a fix with ID
v_name = scalar value calculated by an equal-style variable with name
```

Examples:

```
thermo_style multi
thermo_style custom step temp pe etotal press vol
thermo_style custom step temp etotal c_myTemp v_abc
```

Description:

Set the style and content for printing thermodynamic data to the screen and log file.

Style *one* prints a one-line summary of thermodynamic info that is the equivalent of "thermo_style custom step temp epair emol etotal press". The line contains only numeric values.

Style *multi* prints a multiple-line listing of thermodynamic info that is the equivalent of "thermo_style custom etotal ke temp pe ebond eangle edihed eimp evdwl ecoul elong press". The listing contains numeric values and a string ID for each quantity.

Style *custom* is the most general setting and allows you to specify which of the keywords listed above you want printed on each thermodynamic timestep. Note that the keywords c_ID, f_ID, v_name are references to computes, fixes, and equal-style variables that have been defined elsewhere in the input script or can even be new styles which users have added to LAMMPS (see the Section_modify section of the documentation). Thus the *custom* style provides a flexible means of outputting essentially any desired quantity as a simulation proceeds.

All styles except *custom* have *vol* appended to their list of outputs if the simulation box volume changes during the simulation.

The values printed by the various keywords are instantaneous values, calculated on the current timestep. Time-averaged quantities, which include values from previous timesteps, can be output by using the f_ID keyword and accessing a fix that does time-averaging such as the fix ave/time command.

Options invoked by the thermo_modify command can be used to set the one- or multi-line format of the print-out, the normalization of thermodynamic output (total values versus per-atom values for extensive quantities (ones which scale with the number of atoms in the system), and the numeric precision of each printed value.

NOTE: When you use a "thermo_style" command, all thermodynamic settings are restored to their default values, including those previously set by a thermo_modify command. Thus if your input script specifies a thermo_style command, you should use the thermo_modify command after it.

Several of the thermodynamic quantities require a temperature to be computed: "temp", "press", "ke", "etotal", "enthalpy", "pxx", etc. By default this is done by using a *temperature* compute which is created when LAMMPS

starts up, as if this command had been issued:

```
compute thermo_temp all temp
```

See the compute temp command for details. Note that the ID of this compute is *thermo_temp* and the group is *all*. You can change the attributes of this temperature (e.g. its degrees-of-freedom) via the compute_modify command. Alternatively, you can directly assign a new compute (that calculates temperature) which you have defined, to be used for calculating any thermodynamic quantity that requires a temperature. This is done via the thermo_modify command.

Several of the thermodynamic quantities require a pressure to be computed: "press", "enthalpy", "pxx", etc. By default this is done by using a *pressure* compute which is created when LAMMPS starts up, as if this command had been issued:

```
compute thermo_press all pressure thermo_temp
```

See the compute pressure command for details. Note that the ID of this compute is *thermo_press* and the group is *all*. You can change the attributes of this pressure via the compute_modify command. Alternatively, you can directly assign a new compute (that calculates pressure) which you have defined, to be used for calculating any thermodynamic quantity that requires a pressure. This is done via the thermo_modify command.

Several of the thermodynamic quantities require a potential energy to be computed: "pe", "etotal", "ebond", etc. This is done by using a *pe* compute which is created when LAMMPS starts up, as if this command had been issued:

```
compute thermo_pe all pe
```

See the compute pe command for details. Note that the ID of this compute is *thermo_pe* and the group is *all*. You can change the attributes of this potential energy via the compute_modify command.

The kinetic energy of the system *ke* is inferred from the temperature of the system with 1/2 Kb T of energy for each degree of freedom. Thus, using different compute commands for calculating temperature, via the thermo_modify temp command, may yield different kinetic energies, since different computes that calculate temperature can subtract out different non-thermal components of velocity and/or include different degrees of freedom (translational, rotational, etc).

The potential energy of the system *pe* will include contributions from fixes if the fix_modify thermo option is set for a fix that calculates such a contribution. For example, the fix wall/lj93 fix calculates the energy of atoms interacting with the wall. See the doc pages for "individual fixes" to see which ones contribute.

A long-range tail correction *etail* for the VanderWaal pairwise energy will be non-zero only if the pair_modify tail option is turned on. The *etail* contribution is included in *evdwl*, *epair*, *pe*, and *etotal*, and the corresponding tail correction to the pressure is included in *press* and *pxx*, *pyy*, etc.

The *step*, *elapsed*, and *elaplong* keywords refer to timestep count. *Step* is the current timestep, or iteration count when a minimization is being performed. *Elapsed* is the number of timesteps elapsed since the beginning of this run. *Elaplong* is the number of timesteps elapsed since the beginning of an initial run in a series of runs. See the *start* and *stop* keywords for the run for info on how to invoke a series of runs that keep track of an initial starting time. If these keywords are not used, then *elapsed* and *elaplong* are the same value.

The *dt* keyword is the current timestep size in time units. The *time* keyword is the current elapsed simulation time, also in time units, which is simply (step*dt) if the timestep size has not changed and the timestep has not been reset. If the timestep has changed (e.g. via fix dt/reset) or the timestep has been reset (e.g. via the "reset_timestep"

command), then the simulation time is effectively a cummulative value up to the current point.

The *cpu* keyword is elapsed CPU seconds since the beginning of this run. The *tpcpu* and *spcpu* keywords are measures of how fast your simulation is currently running. The *tpcpu* keyword is simulation time per CPU second, where simulation time is in time units. E.g. for metal units, the *tpcpu* value would be picoseconds per CPU second. The *spcpu* keyword is the number of timesteps per CPU second. Both quantities are on-the-fly metrics, measured relative to the last time they were invoked. Thus if you are printing out thermodyamic output every 100 timesteps, the two keywords will continually output the time and timestep rate for the last 100 steps. The *tpcpu* keyword does not attempt to track any changes in timestep size, e.g. due to using the fix dt/reset command.

The *cpuremain* keyword estimates the CPU time remaining in the current run, based on the time elapsed thus far. It will only be a good estimate if the CPU time/timestep for the rest of the run is similar to the preceding timesteps. On the initial timestep the value will be 0.0 since there is no history to estimate from. For a minimization run performed by the "minimize" command, the estimate is based on the *maxiter* parameter, assuming the minimization will proceed for the maximum number of allowed iterations.

The *part* keyword is useful for multi-replica or multi-partition simulations to indicate which partition this output and this file corresponds to, or for use in a variable to append to a filename for output specific to this partition. See Section_start 7 of the manual for details on running in multi-partition mode.

The *fmax* and *fnorm* keywords are useful for monitoring the progress of an energy minimization. The *fmax* keyword calculates the maximum force in any dimension on any atom in the system, or the infinity-norm of the force vector for the system. The *fnorm* keyword calculates the 2-norm or length of the force vector.

The *nbuild* and *ndanger* keywords are useful for monitoring neighbor list builds during a run. Note that both these values are also printed with the end-of-run statistics. The *nbuild* keyword is the number of re-builds during the current run. The *ndanger* keyword is the number of re-builds that LAMMPS considered potentially "dangerous". If atom movement triggered neighbor list rebuilding (see the neigh_modify command), then dangerous reneighborings are those that were triggered on the first timestep atom movement was checked for. If this count is non-zero you may wish to reduce the delay factor to insure no force interactions are missed by atoms moving beyond the neighbor skin distance before a rebuild takes place.

The keywords *cella*, *cellb*, *cellc*, *cellalpha*, *cellbeta*, *cellgamma*, correspond to the usual crystallographic quantities that define the periodic unit cell of a crystal. See this section of the doc pages for a geometric description of triclinic periodic cells, including a precise defintion of these quantities in terms of the internal LAMMPS cell dimensions *lx*, *ly*, *lz*, *yz*, *xz*, *xy*.

The *c_ID* and *c_ID[I]* and *c_ID[I][J]* keywords allow global values calculated by a compute to be output. As discussed on the compute doc page, computes can calculate global, per-atom, or local values. Only global values can be referenced by this command. However, per-atom compute values can be referenced in a variable and the variable referenced by thermo_style custom, as discussed below.

The ID in the keyword should be replaced by the actual ID of a compute that has been defined elsewhere in the input script. See the compute command for details. If the compute calculates a global scalar, vector, or array, then the keyword formats with 0, 1, or 2 brackets will reference a scalar value from the compute.

Note that some computes calculate "intensive" global quantities like temperature; others calculate "extensive" global quantities like kinetic energy that are summed over all atoms in the compute group. Intensive quantities are printed directly without normalization by thermo_style custom. Extensive quantities may be normalized by the total number of atoms in the simulation (NOT the number of atoms in the compute group) when output, depending on the thermo_modify norm option being used.

The *f_ID* and *f_ID[I]* and *f_ID[I][J]* keywords allow global values calculated by a fix to be output. As discussed on the fix doc page, fixes can calculate global, per-atom, or local values. Only global values can be referenced by this command. However, per-atom fix values can be referenced in a variable and the variable referenced by thermo_style custom, as discussed below.

The ID in the keyword should be replaced by the actual ID of a fix that has been defined elsewhere in the input script. See the fix command for details. If the fix calculates a global scalar, vector, or array, then the keyword formats with 0, 1, or 2 brackets will reference a scalar value from the fix.

Note that some fixes calculate "intensive" global quantities like timestep size; others calculate "extensive" global quantities like energy that are summed over all atoms in the fix group. Intensive quantities are printed directly without normalization by thermo_style custom. Extensive quantities may be normalized by the total number of atoms in the simulation (NOT the number of atoms in the fix group) when output, depending on the thermo_modify norm option being used.

The *v_name* keyword allow the current value of a variable to be output. The name in the keyword should be replaced by the variable name that has been defined elsewhere in the input script. Only equal-style variables can be referenced. See the variable command for details. Variables of style *equal* can reference per-atom properties or thermodynamic keywords, or they can invoke other computes, fixes, or variables when evaluated, so this is a very general means of creating thermodynamic output.

Note that equal-style variables are assumed to be "intensive" global quantities, which are thus printed as-is, without normalization by thermo_style custom. You can include a division by "natoms" in the variable formula if this is not the case.

Restrictions:

This command must come after the simulation box is defined by a read_data, read_restart, or create_box command.

Related commands:

thermo, thermo_modify, fix_modify, compute temp, compute pressure

Default:

```
thermo_style one
```

timer command

Syntax:

```
timer args
```

- *args* = one or more of *off* or *loop* or *normal* or *full* or *sync* or *nosync*

```
  off = do not collect or print any timing information
    loop = collect only the total time for the simulation loop
    normal = collect timer information broken down by sections (default)
    full = like normal but also include CPU and thread utilzation
    sync = explicitly synchronize MPI tasks between sections
    nosync = do not synchronize MPI tasks between sections (default)
```

Examples:

```
timer full sync
timer loop
```

Description:

Select the level of detail LAMMPS performs its CPU timings.

During a simulation run LAMMPS collects information about how much time is spent in different sections of the code and thus can provide valuable information for determining performance and load imbalance problems. This can be done at different levels of detail and accuracy. For more information about the timing output, see this discussion of screen output.

The *off* setting will turn all time measurements off. The *loop* setting will only measure the total time for a run and not collect any detailed per section information. With the *normal* setting, timing information for portions of the timestep (pairwise calculations, neighbor list construction, output, etc) are collected as well as information about load imbalances for those sections across procsessors. The *full* setting adds information about CPU utilization and thread utilization, when multi-threading is enabled.

With the *sync* setting, all MPI tasks are synchronized at each timer call which meaures load imbalance more accuractly, though it can also slow down the simulation. Using the *nosync* setting (which is the default) turns off this synchronization.

Multiple keywords can be specified. For keywords that are mutually exclusive, the last one specified takes effect.

NOTE: Using the *full* and *sync* options provides the most detailed and accurate timing information, but can also have a negative performance impact due to the overhead of the many required system calls. It is thus recommended to use these settings only when testing tests to identify performance bottlenecks. For calculations with few atoms or a very large number of processors, even the *normal* setting can have a measurable negative performance impact. In those cases you can just use the *loop* or *off* setting.

Restrictions: none

Related commands:

run post no, kspace_modify fftbench

Default:

timer normal nosync

timestep command

Syntax:

```
timestep dt
```

- dt = timestep size (time units)

Examples:

```
timestep 2.0
timestep 0.003
```

Description:

Set the timestep size for subsequent molecular dynamics simulations. See the units command for the time units associated with each choice of units that LAMMPS supports.

The default value for the timestep size also depends on the choice of units for the simulation; see the default values below.

When the run style is *respa*, dt is the timestep for the outer loop (largest) timestep.

Restrictions: none

Related commands:

fix dt/reset, run, run_style respa, units

Default:

choice of units	time units	default timestep size
lj	tau	0.005 tau
real	fmsec	1.0 fmsec
metal	psec	0.001 psec
si	sec	1.0e-8 sec (10 nsec)
cgs	sec	1.0e-8 sec (10 nsec)
electron	fmsec	0.001 fmsec
micro	usec	2.0 usec
nano	nsec	0.00045 nsec

Tutorial for Thermalized Drude oscillators in LAMMPS

This tutorial explains how to use Drude oscillators in LAMMPS to simulate polarizable systems using the USER-DRUDE package. As an illustration, the input files for a simulation of 250 phenol molecules are documented. First of all, LAMMPS has to be compiled with the USER-DRUDE package activated. Then, the data file and input scripts have to be modified to include the Drude dipoles and how to handle them.

Overview of Drude induced dipoles

Polarizable atoms acquire an induced electric dipole moment under the action of an external electric field, for example the electric field created by the surrounding particles. Drude oscillators represent these dipoles by two fixed charges: the core (DC) and the Drude particle (DP) bound by a harmonic potential. The Drude particle can be thought of as the electron cloud whose center can be displaced from the position of the the corresponding nucleus.

The sum of the masses of a core-Drude pair should be the mass of the initial (unsplit) atom, $m_C + m_D = m$. The sum of their charges should be the charge of the initial (unsplit) atom, $q_C + q_D = q$. A harmonic potential between the core and Drude partners should be present, with force constant k_D and an equilibrium distance of zero. The (half-)stiffness of the harmonic bond $K_D = k_D/2$ and the Drude charge q_D are related to the atom polarizability α by

$$K_D = \frac{1}{2} \frac{q_D^2}{\alpha}$$

Ideally, the mass of the Drude particle should be small, and the stiffness of the harmonic bond should be large, so that the Drude particle remains close ot the core. The values of Drude mass, Drude charge, and force constant can be chosen following different strategies, as in the following examples of polarizable force fields.

- Lamoureux and Roux suggest adopting a global half-stiffness, K_D = 500 kcal/(mol Å^2) — which corresponds to a force constant k_D = 4184 kJ/(mol Å^2) — for all types of core-Drude bond, a global mass m_D = 0.4 g/mol (or u) for all types of Drude particle, and to calculate the Drude charges for individual atom types from the atom polarizabilities using equation (1). This choice is followed in the polarizable CHARMM force field.
- Schroeder and Steinhauser suggest adopting a global charge q_D = -1.0e and a global mass m_D = 0.1 g/mol (or u) for all Drude particles, and to calculate the force constant for each type of core-Drude bond from equation (1). The timesteps used by these authors are between 0.5 and 2 fs, with the degrees of freedom of the Drude oscillators kept cold at 1 K. In both these force fields hydrogen atoms are treated as non-polarizable.

The motion of of the Drude particles can be calculated by minimizing the energy of the induced dipoles at each timestep, by an interative, self-consistent procedure. The Drude particles can be massless and therefore do not contribute to the kinetic energy. However, the relaxed method is computationall slow. An extended-lagrangian method can be used to calculate the positions of the Drude particles, but this requires them to have mass. It is important in this case to decouple the degrees of freedom associated with the Drude oscillators from those of the normal atoms. Thermalizing the Drude dipoles at temperatures comparable to the rest of the simulation leads to several problems (kinetic energy transfer, very short timestep, etc.), which can be remediated by the "cold Drude" technique (Lamoureux and Roux).

Two closely related models are used to represent polarization through "charges on a spring": the core-shell model and the Drude model. Although the basic idea is the same, the core-shell model is normally used for ionic/crystalline materials, whereas the Drude model is normally used for molecular systems and fluid states. In ionic crystals the symmetry around each ion and the distance between them are such that the core-shell model is sufficiently stable. But to be applicable to molecular/covalent systems the Drude model includes two important

features:

1. The possibility to thermostat the additional degrees of freedom associated with the induced dipoles at very low temperature, in terms of the reduced coordinates of the Drude particles with respect to their cores. This makes the trajectory close to that of relaxed induced dipoles.
2. The Drude dipoles on covalently bonded atoms interact too strongly due to the short distances, so an atom may capture the Drude particle (shell) of a neighbor, or the induced dipoles within the same molecule may align too much. To avoid this, damping at short of the interactions between the point charges composing the induced dipole can be done by Thole functions.

Preparation of the data file

The data file is similar to a standard LAMMPS data file for *atom_style full*. The DPs and the *harmonic bonds* connecting them to their DC should appear in the data file as normal atoms and bonds.

You can use the *polarizer* tool (Python script distributed with the USER-DRUDE package) to convert a non-polarizable data file (here *data.102494.lmp*) to a polarizable data file (*data-p.lmp*)

```
polarizer -q -f phenol.dff data.102494.lmp data-p.lmp
```

This will automatically insert the new atoms and bonds. The masses and charges of DCs and DPs are computed from *phenol.dff*, as well as the DC-DP bond constants. The file *phenol.dff* contains the polarizabilities of the atom types and the mass of the Drude particles, for instance:

```
# units: kJ/mol, A, deg
# kforce is in the form k/2 r_D^2
# type  m_D/u   q_D/e    k_D   alpha/A3  thole
OH      0.4    -1.0    4184.0   0.63     0.67
CA      0.4    -1.0    4184.0   1.36     2.51
CAI     0.4    -1.0    4184.0   1.09     2.51
```

The hydrogen atoms are absent from this file, so they will be treated as non-polarizable atoms. In the non-polarizable data file *data.102494.lmp*, atom names corresponding to the atom type numbers have to be specified as comments at the end of lines of the *Masses* section. You probably need to edit it to add these names. It should look like

```
Masses

1 12.011 # CAI
2 12.011 # CA
3 15.999 # OH
4 1.008  # HA
5 1.008  # HO
```

Basic input file

The atom style should be set to (or derive from) *full*, so that you can define atomic charges and molecular bonds, angles, dihedrals...

The *polarizer* tool also outputs certain lines related to the input script (the use of these lines will be explained below). In order for LAMMPS to recognize that you are using Drude oscillators, you should use the fix *drude*. The command is

```
fix DRUDE all drude C C C N N D D D
```

The N, C, D following the *drude* keyword have the following meaning: There is one tag for each atom type. This tag is C for DCs, D for DPs and N for non-polarizable atoms. Here the atom types 1 to 3 (C and O atoms) are DC, atom types 4 and 5 (H atoms) are non-polarizable and the atom types 6 to 8 are the newly created DPs.

By recognizing the fix *drude*, LAMMPS will find and store matching DC-DP pairs and will treat DP as equivalent to their DC in the *special bonds* relations. It may be necessary to extend the space for storing such special relations. In this case extra space should be reserved by using the *extra* keyword of the *special_bonds* command. With our phenol, there is 1 more special neighbor for which space is required. Otherwise LAMMPS crashes and gives the required value.

```
special_bonds lj/coul 0.0 0.0 0.5 extra 1
```

Let us assume we want to run a simple NVT simulation at 300 K. Note that Drude oscillators need to be thermalized at a low temperature in order to approximate a self-consistent field (SCF), therefore it is not possible to simulate an NVE ensemble with this package. Since dipoles are approximated by a charged DC-DP pair, the *pair_style* must include Coulomb interactions, for instance *lj/cut/coul/long* with *kspace_style pppm*. For example, with a cutoff of 10. and a precision 1.e-4:

```
pair_style lj/cut/coul/long 10.0
kspace_style pppm 1.0e-4
```

As compared to the non-polarizable input file, *pair_coeff* lines need to be added for the DPs. Since the DPs have no Lennard-Jones interactions, their *epsilon* is 0. so the only *pair_coeff* line that needs to be added is

```
pair_coeff * 6* 0.0 0.0 # All-DPs
```

Now for the thermalization, the simplest choice is to use the fix langevin/drude.

```
fix LANG all langevin/drude 300. 100 12435 1. 20 13977
```

This applies a Langevin thermostat at temperature 300. to the centers of mass of the DC-DP pairs, with relaxation time 100 and with random seed 12345. This fix applies also a Langevin thermostat at temperature 1. to the relative motion of the DPs around their DCs, with relaxation time 20 and random seed 13977. Only the DCs and non-polarizable atoms need to be in this fix's group. LAMMPS will thermostate the DPs together with their DC. For this, ghost atoms need to know their velocities. Thus you need to add the following command:

```
comm_modify vel yes
```

In order to avoid that the center of mass of the whole system drifts due to the random forces of the Langevin thermostat on DCs, you can add the *zero yes* option at the end of the fix line.

If the fix *shake* is used to constrain the C-H bonds, it should be invoked after the fix *langevin/drude* for more accuracy.

```
fix SHAKE ATOMS shake 0.0001 20 0 t 4 5
```

NOTE: The group of the fix *shake* must not include the DPs. If the group *ATOMS* is defined by non-DPs atom types, you could use

Since the fix *langevin/drude* does not perform time integration (just modification of forces but no position/velocity updates), the fix *nve* should be used in conjunction.

```
fix NVE all nve
```

Finally, do not forget to update the atom type elements if you use them in a *dump_modify ... element ...* command, by adding the element type of the DPs. Here for instance

```
dump DUMP all custom 10 dump.lammpstrj id mol type element x y z ix iy iz
dump_modify DUMP element C C O H H D D D
```

The input file should now be ready for use!

You will notice that the global temperature *thermo_temp* computed by LAMMPS is not 300. K as wanted. This is because LAMMPS treats DPs as standard atoms in his default compute. If you want to output the temperatures of the DC-DP pair centers of mass and of the DPs relative to their DCs, you should use the compute temp_drude

```
compute TDRUDE all temp/drude
```

And then output the correct temperatures of the Drude oscillators using *thermo_style custom* with respectively *c_TDRUDE[1]* and *c_TDRUDE[2]*. These should be close to 300.0 and 1.0 on average.

```
thermo_style custom step temp c_TDRUDE[1] c_TDRUDE[2]
```

Thole screening

Dipolar interactions represented by point charges on springs may not be stable, for example if the atomic polarizability is too high for instance, a DP can escape from its DC and be captured by another DC, which makes the force and energy diverge and the simulation crash. Even without reaching this extreme case, the correlation between nearby dipoles on the same molecule may be exagerated. Often, special bond relations prevent bonded neighboring atoms to see the charge of each other's DP, so that the problem does not always appear. It is possible to use screened dipole dipole interactions by using the *pair_style thole*. This is implemented as a correction to the Coulomb pair_styles, which dampens at short distance the interactions between the charges representing the induced dipoles. It is to be used as *hybrid/overlay* with any standard *coul* pair style. In our example, we would use

```
pair_style hybrid/overlay lj/cut/coul/long 10.0 thole 2.6 10.0
```

This tells LAMMPS that we are using two pair_styles. The first one is as above (*lj/cut/coul/long 10.0*). The second one is a *thole* pair_style with default screening factor 2.6 (Noskov) and cutoff 10.0.

Since *hybrid/overlay* does not support mixing rules, the interaction coefficients of all the pairs of atom types with i < j should be explicitly defined. The output of the *polarizer* script can be used to complete the *pair_coeff* section of the input file. In our example, this will look like:

```
pair_coeff    1    1 lj/cut/coul/long    0.0700   3.550
pair_coeff    1    2 lj/cut/coul/long    0.0700   3.550
pair_coeff    1    3 lj/cut/coul/long    0.1091   3.310
pair_coeff    1    4 lj/cut/coul/long    0.0458   2.985
pair_coeff    2    2 lj/cut/coul/long    0.0700   3.550
pair_coeff    2    3 lj/cut/coul/long    0.1091   3.310
pair_coeff    2    4 lj/cut/coul/long    0.0458   2.985
pair_coeff    3    3 lj/cut/coul/long    0.1700   3.070
pair_coeff    3    4 lj/cut/coul/long    0.0714   2.745
pair_coeff    4    4 lj/cut/coul/long    0.0300   2.420
pair_coeff    *    5 lj/cut/coul/long    0.0000   0.000
pair_coeff    *   6* lj/cut/coul/long    0.0000   0.000
pair_coeff    1    1 thole   1.090   2.510
pair_coeff    1    2 thole   1.218   2.510
pair_coeff    1    3 thole   0.829   1.590
pair_coeff    1    6 thole   1.090   2.510
pair_coeff    1    7 thole   1.218   2.510
pair_coeff    1    8 thole   0.829   1.590
```

```
pair_coeff    2    2 thole   1.360   2.510
pair_coeff    2    3 thole   0.926   1.590
pair_coeff    2    6 thole   1.218   2.510
pair_coeff    2    7 thole   1.360   2.510
pair_coeff    2    8 thole   0.926   1.590
pair_coeff    3    3 thole   0.630   0.670
pair_coeff    3    6 thole   0.829   1.590
pair_coeff    3    7 thole   0.926   1.590
pair_coeff    3    8 thole   0.630   0.670
pair_coeff    6    6 thole   1.090   2.510
pair_coeff    6    7 thole   1.218   2.510
pair_coeff    6    8 thole   0.829   1.590
pair_coeff    7    7 thole   1.360   2.510
pair_coeff    7    8 thole   0.926   1.590
pair_coeff    8    8 thole   0.630   0.670
```

For the *thole* pair style the coefficients are

1. the atom polarizability in units of cubic length
2. the screening factor of the Thole function (optional, default value specified by the pair_style command)
3. the cutoff (optional, default value defined by the pair_style command)

The special neighbors have charge-charge and charge-dipole interactions screened by the *coul* factors of the *special_bonds* command (0.0, 0.0, and 0.5 in the example above). Without using the pair_style *thole*, dipole-dipole interactions are screened by the same factor. By using the pair_style *thole*, dipole-dipole interactions are screened by Thole's function, whatever their special relationship (except within each DC-DP pair of course). Consider for example 1-2 neighbors: using the pair_style *thole*, their dipoles will see each other (despite the *coul* factor being 0.) and the interactions between these dipoles will be damped by Thole's function.

Thermostats and barostats

Using a Nose-Hoover barostat with the *langevin/drude* thermostat is straightforward using fix *nph* instead of *nve*. For example:

```
fix NPH all nph iso 1. 1. 500
```

It is also possible to use a Nose-Hoover instead of a Langevin thermostat. This requires to use *fix drude/transform* just before and after the time intergation fixes. The *fix drude/transform/direct* converts the atomic masses, positions, velocities and forces into a reduced representation, where the DCs transform into the centers of mass of the DC-DP pairs and the DPs transform into their relative position with respect to their DC. The *fix drude/transform/inverse* performs the reverse transformation. For a NVT simulation, with the DCs and atoms at 300 K and the DPs at 1 K relative to their DC one would use

```
fix DIRECT all drude/transform/direct
fix NVT1 ATOMS nvt temp 300. 300. 100
fix NVT2 DRUDES nvt temp 1. 1. 20
fix INVERSE all drude/transform/inverse
```

For our phenol example, the groups would be defined as

```
group ATOMS  type 1 2 3 4 5 # DCs and non-polarizable atoms
group CORES  type 1 2 3     # DCs
group DRUDES type 6 7 8     # DPs
```

Note that with the fixes *drude/transform*, it is not required to specify *comm_modify vel yes* because the fixes do it anyway (several times and for the forces also). To avoid the flying ice cube artifact (Lamoureux), where the

atoms progressively freeze and the center of mass of the whole system drifts faster and faster, the *fix momentum* can be used. For instance:

```
fix MOMENTUM all momentum 100 linear 1 1 1
```

It is a bit more tricky to run a NPT simulation with Nose-Hoover barostat and thermostat. First, the volume should be integrated only once. So the fix for DCs and atoms should be *npt* while the fix for DPs should be *nvt* (or vice versa). Second, the *fix npt* computes a global pressure and thus a global temperature whatever the fix group. We do want the pressure to correspond to the whole system, but we want the temperature to correspond to the fix group only. We must then use the *fix_modify* command for this. In the end, the block of instructions for thermostating and barostating will look like

```
compute TATOMS ATOMS temp
fix DIRECT all drude/transform/direct
fix NPT ATOMS npt temp 300. 300. 100 iso 1. 1. 500
fix_modify NPT temp TATOMS press thermo_press
fix NVT DRUDES nvt temp 1. 1. 20
fix INVERSE all drude/transform/inverse
```

Rigid bodies

You may want to simulate molecules as rigid bodies (but polarizable). Common cases are water models such as SWM4-NDP, which is a kind of polarizable TIP4P water. The rigid bodies and the DPs should be integrated separately, even with the Langevin thermostat. Let us review the different thermostats and ensemble combinations.

NVT ensemble using Langevin thermostat:

```
comm_modify vel yes
fix LANG all langevin/drude 300. 100 12435 1. 20 13977
fix RIGID ATOMS rigid/nve/small molecule
fix NVE DRUDES nve
```

NVT ensemble using Nose-Hoover thermostat:

```
fix DIRECT all drude/transform/direct
fix RIGID ATOMS rigid/nvt/small molecule temp 300. 300. 100
fix NVT DRUDES nvt temp 1. 1. 20
fix INVERSE all drude/transform/inverse
```

NPT ensemble with Langevin thermostat:

```
comm_modify vel yes
fix LANG all langevin/drude 300. 100 12435 1. 20 13977
fix RIGID ATOMS rigid/nph/small molecule iso 1. 1. 500
fix NVE DRUDES nve
```

NPT ensemble using Nose-Hoover thermostat:

```
compute TATOM ATOMS temp
fix DIRECT all drude/transform/direct
fix RIGID ATOMS rigid/npt/small molecule temp 300. 300. 100 iso 1. 1. 500
fix_modify RIGID temp TATOM press thermo_press
fix NVT DRUDES nvt temp 1. 1. 20
fix INVERSE all drude/transform/inverse
```

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uncompute command

Syntax:

```
uncompute compute-ID
```

- compute-ID = ID of a previously defined compute

Examples:

```
uncompute 2
uncompute lower-boundary
```

Description:

Delete a compute that was previously defined with a compute command. This also wipes out any additional changes made to the compute via the compute_modify command.

Restrictions: none

Related commands:

compute

Default: none

undump command

Syntax:

```
undump dump-ID
```

- dump-ID = ID of previously defined dump

Examples:

```
undump mine
undump 2
```

Description:

Turn off a previously defined dump so that it is no longer active. This closes the file associated with the dump.

Restrictions: none

Related commands:

dump

Default: none

unfix command

Syntax:

```
unfix fix-ID
```

- fix-ID = ID of a previously defined fix

Examples:

```
unfix 2
unfix lower-boundary
```

Description:

Delete a fix that was previously defined with a fix command. This also wipes out any additional changes made to the fix via the fix_modify command.

Restrictions: none

Related commands:

fix

Default: none

units command

Syntax:

```
units style
```

- style = *lj* or *real* or *metal* or *si* or *cgs* or *electron* or *micro* or *nano*

Examples:

```
units metal
units lj
```

Description:

This command sets the style of units used for a simulation. It determines the units of all quantities specified in the input script and data file, as well as quantities output to the screen, log file, and dump files. Typically, this command is used at the very beginning of an input script.

For all units except *lj*, LAMMPS uses physical constants from www.physics.nist.gov. For the definition of Kcal in real units, LAMMPS uses the thermochemical calorie = 4.184 J.

The choice you make for units simply sets some internal conversion factors within LAMMPS. This means that any simulation you perform for one choice of units can be duplicated with any other unit setting LAMMPS supports. In this context "duplicate" means the particles will have identical trajectories and all output generated by the simulation will be identical. This will be the case for some number of timesteps until round-off effects accumulate, since the conversion factors for two different unit systems are not identical to infinite precision.

To perform the same simulation in a different set of units you must change all the unit-based input parameters in your input script and other input files (data file, potential files, etc) correctly to the new units. And you must correctly convert all output from the new units to the old units when comparing to the original results. That is often not simple to do.

For style *lj*, all quantities are unitless. Without loss of generality, LAMMPS sets the fundamental quantities mass, sigma, epsilon, and the Boltzmann constant = 1. The masses, distances, energies you specify are multiples of these fundamental values. The formulas relating the reduced or unitless quantity (with an asterisk) to the same quantity with units is also given. Thus you can use the mass & sigma & epsilon values for a specific material and convert the results from a unitless LJ simulation into physical quantities.

- mass = mass or m
- distance = sigma, where x* = x / sigma
- time = tau, where t* = t (epsilon / m / sigma^2)^1/2
- energy = epsilon, where E* = E / epsilon
- velocity = sigma/tau, where v* = v tau / sigma
- force = epsilon/sigma, where f* = f sigma / epsilon
- torque = epsilon, where t* = t / epsilon
- temperature = reduced LJ temperature, where T* = T Kb / epsilon
- pressure = reduced LJ pressure, where P* = P sigma^3 / epsilon
- dynamic viscosity = reduced LJ viscosity, where eta* = eta sigma^3 / epsilon / tau
- charge = reduced LJ charge, where q* = q / (4 pi perm0 sigma epsilon)^1/2

- dipole = reduced LJ dipole, moment where *mu = mu / (4 pi perm0 sigma^3 epsilon)^1/2
- electric field = force/charge, where E* = E (4 pi perm0 sigma epsilon)^1/2 sigma / epsilon
- density = mass/volume, where rho* = rho sigma^dim

Note that for LJ units, the default mode of thermodyamic output via the thermo_style command is to normalize energies by the number of atoms, i.e. energy/atom. This can be changed via the thermo_modify norm command.

For style *real*, these are the units:

- mass = grams/mole
- distance = Angstroms
- time = femtoseconds
- energy = Kcal/mole
- velocity = Angstroms/femtosecond
- force = Kcal/mole-Angstrom
- torque = Kcal/mole
- temperature = Kelvin
- pressure = atmospheres
- dynamic viscosity = Poise
- charge = multiple of electron charge (1.0 is a proton)
- dipole = charge*Angstroms
- electric field = volts/Angstrom
- density = gram/cm^dim

For style *metal*, these are the units:

- mass = grams/mole
- distance = Angstroms
- time = picoseconds
- energy = eV
- velocity = Angstroms/picosecond
- force = eV/Angstrom
- torque = eV
- temperature = Kelvin
- pressure = bars
- dynamic viscosity = Poise
- charge = multiple of electron charge (1.0 is a proton)
- dipole = charge*Angstroms
- electric field = volts/Angstrom
- density = gram/cm^dim

For style *si*, these are the units:

- mass = kilograms
- distance = meters
- time = seconds
- energy = Joules
- velocity = meters/second
- force = Newtons
- torque = Newton-meters
- temperature = Kelvin
- pressure = Pascals

- dynamic viscosity = Pascal*second
- charge = Coulombs (1.6021765e-19 is a proton)
- dipole = Coulombs*meters
- electric field = volts/meter
- density = kilograms/meter^dim

For style *cgs*, these are the units:

- mass = grams
- distance = centimeters
- time = seconds
- energy = ergs
- velocity = centimeters/second
- force = dynes
- torque = dyne-centimeters
- temperature = Kelvin
- pressure = dyne/cm^2 or barye = 1.0e-6 bars
- dynamic viscosity = Poise
- charge = statcoulombs or esu (4.8032044e-10 is a proton)
- dipole = statcoul-cm = 10^18 debye
- electric field = statvolt/cm or dyne/esu
- density = grams/cm^dim

For style *electron*, these are the units:

- mass = atomic mass units
- distance = Bohr
- time = femtoseconds
- energy = Hartrees
- velocity = Bohr/atomic time units [1.03275e-15 seconds]
- force = Hartrees/Bohr
- temperature = Kelvin
- pressure = Pascals
- charge = multiple of electron charge (1.0 is a proton)
- dipole moment = Debye
- electric field = volts/cm

For style *micro*, these are the units:

- mass = picograms
- distance = micrometers
- time = microseconds
- energy = picogram-micrometer^2/microsecond^2
- velocity = micrometers/microsecond
- force = picogram-micrometer/microsecond^2
- torque = picogram-micrometer^2/microsecond^2
- temperature = Kelvin
- pressure = picogram/(micrometer-microsecond^2)
- dynamic viscosity = picogram/(micrometer-microsecond)
- charge = picocoulombs (1.6021765e-7 is a proton)
- dipole = picocoulomb-micrometer
- electric field = volt/micrometer

- density = picograms/micrometer^dim

For style *nano*, these are the units:

- mass = attograms
- distance = nanometers
- time = nanoseconds
- energy = attogram-nanometer^2/nanosecond^2
- velocity = nanometers/nanosecond
- force = attogram-nanometer/nanosecond^2
- torque = attogram-nanometer^2/nanosecond^2
- temperature = Kelvin
- pressure = attogram/(nanometer-nanosecond^2)
- dynamic viscosity = attogram/(nanometer-nanosecond)
- charge = multiple of electron charge (1.0 is a proton)
- dipole = charge-nanometer
- electric field = volt/nanometer
- density = attograms/nanometer^dim

The units command also sets the timestep size and neighbor skin distance to default values for each style:

- For style *lj* these are dt = 0.005 tau and skin = 0.3 sigma.
- For style *real* these are dt = 1.0 fmsec and skin = 2.0 Angstroms.
- For style *metal* these are dt = 0.001 psec and skin = 2.0 Angstroms.
- For style *si* these are dt = 1.0e-8 sec and skin = 0.001 meters.
- For style *cgs* these are dt = 1.0e-8 sec and skin = 0.1 cm.
- For style *electron* these are dt = 0.001 fmsec and skin = 2.0 Bohr.
- For style *micro* these are dt = 2.0 microsec and skin = 0.1 micrometers.
- For style *nano* these are dt = 0.00045 nanosec and skin = 0.1 nanometers.

Restrictions:

This command cannot be used after the simulation box is defined by a read_data or create_box command.

Related commands: none

Default:

```
units lj
```

variable command

Syntax:

```
variable name style args ...
```

- name = name of variable to define
- style = *delete* or *index* or *loop* or *world* or *universe* or *uloop* or *string* or *format* or *getenv* or *file* or *atomfile* or *python* or *equal* or *atom*

```
delete = no args
  index args = one or more strings
  loop args = N
    N = integer size of loop, loop from 1 to N inclusive
  loop args = N pad
    N = integer size of loop, loop from 1 to N inclusive
    pad = all values will be same length, e.g. 001, 002, ..., 100
  loop args = N1 N2
    N1,N2 = loop from N1 to N2 inclusive
  loop args = N1 N2 pad
    N1,N2 = loop from N1 to N2 inclusive
    pad = all values will be same length, e.g. 050, 051, ..., 100
  world args = one string for each partition of processors
  universe args = one or more strings
  uloop args = N
    N = integer size of loop
  uloop args = N pad
    N = integer size of loop
    pad = all values will be same length, e.g. 001, 002, ..., 100
  string arg = one string
  format args = vname fstr
    vname = name of equal-style variable to evaluate
    fstr = C-style format string
  getenv arg = one string
  file arg = filename
  atomfile arg = filename
  python arg = function
  equal or atom args = one formula containing numbers, thermo keywords, math operations, group
    numbers = 0.0, 100, -5.4, 2.8e-4, etc
    constants = PI, version, on, off, true, false, yes, no
    thermo keywords = vol, ke, press, etc from thermo_style
    math operators = (), -x, x+y, x-y, x*y, x/y, x^y, x%y,
                     x == y, x != y, x &lt y, x &lt= y, x &gt y, x &gt= y, x && y, x || y, !x
    math functions = sqrt(x), exp(x), ln(x), log(x), abs(x),
                     sin(x), cos(x), tan(x), asin(x), acos(x), atan(x), atan2(y,x),
                     random(x,y,z), normal(x,y,z), ceil(x), floor(x), round(x)
                     ramp(x,y), stagger(x,y), logfreq(x,y,z), logfreq2(x,y,z),
                     stride(x,y,z), stride2(x,y,z,a,b,c),
                     vdisplace(x,y), swiggle(x,y,z), cwiggle(x,y,z)
    group functions = count(group), mass(group), charge(group),
                      xcm(group,dim), vcm(group,dim), fcm(group,dim),
                      bound(group,dir), gyration(group), ke(group),
                      angmom(group,dim), torque(group,dim),
                      inertia(group,dimdim), omega(group,dim)
    region functions = count(group,region), mass(group,region), charge(group,region),
                       xcm(group,dim,region), vcm(group,dim,region), fcm(group,dim,region),
                       bound(group,dir,region), gyration(group,region), ke(group,reigon),
                       angmom(group,dim,region), torque(group,dim,region),
                       inertia(group,dimdim,region), omega(group,dim,region)
```

```
special functions = sum(x), min(x), max(x), ave(x), trap(x), slope(x), gmask(x), rmask(x),
feature functions = is_active(category,feature,exact), is_defined(category,id,exact)
atom value = id[i], mass[i], type[i], mol[i], x[i], y[i], z[i], vx[i], vy[i], vz[i], fx[i]
atom vector = id, mass, type, mol, x, y, z, vx, vy, vz, fx, fy, fz, q
compute references = c_ID, c_ID[i], c_ID[i][j]
fix references = f_ID, f_ID[i], f_ID[i][j]
variable references = v_name, v_name[i]
```

Examples:

```
variable x index run1 run2 run3 run4 run5 run6 run7 run8
variable LoopVar loop $n
variable beta equal temp/3.0
variable b1 equal x[234]+0.5*vol
variable b1 equal "x[234] + 0.5*vol"
variable b equal xcm(mol1,x)/2.0
variable b equal c_myTemp
variable b atom x*y/vol
variable foo string myfile
variable myPy python increase
variable f file values.txt
variable temp world 300.0 310.0 320.0 ${Tfinal}
variable x universe 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
variable x uloop 15 pad
variable str format x %.6g
variable x delete
```

Description:

This command assigns one or more strings to a variable name for evaluation later in the input script or during a simulation.

Variables can thus be useful in several contexts. A variable can be defined and then referenced elsewhere in an input script to become part of a new input command. For variable styles that store multiple strings, the next command can be used to increment which string is assigned to the variable. Variables of style *equal* store a formula which when evaluated produces a single numeric value which can be output either directly (see the print, fix print, and run every commands) or as part of thermodynamic output (see the thermo_style command), or used as input to an averaging fix (see the fix ave/time command). Variables of style *atom* store a formula which when evaluated produces one numeric value per atom which can be output to a dump file (see the dump custom command) or used as input to an averaging fix (see the fix ave/spatial and fix ave/atom commands). Variables of style *atomfile* can be used anywhere in an input script that atom-style variables are used; they get their per-atom values from a file rather than from a formula. Variables can be hooked to Python functions using code you provide, so that the variable gets its value from the evaluation of the Python code.

NOTE: As discussed in Section 3.2 of the manual, an input script can use "immediate" variables, specified as $(formula) with parenthesis, where the formula has the same syntax as equal-style variables described on this page. This is a convenient way to evaluate a formula immediately without using the variable command to define a named variable and then evaluate that variable. See below for a more detailed discussion of this feature.

In the discussion that follows, the "name" of the variable is the arbitrary string that is the 1st argument in the variable command. This name can only contain alphanumeric characters and underscores. The "string" is one or more of the subsequent arguments. The "string" can be simple text as in the 1st example above, it can contain other variables as in the 2nd example, or it can be a formula as in the 3rd example. The "value" is the numeric quantity resulting from evaluation of the string. Note that the same string can generate different values when it is evaluated at different times during a simulation.

NOTE: When the input script line is encountered that defines a variable of style *equal* or *atom* or *python* that contains a formula or Python code, the formula is NOT immediately evaluated. It will be evaluated every time when the variable is **used** instead. If you simply want to evaluate a formula in place you can use as so-called. See the section below about "Immediate Evaluation of Variables" for more details on the topic. This is also true of a *format* style variable since it evaluates another variable when it is invoked.

NOTE: Variables of style *equal* and *atom* can be used as inputs to various other LAMMPS commands which evaluate their formulas as needed, e.g. at different timesteps during a run. Variables of style *python* can be used in place of an equal-style variable so long as the associated Python function, as defined by the python command, returns a numeric value. Thus any command that states it can use an equal-style variable as an argument, can also use such a python-style variable. This means that when the LAMMPS command evaluates the variable, the Python function will be executed.

NOTE: When a variable command is encountered in the input script and the variable name has already been specified, the command is ignored. This means variables can NOT be re-defined in an input script (with two exceptions, read further). This is to allow an input script to be processed multiple times without resetting the variables; see the jump or include commands. It also means that using the command-line switch -var will override a corresponding index variable setting in the input script.

There are two exceptions to this rule. First, variables of style *string*, *getenv*, *equal*, *atom*, and *python* ARE redefined each time the command is encountered. This allows these style of variables to be redefined multiple times in an input script. In a loop, this means the formula associated with an *equal* or *atom* style variable can change if it contains a substitution for another variable, e.g. $x or v_x.

Second, as described below, if a variable is iterated on to the end of its list of strings via the next command, it is removed from the list of active variables, and is thus available to be re-defined in a subsequent variable command. The *delete* style does the same thing.

This section of the manual explains how occurrences of a variable name in an input script line are replaced by the variable's string. The variable name can be referenced as $x if the name "x" is a single character, or as ${LoopVar} if the name "LoopVar" is one or more characters.

As described below, for variable styles *index*, *loop*, *file*, *universe*, and *uloop*, which string is assigned to a variable can be incremented via the next command. When there are no more strings to assign, the variable is exhausted and a flag is set that causes the next jump command encountered in the input script to be skipped. This enables the construction of simple loops in the input script that are iterated over and then exited from.

As explained above, an exhausted variable can be re-used in an input script. The *delete* style also removes the variable, the same as if it were exhausted, allowing it to be redefined later in the input script or when the input script is looped over. This can be useful when breaking out of a loop via the if and jump commands before the variable would become exhausted. For example,

```
label       loop
variable    a loop 5
print       "A = $a"
if          "$a > 2" then "jump in.script break"
next        a
jump        in.script loop
label       break
variable    a delete
```

This section describes how all the various variable styles are defined and what they store. Except for the *equal* and *atom* styles, which are explaine in the next section.

Many of the styles store one or more strings. Note that a single string can contain spaces (multiple words), if it is enclosed in quotes in the variable command. When the variable is substituted for in another input script command, its returned string will then be interpreted as multiple arguments in the expanded command.

For the *index* style, one or more strings are specified. Initially, the 1st string is assigned to the variable. Each time a next command is used with the variable name, the next string is assigned. All processors assign the same string to the variable.

Index style variables with a single string value can also be set by using the command-line switch -var; see this section for details.

The *loop* style is identical to the *index* style except that the strings are the integers from 1 to N inclusive, if only one argument N is specified. This allows generation of a long list of runs (e.g. 1000) without having to list N strings in the input script. Initially, the string "1" is assigned to the variable. Each time a next command is used with the variable name, the next string ("2", "3", etc) is assigned. All processors assign the same string to the variable. The *loop* style can also be specified with two arguments N1 and N2. In this case the loop runs from N1 to N2 inclusive, and the string N1 is initially assigned to the variable. N1 <= N2 and N2 >= 0 is required.

For the *world* style, one or more strings are specified. There must be one string for each processor partition or "world". See this section of the manual for information on running LAMMPS with multiple partitions via the "-partition" command-line switch. This variable command assigns one string to each world. All processors in the world are assigned the same string. The next command cannot be used with *equal* style variables, since there is only one value per world. This style of variable is useful when you wish to run different simulations on different partitions, or when performing a parallel tempering simulation (see the temper command), to assign different temperatures to different partitions.

For the *universe* style, one or more strings are specified. There must be at least as many strings as there are processor partitions or "worlds". See this page for information on running LAMMPS with multiple partitions via the "-partition" command-line switch. This variable command initially assigns one string to each world. When a next command is encountered using this variable, the first processor partition to encounter it, is assigned the next available string. This continues until all the variable strings are consumed. Thus, this command can be used to run 50 simulations on 8 processor partitions. The simulations will be run one after the other on whatever partition becomes available, until they are all finished. *Universe* style variables are incremented using the files "tmp.lammps.variable" and "tmp.lammps.variable.lock" which you will see in your directory during such a LAMMPS run.

The *uloop* style is identical to the *universe* style except that the strings are the integers from 1 to N. This allows generation of long list of runs (e.g. 1000) without having to list N strings in the input script.

For the *string* style, a single string is assigned to the variable. The only difference between this and using the *index* style with a single string is that a variable with *string* style can be redefined. E.g. by another command later in the input script, or if the script is read again in a loop.

For the *format* style, an equal-style variable is specified along with a C-style format string, e.g. "%f" or "%.10g", which must be appropriate for formatting a double-precision floating-point value. This allows an equal-style variable to be formatted specifically for output as a string, e.g. by the print command, if the default format "%.15g" has too much precision.

For the *getenv* style, a single string is assigned to the variable which should be the name of an environment variable. When the variable is evaluated, it returns the value of the environment variable, or an empty string if it not defined. This style of variable can be used to adapt the behavior of LAMMPS input scripts via environment variable settings, or to retrieve information that has been previously stored with the shell putenv command. Note

that because environment variable settings are stored by the operating systems, they persist beyond a clear command.

For the *file* style, a filename is provided which contains a list of strings to assign to the variable, one per line. The strings can be numeric values if desired. See the discussion of the next() function below for equal-style variables, which will convert the string of a file-style variable into a numeric value in a formula.

When a file-style variable is defined, the file is opened and the string on the first line is read and stored with the variable. This means the variable can then be evaluated as many times as desired and will return that string. There are two ways to cause the next string from the file to be read: use the next command or the next() function in an equal- or atom-style variable, as discussed below.

The rules for formatting the file are as follows. A comment character "#" can be used anywhere on a line; text starting with the comment character is stripped. Blank lines are skipped. The first "word" of a non-blank line, delimited by white space, is the "string" assigned to the variable.

For the *atomfile* style, a filename is provided which contains one or more sets of values, to assign on a per-atom basis to the variable. The format of the file is described below.

When an atomfile-style variable is defined, the file is opened and the first set of per-atom values are read and stored with the variable. This means the variable can then be evaluated as many times as desired and will return those values. There are two ways to cause the next set of per-atom values from the file to be read: use the next command or the next() function in an atom-style variable, as discussed below.

The rules for formatting the file are as follows. Each time a set of per-atom values is read, a non-blank line is searched for in the file. A comment character "#" can be used anywhere on a line; text starting with the comment character is stripped. Blank lines are skipped. The first "word" of a non-blank line, delimited by white space, is read as the count N of per-atom lines to immediately follow. N can be be the total number of atoms in the system, or only a subset. The next N lines have the following format

```
ID value
```

where ID is an atom ID and value is the per-atom numeric value that will be assigned to that atom. IDs can be listed in any order.

NOTE: Every time a set of per-atom lines is read, the value for all atoms is first set to 0.0. Thus values for atoms whose ID does not appear in the set, will remain 0.0.

For the *python* style a Python function name is provided. This needs to match a function name specified in a python command which returns a value to this variable as defined by its *return* keyword. For exampe these two commands would be self-consistent:

```
variable foo python myMultiply
python myMultiply return v_foo format f file funcs.py
```

The two commands can appear in either order so long as both are specified before the Python function is invoked for the first time.

Each time the variable is evaluated, the associated Python function is invoked, and the value it returns is also returned by the variable. Since the Python function can use other LAMMPS variables as input, or query interal LAMMPS quantities to perform its computation, this means the variable can return a different value each time it is evaluated.

The type of value stored in the variable is determined by the *format* keyword of the python command. It can be an integer (i), floating point (f), or string (s) value. As mentioned above, if it is a numeric value (integer or floating point), then the python-style variable can be used in place of an equal-style variable anywhere in an input script, e.g. as an argument to another command that allows for equal-style variables.

For the *equal* and *atom* styles, a single string is specified which represents a formula that will be evaluated afresh each time the variable is used. If you want spaces in the string, enclose it in double quotes so the parser will treat it as a single argument. For *equal* style variables the formula computes a scalar quantity, which becomes the value of the variable whenever it is evaluated. For *atom* style variables the formula computes one quantity for each atom whenever it is evaluated.

Note that *equal* and *atom* variables can produce different values at different stages of the input script or at different times during a run. For example, if an *equal* variable is used in a fix print command, different values could be printed each timestep it was invoked. If you want a variable to be evaluated immediately, so that the result is stored by the variable instead of the string, see the section below on "Immediate Evaluation of Variables".

The next command cannot be used with *equal* or *atom* style variables, since there is only one string.

The formula for an *equal* or *atom* variable can contain a variety of quantities. The syntax for each kind of quantity is simple, but multiple quantities can be nested and combined in various ways to build up formulas of arbitrary complexity. For example, this is a valid (though strange) variable formula:

```
variable x equal "pe + c_MyTemp / vol^(1/3)"
```

Specifically, an formula can contain numbers, thermo keywords, math operators, math functions, group functions, region functions, atom values, atom vectors, compute references, fix references, and references to other variables.

Number	0.2, 100, 1.0e20, -15.4, etc
Constant	PI, version, on, off, true, false, yes, no
Thermo keywords	vol, pe, ebond, etc
Math operators	(), -x, x+y, x-y, x*y, x/y, x^y, x%y,
Math operators	(), -x, x+y, x-y, x*y, x/y, x^y, x%y, x == y, x != y, x &lt y, x &lt= y, x &gt y, x &gt= y, x && y, x || y, !x
Math functions	sqrt(x), exp(x), ln(x), log(x), abs(x), sin(x), cos(x), tan(x), asin(x), acos(x), atan(x), atan2(y,x), random(x,y,z), normal(x,y,z), ceil(x), floor(x), round(x), ramp(x,y), stagger(x,y), logfreq(x,y,z), logfreq2(x,y,z), stride(x,y,z), stride2(x,y,z,a,b,c), vdisplace(x,y), swiggle(x,y,z), cwiggle(x,y,z)
Group functions	count(ID), mass(ID), charge(ID), xcm(ID,dim), vcm(ID,dim), fcm(ID,dim), bound(ID,dir), gyration(ID), ke(ID), angmom(ID,dim), torque(ID,dim), inertia(ID,dimdim), omega(ID,dim)
Region functions	count(ID,IDR), mass(ID,IDR), charge(ID,IDR), xcm(ID,dim,IDR), vcm(ID,dim,IDR), fcm(ID,dim,IDR), bound(ID,dir,IDR), gyration(ID,IDR), ke(ID,IDR), angmom(ID,dim,IDR), torque(ID,dim,IDR), inertia(ID,dimdim,IDR), omega(ID,dim,IDR)
Special functions	sum(x), min(x), max(x), ave(x), trap(x), slope(x), gmask(x), rmask(x), grmask(x,y), next(x)
Atom values	id[i], mass[i], type[i], mol[i], x[i], y[i], z[i], vx[i], vy[i], vz[i], fx[i], fy[i], fz[i], q[i]
Atom vectors	id, mass, type, mol, x, y, z, vx, vy, vz, fx, fy, fz, q
Compute references	c_ID, c_ID[i], c_ID[i][j]

Fix references	f_ID, f_ID[i], f_ID[i][j]
Other variables	v_name, v_name[i]

Most of the formula elements produce a scalar value. A few produce a per-atom vector of values. These are the atom vectors, compute references that represent a per-atom vector, fix references that represent a per-atom vector, and variables that are atom-style variables. Math functions that operate on scalar values produce a scalar value; math function that operate on per-atom vectors do so element-by-element and produce a per-atom vector.

A formula for equal-style variables cannot use any formula element that produces a per-atom vector. A formula for an atom-style variable can use formula elements that produce either a scalar value or a per-atom vector. Atom-style variables are evaluated by other commands that define a group on which they operate, e.g. a dump or compute or fix command. When they invoke the atom-style variable, only atoms in the group are inlcuded in the formula evaluation. The variable evaluates to 0.0 for atoms not in the group.

Constants are set at compile time and cannot be changed. *PI* will return the number 3.14159265358979323846; *on*, *true* or *yes* will return 1.0; *off*, *false* or *no* will return 0.0; *version* will return a numeric version code of the current LAMMPS version (e.g. version 2 Sep 2015 will return the number 20150902). The corresponding value for newer versions of LAMMPS will be larger, for older versions of LAMMPS will be smaller. This can be used to have input scripts adapt automatically to LAMMPS versions, when non-backwards compatible syntax changes are introduced. Here is an illustrative example (which will not work, since the *version* has been introduced more recently):

```
if $(version
```

The thermo keywords allowed in a formula are those defined by the thermo_style custom command. Thermo keywords that require a compute to calculate their values such as "temp" or "press", use computes stored and invoked by the thermo_style command. This means that you can only use those keywords in a variable if the style you are using with the thermo_style command (and the thermo keywords associated with that style) also define and use the needed compute. Note that some thermo keywords use a compute indirectly to calculate their value (e.g. the enthalpy keyword uses temp, pe, and pressure). If a variable is evaluated directly in an input script (not during a run), then the values accessed by the thermo keyword must be current. See the discussion below about "Variable Accuracy".

Math Operators

Math operators are written in the usual way, where the "x" and "y" in the examples can themselves be arbitrarily complex formulas, as in the examples above. In this syntax, "x" and "y" can be scalar values or per-atom vectors. For example, "ke/natoms" is the division of two scalars, where "vy+vz" is the element-by-element sum of two per-atom vectors of y and z velocities.

Operators are evaluated left to right and have the usual C-style precedence: unary minus and unary logical NOT operator "!" have the highest precedence, exponentiation "^" is next; multiplication and division and the modulo operator "%" are next; addition and subtraction are next; the 4 relational operators "", and ">=" are next; the two remaining relational operators "==" and "!=" are next; then the logical AND operator "&&"; and finally the logical OR operator "||" has the lowest precedence. Parenthesis can be used to group one or more portions of a formula and/or enforce a different order of evaluation than what would occur with the default precedence.

NOTE: Because a unary minus is higher precedence than exponentiation, the formula "-2^2" will evaluate to 4, not -4. This convention is compatible with some programming languages, but not others. As mentioned, this behavior can be easily overridden with parenthesis; the formula "-(2^2)" will evaluate to -4.

The 6 relational operators return either a 1.0 or 0.0 depending on whether the relationship between x and y is TRUE or FALSE. For example the expression x

These relational and logical operators can be used as a masking or selection operation in a formula. For example, the number of atoms whose properties satifsy one or more criteria could be calculated by taking the returned per-atom vector of ones and zeroes and passing it to the compute reduce command.

Math Functions

Math functions are specified as keywords followed by one or more parenthesized arguments "x", "y", "z", each of which can themselves be arbitrarily complex formulas. In this syntax, the arguments can represent scalar values or per-atom vectors. In the latter case, the math operation is performed on each element of the vector. For example, "sqrt(natoms)" is the sqrt() of a scalar, where "sqrt(y*z)" yields a per-atom vector with each element being the sqrt() of the product of one atom's y and z coordinates.

Most of the math functions perform obvious operations. The ln() is the natural log; log() is the base 10 log.

The random(x,y,z) function takes 3 arguments: x = lo, y = hi, and z = seed. It generates a uniform random number between lo and hi. The normal(x,y,z) function also takes 3 arguments: x = mu, y = sigma, and z = seed. It generates a Gaussian variate centered on mu with variance sigma^2. In both cases the seed is used the first time the internal random number generator is invoked, to initialize it. For equal-style variables, every processor uses the same seed so that they each generate the same sequence of random numbers. For atom-style variables, a unique seed is created for each processor, based on the specified seed. This effectively generates a different random number for each atom being looped over in the atom-style variable.

NOTE: Internally, there is just one random number generator for all equal-style variables and one for all atom-style variables. If you define multiple variables (of each style) which use the random() or normal() math functions, then the internal random number generators will only be initialized once, which means only one of the specified seeds will determine the sequence of generated random numbers.

The ceil(), floor(), and round() functions are those in the C math library. Ceil() is the smallest integer not less than its argument. Floor() if the largest integer not greater than its argument. Round() is the nearest integer to its argument.

The ramp(x,y) function uses the current timestep to generate a value linearly intepolated between the specified x,y values over the course of a run, according to this formula:

```
value = x + (y-x) * (timestep-startstep) / (stopstep-startstep)
```

The run begins on startstep and ends on stopstep. Startstep and stopstep can span multiple runs, using the *start* and *stop* keywords of the run command. See the run command for details of how to do this.

The stagger(x,y) function uses the current timestep to generate a new timestep. X,y > 0 and x > y are required. The generated timesteps increase in a staggered fashion, as the sequence x,x+y,2x,2x+y,3x,3x+y,etc. For any current timestep, the next timestep in the sequence is returned. Thus if stagger(1000,100) is used in a variable by the dump_modify every command, it will generate the sequence of output timesteps:

```
100,1000,1100,2000,2100,3000,etc
```

The logfreq(x,y,z) function uses the current timestep to generate a new timestep. X,y,z > 0 and y < z are required. The generated timesteps are on a base-z logarithmic scale, starting with x, and the y value is how many of the z-1 possible timesteps within one logarithmic interval are generated. I.e. the timesteps follow the sequence x,2x,3x,...y*x,x*z,2x*z,3x*z,...y*x*z,x*z^2,2x*z^2,etc. For any current timestep, the next timestep in the

sequence is returned. Thus if logfreq(100,4,10) is used in a variable by the dump_modify every command, it will generate this sequence of output timesteps:

```
100,200,300,400,1000,2000,3000,4000,10000,20000,etc
```

The logfreq2(x,y,z) function is similar to logfreq, except a single logarithmic interval is divided into y equally-spaced timesteps and all of them are output. Y < z is not required. Thus, if logfreq2(100,18,10) is used in a variable by the dump_modify every command, then the interval between 100 and 1000 is divided as 900/18 = 50 steps, and it will generate the sequence of output timesteps:

```
100,150,200,...950,1000,1500,2000,...9500,10000,15000,etc
```

The stride(x,y,z) function uses the current timestep to generate a new timestep. X,y >= 0 and z > 0 and x <= y are required. The generated timesteps increase in increments of z, from x to y, i.e. it generates the sequece x,x+z,x+2z,...,y. If y-x is not a multiple of z, then similar to the way a for loop operates, the last value will be one that does not exceed y. For any current timestep, the next timestep in the sequence is returned. Thus if stride(1000,2000,100) is used in a variable by the dump_modify every command, it will generate the sequence of output timesteps:

```
1000,1100,1200, ... ,1900,2000
```

The stride2(x,y,z,a,b,c) function is similar to the stride() function except it generates two sets of strided timesteps, one at a coarser level and one at a finer level. Thus it is useful for debugging, e.g. to produce output every timestep at the point in simulation when a problem occurs. X,y >= 0 and z > 0 and x <= y are required, as are a,b >= 0 and c > 0 and a < b. Also, a >= x and b <= y are required so that the second stride is inside the first. The generated timesteps increase in increments of z, starting at x, until a is reached. At that point the timestep increases in increments of c, from a to b, then after b, increments by z are resumed until y is reached. For any current timestep, the next timestep in the sequence is returned. Thus if stride(1000,2000,100,1350,1360,1) is used in a variable by the dump_modify every command, it will generate the sequence of output timesteps:

```
1000,1100,1200,1300,1350,1351,1352, ... 1359,1360,1400,1500, ... ,2000
```

The vdisplace(x,y) function takes 2 arguments: x = value0 and y = velocity, and uses the elapsed time to change the value by a linear displacement due to the applied velocity over the course of a run, according to this formula:

```
value = value0 + velocity*(timestep-startstep)*dt
```

where dt = the timestep size.

The run begins on startstep. Startstep can span multiple runs, using the *start* keyword of the run command. See the run command for details of how to do this. Note that the thermo_style keyword elaplong = timestep-startstep.

The swiggle(x,y,z) and cwiggle(x,y,z) functions each take 3 arguments: x = value0, y = amplitude, z = period. They use the elapsed time to oscillate the value by a sin() or cos() function over the course of a run, according to one of these formulas, where omega = 2 PI / period:

```
value = value0 + Amplitude * sin(omega*(timestep-startstep)*dt)
value = value0 + Amplitude * (1 - cos(omega*(timestep-startstep)*dt))
```

where dt = the timestep size.

The run begins on startstep. Startstep can span multiple runs, using the *start* keyword of the run command. See the run command for details of how to do this. Note that the thermo_style keyword elaplong = timestep-startstep.

Group and Region Functions

Group functions are specified as keywords followed by one or two parenthesized arguments. The first argument *ID* is the group-ID. The *dim* argument, if it exists, is *x* or *y* or *z*. The *dir* argument, if it exists, is *xmin*, *xmax*, *ymin*, *ymax*, *zmin*, or *zmax*. The *dimdim* argument, if it exists, is *xx* or *yy* or *zz* or *xy* or *yz* or *xz*.

The group function count() is the number of atoms in the group. The group functions mass() and charge() are the total mass and charge of the group. Xcm() and vcm() return components of the position and velocity of the center of mass of the group. Fcm() returns a component of the total force on the group of atoms. Bound() returns the min/max of a particular coordinate for all atoms in the group. Gyration() computes the radius-of-gyration of the group of atoms. See the compute gyration command for a definition of the formula. Angmom() returns components of the angular momentum of the group of atoms around its center of mass. Torque() returns components of the torque on the group of atoms around its center of mass, based on current forces on the atoms. Inertia() returns one of 6 components of the symmetric inertia tensor of the group of atoms around its center of mass, ordered as Ixx,Iyy,Izz,Ixy,Iyz,Ixz. Omega() returns components of the angular velocity of the group of atoms around its center of mass.

Region functions are specified exactly the same way as group functions except they take an extra final argument *IDR* which is the region ID. The function is computed for all atoms that are in both the group and the region. If the group is "all", then the only criteria for atom inclusion is that it be in the region.

Special Functions

Special functions take specific kinds of arguments, meaning their arguments cannot be formulas themselves.

The sum(x), min(x), max(x), ave(x), trap(x), and slope(x) functions each take 1 argument which is of the form "c_ID" or "c_ID[N]" or "f_ID" or "f_ID[N]". The first two are computes and the second two are fixes; the ID in the reference should be replaced by the ID of a compute or fix defined elsewhere in the input script. The compute or fix must produce either a global vector or array. If it produces a global vector, then the notation without "[N]" should be used. If it produces a global array, then the notation with "[N]" should be used, when N is an integer, to specify which column of the global array is being referenced.

These functions operate on the global vector of inputs and reduce it to a single scalar value. This is analagous to the operation of the compute reduce command, which invokes the same functions on per-atom and local vectors.

The sum() function calculates the sum of all the vector elements. The min() and max() functions find the minimum and maximum element respectively. The ave() function is the same as sum() except that it divides the result by the length of the vector.

The trap() function is the same as sum() except the first and last elements are multiplied by a weighting factor of 1/2 when performing the sum. This effectively implements an integration via the trapezoidal rule on the global vector of data. I.e. consider a set of points, equally spaced by 1 in their x coordinate: (1,V1), (2,V2), ..., (N,VN), where the Vi are the values in the global vector of length N. The integral from 1 to N of these points is trap(). When appropriately normalized by the timestep size, this function is useful for calculating integrals of time-series data, like that generated by the fix ave/correlate command.

The slope() function uses linear regression to fit a line to the set of points, equally spaced by 1 in their x coordinate: (1,V1), (2,V2), ..., (N,VN), where the Vi are the values in the global vector of length N. The returned value is the slope of the line. If the line has a single point or is vertical, it returns 1.0e20.

The gmask(x) function takes 1 argument which is a group ID. It can only be used in atom-style variables. It returns a 1 for atoms that are in the group, and a 0 for atoms that are not.

The rmask(x) function takes 1 argument which is a region ID. It can only be used in atom-style variables. It returns a 1 for atoms that are in the geometric region, and a 0 for atoms that are not.

The grmask(x,y) function takes 2 arguments. The first is a group ID, and the second is a region ID. It can only be used in atom-style variables. It returns a 1 for atoms that are in both the group and region, and a 0 for atoms that are not in both.

The next(x) function takes 1 argument which is a variable ID (not "v_foo", just "foo"). It must be for a file-style or atomfile-style variable. Each time the next() function is invoked (i.e. each time the equal-style or atom-style variable is evaluated), the following steps occur.

For file-style variables, the current string value stored by the file-style variable is converted to a numeric value and returned by the function. And the next string value in the file is read and stored. Note that if the line previously read from the file was not a numeric string, then it will typically evaluate to 0.0, which is likely not what you want.

For atomfile-style variables, the current per-atom values stored by the atomfile-style variable are returned by the function. And the next set of per-atom values in the file is read and stored.

Since file-style and atomfile-style variables read and store the first line of the file or first set of per-atoms values when they are defined in the input script, these are the value(s) that will be returned the first time the next() function is invoked. If next() is invoked more times than there are lines or sets of lines in the file, the variable is deleted, similar to how the next command operates.

Feature Functions

Feature functions allow to probe the running LAMMPS executable for whether specific features are either active, defined, or available. The functions take two arguments, a *category* and a corresponding *argument*. The arguments are strings thus cannot be formulas themselves (only $-style immediate variable expansion is possible). Return value is either 1.0 or 0.0 depending on whether the function evaluates to true or false, respectively.

The *is_active()* function allows to query for active settings which are grouped by categories. Currently supported categories and arguments are:

- *package* (argument = *cuda* or *gpu* or *intel* or *kokkos* or *omp*)
- *newton* (argument = *pair* or *bond* or *any*)
- *pair* (argument = *single* or *respa* or *manybody* or *tail* or *shift*)
- *comm_style* (argument = *brick* or *tiled*)
- *min_style* (argument = any of the compiled in minimizer styles)
- *run_style* (argument = any of the compiled in run styles)
- *atom_style* (argument = any of the compiled in atom styles)
- *pair_style* (argument = any of the compiled in pair styles)
- *bond_style* (argument = any of the compiled in bond styles)
- *angle_style* (argument = any of the compiled in angle styles)
- *dihedral_style* (argument = any of the compiled in dihedral styles)
- *improper_style* (argument = any of the compiled in improper styles)
- *kspace_style* (argument = any of the compiled in kspace styles)

Most of the settings are self-explanatory, the *single* argument in the *pair* category allows to check whether a pair style supports a Pair::single() function as needed by compute group/group and others features or LAMMPS, *respa* allows to check whether the inner/middle/outer mode of r-RESPA is supported. In the various style categories, the checking is also done using suffix flags, if available and enabled.

Example 1: disable use of suffix for pppm when using GPU package (i.e. run it on the CPU concurrently to running the pair style on the GPU), but do use the suffix otherwise (e.g. with USER-OMP).

```
pair_style lj/cut/coul/long 14.0
if $(is_active(package,gpu)) then "suffix off"
kspace_style pppm
```

Example 2: use r-RESPA with inner/outer cutoff, if supported by pair style, otherwise fall back to using pair and reducing the outer time step

```
timestep $(2.0*(1.0+*is_active(pair,respa))
if $(is_active(pair,respa)) then "run_style respa 4 3 2 2  improper 1 inner 2 5.5 7.0 outer 3 kspace
```

The *is_defined()* function allows to query categories like *compute*, *dump*, *fix*, *group*, *region*, and *variable* whether an entry with the provided name or id is defined.

The *is_available()* function allows to query whether a specific optional feature is available, i.e. compiled in. This currently works for the following categories: *command*, *compute*, *fix*, and *pair_style*. For all categories except *command* also appending active suffixes is tried before reporting failure.

Atom Values and Vectors

Atom values take an integer argument I from 1 to N, where I is the atom-ID, e.g. x[243], which means use the x coordinate of the atom with ID = 243. Or they can take a variable name, specified as v_name, where name is the name of the variable, like x[v_myIndex]. The variable can be of any style except atom or atom-file variables. The variable is evaluated and the result is expected to be numeric and is cast to an integer (i.e. 3.4 becomes 3), to use an an index, which must be a value from 1 to N. Note that a "formula" cannot be used as the argument between the brackets, e.g. x[243+10] or x[v_myIndex+1] are not allowed. To do this a single variable can be defined that contains the needed formula.

Note that the 0 < atom-ID <= N, where N is the largest atom ID in the system. If an ID is specified for an atom that does not currently exist, then the generated value is 0.0.

Atom vectors generate one value per atom, so that a reference like "vx" means the x-component of each atom's velocity will be used when evaluating the variable.

The meaning of the different atom values and vectors is mostly self-explanatory. Mol refers to the molecule ID of an atom, and is only defined if an atom_style is being used that defines molecule IDs.

Note that many other atom attributes can be used as inputs to a variable by using the compute property/atom command and then specifying a quantity from that compute.

Compute References

Compute references access quantities calculated by a compute. The ID in the reference should be replaced by the ID of a compute defined elsewhere in the input script. As discussed in the doc page for the compute command, computes can produce global, per-atom, or local values. Only global and per-atom values can be used in a variable. Computes can also produce a scalar, vector, or array. An equal-style variable can only use scalar values,

which means a global scalar, or an element of a global or per-atom vector or array. Atom-style variables can use the same scalar values. They can also use per-atom vector values. A vector value can be a per-atom vector itself, or a column of an per-atom array. See the doc pages for individual computes to see what kind of values they produce.

Examples of different kinds of compute references are as follows. There is no ambiguity as to what a reference means, since computes only produce global or per-atom quantities, never both.

c_ID	global scalar, or per-atom vector
c_ID[I]	Ith element of global vector, or atom I's value in per-atom vector, or Ith column from per-atom array
c_ID[I][J]	I,J element of global array, or atom I's Jth value in per-atom array

For I and J, integers can be specified or a variable name, specified as v_name, where name is the name of the variable. The rules for this syntax are the same as for the "Atom Values and Vectors" discussion above.

If a variable containing a compute is evaluated directly in an input script (not during a run), then the values accessed by the compute must be current. See the discussion below about "Variable Accuracy".

Fix References

Fix references access quantities calculated by a fix. The ID in the reference should be replaced by the ID of a fix defined elsewhere in the input script. As discussed in the doc page for the fix command, fixes can produce global, per-atom, or local values. Only global and per-atom values can be used in a variable. Fixes can also produce a scalar, vector, or array. An equal-style variable can only use scalar values, which means a global scalar, or an element of a global or per-atom vector or array. Atom-style variables can use the same scalar values. They can also use per-atom vector values. A vector value can be a per-atom vector itself, or a column of an per-atom array. See the doc pages for individual fixes to see what kind of values they produce.

The different kinds of fix references are exactly the same as the compute references listed in the above table, where "c_" is replaced by "f_". Again, there is no ambiguity as to what a reference means, since fixes only produce global or per-atom quantities, never both.

f_ID	global scalar, or per-atom vector
f_ID[I]	Ith element of global vector, or atom I's value in per-atom vector, or Ith column from per-atom array
f_ID[I][J]	I,J element of global array, or atom I's Jth value in per-atom array

For I and J, integers can be specified or a variable name, specified as v_name, where name is the name of the variable. The rules for this syntax are the same as for the "Atom Values and Vectors" discussion above.

If a variable containing a fix is evaluated directly in an input script (not during a run), then the values accessed by the fix should be current. See the discussion below about "Variable Accuracy".

Note that some fixes only generate quantities on certain timesteps. If a variable attempts to access the fix on non-allowed timesteps, an error is generated. For example, the fix ave/time command may only generate averaged quantities every 100 steps. See the doc pages for individual fix commands for details.

Variable References

Variable references access quantities stored or calculated by other variables, which will cause those variables to be evaluated. The name in the reference should be replaced by the name of a variable defined elsewhere in the input script.

As discussed on this doc page, equal-style variables generate a global scalar numeric value; atom-style and atomfile-style variables generate a per-atom vector of numeric values; all other variables store a string. The formula for an equal-style variable can use any style of variable except an atom-style or atomfile-style (unless only a single value from the variable is accessed via a subscript). If a string-storing variable is used, the string is converted to a numeric value. Note that this will typically produce a 0.0 if the string is not a numeric string, which is likely not what you want. The formula for an atom-style variable can use any style of variable, including other atom-style or atomfile-style variables.

Examples of different kinds of variable references are as follows. There is no ambiguity as to what a reference means, since variables produce only a global scalar or a per-atom vector, never both.

v_name	scalar, or per-atom vector
v_name[I]	atom I's value in per-atom vector

For I, an integer can be specified or a variable name, specified as v_name, where name is the name of the variable. The rules for this syntax are the same as for the "Atom Values and Vectors" discussion above.

Immediate Evaluation of Variables:

If you want an equal-style variable to be evaluated immediately, it may be the case that you do not need to define a variable at all. See Section 3.2 of the manual, which describes the use of "immediate" variables in an input script, specified as $(formula) with parenthesis, where the formula has the same syntax as equal-style variables described on this page. This effectively evaluates a formula immediately without using the variable command to define a named variable.

More generally, there is a difference between referencing a variable with a leading $ sign (e.g. $x or ${abc}) versus with a leading "v_" (e.g. v_x or v_abc). The former can be used in any input script command, including a variable command. The input script parser evaluates the reference variable immediately and substitutes its value into the command. As explained in Section commands 3.2 for "Parsing rules", you can also use un-named "immediate" variables for this purpose. For example, a string like this $((xlo+xhi)/2+sqrt(v_area)) in an input script command evaluates the string between the parenthesis as an equal-style variable formula.

Referencing a variable with a leading "v_" is an optional or required kind of argument for some commands (e.g. the fix ave/spatial or dump custom or thermo_style commands) if you wish it to evaluate a variable periodically during a run. It can also be used in a variable formula if you wish to reference a second variable. The second variable will be evaluated whenever the first variable is evaluated.

As an example, suppose you use this command in your input script to define the variable "v" as

```
variable v equal vol
```

before a run where the simulation box size changes. You might think this will assign the initial volume to the variable "v". That is not the case. Rather it assigns a formula which evaluates the volume (using the thermo_style keyword "vol") to the variable "v". If you use the variable "v" in some other command like fix ave/time then the current volume of the box will be evaluated continuously during the run.

If you want to store the initial volume of the system, you can do it this way:

```
variable v equal vol
variable v0 equal $v
```

The second command will force "v" to be evaluated (yielding the initial volume) and assign that value to the variable "v0". Thus the command

```
thermo_style custom step v_v v_v0
```

would print out both the current and initial volume periodically during the run.

Note that it is a mistake to enclose a variable formula in double quotes if it contains variables preceeded by $ signs. For example,

```
variable vratio equal "${vfinal}/${v0}"
```

This is because the quotes prevent variable substitution (see this section on parsing input script commands), and thus an error will occur when the formula for "vratio" is evaluated later.

Variable Accuracy:

Obviously, LAMMPS attempts to evaluate variables containing formulas (*equal* and *atom* style variables) accurately whenever the evaluation is performed. Depending on what is included in the formula, this may require invoking a compute, either directly or indirectly via a thermo keyword, or accessing a value previously calculated by a compute, or accessing a value calculated and stored by a fix. If the compute is one that calculates the pressure or energy of the system, then these quantities need to be tallied during the evaluation of the interatomic potentials (pair, bond, etc) on timesteps that the variable will need the values.

LAMMPS keeps track of all of this during a run or energy minimization. An error will be generated if you attempt to evaluate a variable on timesteps when it cannot produce accurate values. For example, if a thermo_style custom command prints a variable which accesses values stored by a fix ave/time command and the timesteps on which thermo output is generated are not multiples of the averaging frequency used in the fix command, then an error will occur.

An input script can also request variables be evaluated before or after or in between runs, e.g. by including them in a print command. In this case, if a compute is needed to evaluate a variable (either directly or indirectly), LAMMPS will not invoke the compute, but it will use a value previously calculated by the compute, and can do this only if it was invoked on the current timestep. Fixes will always provide a quantity needed by a variable, but the quantity may or may not be current. This leads to one of three kinds of behavior:

(1) The variable may be evaluated accurately. If it contains references to a compute or fix, and these values were calculated on the last timestep of a preceeding run, then they will be accessed and used by the variable and the result will be accurate.

(2) LAMMPS may not be able to evaluate the variable and will generate an error message stating so. For example, if the variable requires a quantity from a compute that has not been invoked on the current timestep, LAMMPS will generate an error. This means, for example, that such a variable cannot be evaluated before the first run has occurred. Likewise, in between runs, a variable containing a compute cannot be evaluated unless the compute was invoked on the last timestep of the preceding run, e.g. by thermodynamic output.

One way to get around this problem is to perform a 0-timestep run before using the variable. For example, these commands

```
variable t equal temp
print "Initial temperature = $t"
run 1000
```

will generate an error if the run is the first run specified in the input script, because generating a value for the "t" variable requires a compute for calculating the temperature to be invoked.

However, this sequence of commands would be fine:

```
run 0
variable t equal temp
print "Initial temperature = $t"
run 1000
```

The 0-timestep run initializes and invokes various computes, including the one for temperature, so that the value it stores is current and can be accessed by the variable "t" after the run has completed. Note that a 0-timestep run does not alter the state of the system, so it does not change the input state for the 1000-timestep run that follows. Also note that the 0-timestep run must actually use and invoke the compute in question (e.g. via thermo or dump output) in order for it to enable the compute to be used in a variable after the run. Thus if you are trying to print a variable that uses a compute you have defined, you can insure it is invoked on the last timestep of the preceding run by including it in thermodynamic output.

Unlike computes, fixes will never generate an error if their values are accessed by a variable in between runs. They always return some value to the variable. However, the value may not be what you expect if the fix has not yet calculated the quantity of interest or it is not current. For example, the fix indent command stores the force on the indenter. But this is not computed until a run is performed. Thus if a variable attempts to print this value before the first run, zeroes will be output. Again, performing a 0-timestep run before printing the variable has the desired effect.

(3) The variable may be evaluated incorrectly and LAMMPS may have no way to detect this has occurred. Consider the following sequence of commands:

```
pair_coeff 1 1 1.0 1.0
run 1000
pair_coeff 1 1 1.5 1.0
variable e equal pe
print "Final potential energy = $e"
```

The first run is performed using one setting for the pairwise potential defined by the pair_style and pair_coeff commands. The potential energy is evaluated on the final timestep and stored by the compute pe compute (this is done by the thermo_style command). Then a pair coefficient is changed, altering the potential energy of the system. When the potential energy is printed via the "e" variable, LAMMPS will use the potential energy value stored by the compute pe compute, thinking it is current. There are many other commands which could alter the state of the system between runs, causing a variable to evaluate incorrectly.

The solution to this issue is the same as for case (2) above, namely perform a 0-timestep run before the variable is evaluated to insure the system is up-to-date. For example, this sequence of commands would print a potential energy that reflected the changed pairwise coefficient:

```
pair_coeff 1 1 1.0 1.0
run 1000
pair_coeff 1 1 1.5 1.0
run 0
variable e equal pe
print "Final potential energy = $e"
```

Restrictions:

Indexing any formula element by global atom ID, such as an atom value, requires the atom style to use a global mapping in order to look up the vector indices. By default, only atom styles with molecular information create global maps. The atom_modify map command can override the default.

All *universe*- and *uloop*-style variables defined in an input script must have the same number of values.

Related commands:

next, jump, include, temper, fix print, print

Default: none

velocity command

Syntax:

```
velocity group-ID style args keyword value ...
```

- group-ID = ID of group of atoms whose velocity will be changed
- style = *create* or *set* or *scale* or *ramp* or *zero*

```
  create args = temp seed
      temp = temperature value (temperature units)
      seed = random # seed (positive integer)
    set args = vx vy vz
      vx,vy,vz = velocity value or NULL (velocity units)
      any of vx,vy,vz van be a variable (see below)
    scale arg = temp
      temp = temperature value (temperature units)
    ramp args = vdim vlo vhi dim clo chi
      vdim = vx or vy or vz
      vlo,vhi = lower and upper velocity value (velocity units)
      dim = x or y or z
      clo,chi = lower and upper coordinate bound (distance units)
    zero arg = linear or angular
      linear = zero the linear momentum
      angular = zero the angular momentum
```

- zero or more keyword/value pairs may be appended
- keyword = *dist* or *sum* or *mom* or *rot* or *temp* or *bias* or *loop* or *units*

```
  dist value = uniform or gaussian
    sum value = no or yes
    mom value = no or yes
    rot value = no or yes
    temp value = temperature compute ID
    bias value = no or yes
    loop value = all or local or geom
    rigid value = fix-ID
      fix-ID = ID of rigid body fix
    units value = box or lattice
```

Examples:

```
velocity all create 300.0 4928459 rot yes dist gaussian
velocity border set NULL 4.0 v_vz sum yes units box
velocity flow scale 300.0
velocity flow ramp vx 0.0 5.0 y 5 25 temp mytemp
velocity all zero linear
```

Description:

Set or change the velocities of a group of atoms in one of several styles. For each style, there are required arguments and optional keyword/value parameters. Not all options are used by each style. Each option has a default as listed below.

The *create* style generates an ensemble of velocities using a random number generator with the specified seed as the specified temperature.

The *set* style sets the velocities of all atoms in the group to the specified values. If any component is specified as NULL, then it is not set. Any of the vx,vy,vz velocity components can be specified as an equal-style or atom-style variable. If the value is a variable, it should be specified as v_name, where name is the variable name. In this case, the variable will be evaluated, and its value used to determine the velocity component. Note that if a variable is used, the velocity it calculates must be in box units, not lattice units; see the discussion of the *units* keyword below.

Equal-style variables can specify formulas with various mathematical functions, and include thermo_style command keywords for the simulation box parameters or other parameters.

Atom-style variables can specify the same formulas as equal-style variables but can also include per-atom values, such as atom coordinates. Thus it is easy to specify a spatially-dependent velocity field.

The *scale* style computes the current temperature of the group of atoms and then rescales the velocities to the specified temperature.

The *ramp* style is similar to that used by the compute temp/ramp command. Velocities ramped uniformly from vlo to vhi are applied to dimension vx, or vy, or vz. The value assigned to a particular atom depends on its relative coordinate value (in dim) from clo to chi. For the example above, an atom with y-coordinate of 10 (1/4 of the way from 5 to 25), would be assigned a x-velocity of 1.25 (1/4 of the way from 0.0 to 5.0). Atoms outside the coordinate bounds (less than 5 or greater than 25 in this case), are assigned velocities equal to vlo or vhi (0.0 or 5.0 in this case).

The *zero* style adjusts the velocities of the group of atoms so that the aggregate linear or angular momentum is zero. No other changes are made to the velocities of the atoms. If the *rigid* option is specified (see below), then the zeroing is performed on individual rigid bodies, as defined by the fix rigid or fix rigid/small commands. In other words, zero linear will set the linear momentum of each rigid body to zero, and zero angular will set the angular momentum of each rigid body to zero. This is done by adjusting the velocities of the atoms in each rigid body.

All temperatures specified in the velocity command are in temperature units; see the units command. The units of velocities and coordinates depend on whether the *units* keyword is set to *box* or *lattice*, as discussed below.

For all styles, no atoms are assigned z-component velocities if the simulation is 2d; see the dimension command.

The keyword/value options are used in the following ways by the various styles.

The *dist* keyword is used by *create*. The ensemble of generated velocities can be a *uniform* distribution from some minimum to maximum value, scaled to produce the requested temperature. Or it can be a *gaussian* distribution with a mean of 0.0 and a sigma scaled to produce the requested temperature.

The *sum* keyword is used by all styles, except *zero*. The new velocities will be added to the existing ones if sum = yes, or will replace them if sum = no.

The *mom* and *rot* keywords are used by *create*. If mom = yes, the linear momentum of the newly created ensemble of velocities is zeroed; if rot = yes, the angular momentum is zeroed.

*line

If specified, the *temp* keyword is used by *create* and *scale* to specify a compute that calculates temperature in a desired way, e.g. by first subtracting out a velocity bias, as discussed in Section howto 16 of the doc pages. If this keyword is not specified, *create* and *scale* calculate temperature using a compute that is defined internally as

follows:

```
compute velocity_temp group-ID temp
```

where group-ID is the same ID used in the velocity command. i.e. the group of atoms whose velocity is being altered. This compute is deleted when the velocity command is finished. See the compute temp command for details. If the calculated temperature should have degrees-of-freedom removed due to fix constraints (e.g. SHAKE or rigid-body constraints), then the appropriate fix command must be specified before the velocity command is issued.

The *bias* keyword with a *yes* setting is used by *create* and *scale*, but only if the *temp* keyword is also used to specify a compute that calculates temperature in a desired way. If the temperature compute also calculates a velocity bias, the the bias is subtracted from atom velocities before the *create* and *scale* operations are performed. After the operations, the bias is added back to the atom velocities. See Section howto 16 of the doc pages for more discussion of temperature computes with biases. Note that the velocity bias is only applied to atoms in the temperature compute specified with the *temp* keyword.

As an example, assume atoms are currently streaming in a flow direction (which could be separately initialized with the *ramp* style), and you wish to initialize their thermal velocity to a desired temperature. In this context thermal velocity means the per-particle velocity that remains when the streaming velocity is subtracted. This can be done using the *create* style with the *temp* keyword specifying the ID of a compute temp/ramp or compute temp/profile command, and the *bias* keyword set to a *yes* value.

The *loop* keyword is used by *create* in the following ways.

If loop = all, then each processor loops over all atoms in the simulation to create velocities, but only stores velocities for atoms it owns. This can be a slow loop for a large simulation. If atoms were read from a data file, the velocity assigned to a particular atom will be the same, independent of how many processors are being used. This will not be the case if atoms were created using the create_atoms command, since atom IDs will likely be assigned to atoms differently.

If loop = local, then each processor loops over only its atoms to produce velocities. The random number seed is adjusted to give a different set of velocities on each processor. This is a fast loop, but the velocity assigned to a particular atom will depend on which processor owns it. Thus the results will always be different when a simulation is run on a different number of processors.

If loop = geom, then each processor loops over only its atoms. For each atom a unique random number seed is created, based on the atom's xyz coordinates. A velocity is generated using that seed. This is a fast loop and the velocity assigned to a particular atom will be the same, independent of how many processors are used. However, the set of generated velocities may be more correlated than if the *all* or *local* keywords are used.

Note that the *loop geom* keyword will not necessarily assign identical velocities for two simulations run on different machines. This is because the computations based on xyz coordinates are sensitive to tiny differences in the double-precision value for a coordinate as stored on a particular machine.

The *rigid* keyword only has meaning when used with the *zero* style. It allows specification of a fix-ID for one of the rigid-body fix variants which defines a set of rigid bodies. The zeroing of linear or angular momentum is then performed for each rigid body defined by the fix, as described above.

The *units* keyword is used by *set* and *ramp*. If units = box, the velocities and coordinates specified in the velocity command are in the standard units described by the units command (e.g. Angstroms/fmsec for real units). If units = lattice, velocities are in units of lattice spacings per time (e.g. spacings/fmsec) and coordinates are in lattice

spacings. The lattice command must have been previously used to define the lattice spacing.

Restrictions:

Assigning a temperature via the *create* style to a system with rigid bodies or SHAKE constraints may not have the desired outcome for two reasons. First, the velocity command can be invoked before all of the relevant fixes are created and initialized and the number of adjusted degrees of freedom (DOFs) is known. Thus it is not possible to compute the target temperature correctly. Second, the assigned velocities may be partially canceled when constraints are first enforced, leading to a different temperature than desired. A workaround for this is to perform a run 0 command, which insures all DOFs are accounted for properly, and then rescale the temperature to the desired value before performing a simulation. For example:

```
velocity all create 300.0 12345
run 0                           # temperature may not be 300K
velocity all scale 300.0        # now it should be
```

Related commands:

fix rigid, fix shake, lattice

Default:

The keyword defaults are dist = uniform, sum = no, mom = yes, rot = no, bias = no, loop = all, and units = lattice. The temp and rigid keywords are not defined by default.

write_data command

Syntax:

```
write_data file keyword value ...
```

- file = name of data file to write out
- zero or more keyword/value pairs may be appended
- keyword = *pair* or *nocoeff*

```
  nocoeff = do not write out force field info
    pair value = ii or ij
      ii = write one line of pair coefficient info per atom type
      ij = write one line of pair coefficient info per IJ atom type pair
```

Examples:

```
write_data data.polymer
write_data data.*
```

Description:

Write a data file in text format of the current state of the simulation. Data files can be read by the read data command to begin a simulation. The read_data command also describes their format.

Similar to dump files, the data filename can contain a "*" wild-card character. The "*" is replaced with the current timestep value.

NOTE: The write-data command is not yet fully implemented in two respects. First, most pair styles do not yet write their coefficient information into the data file. This means you will need to specify that information in your input script that reads the data file, via the pair_coeff command. Second, a few of the atom styles (body, ellipsoid, line, tri) that store auxiliary "bonus" information about aspherical particles, do not yet write the bonus info into the data file. Both these functionalities will be added to the write_data command later.

Because a data file is in text format, if you use a data file written out by this command to restart a simulation, the initial state of the new run will be slightly different than the final state of the old run (when the file was written) which was represented internally by LAMMPS in binary format. A new simulation which reads the data file will thus typically diverge from a simulation that continued in the original input script.

If you want to do more exact restarts, using binary files, see the restart, write_restart, and read_restart commands. You can also convert binary restart files to text data files, after a simulation has run, using the -r command-line switch.

NOTE: Only limited information about a simulation is stored in a data file. For example, no information about atom groups and fixes are stored. Binary restart files store more information.

Bond interactions (angle, etc) that have been turned off by the fix shake or delete_bonds command will be written to a data file as if they are turned on. This means they will need to be turned off again in a new run after the data file is read.

Bonds that are broken (e.g. by a bond-breaking potential) are not written to the data file. Thus these bonds will not exist when the data file is read.

The *nocoeff* keyword requests that no force field parameters should be written to the data file. This can be very helpful, if one wants to make significant changes to the force field or if the parameters are read in separately anyway, e.g. from an include file.

The *pair* keyword lets you specify in what format the pair coefficient information is written into the data file. If the value is specified as *ii*, then one line per atom type is written, to specify the coefficients for each of the I=J interactions. This means that no cross-interactions for I != J will be specified in the data file and the pair style will apply its mixing rule, as documented on individual pair_style doc pages. Of course this behavior can be overridden in the input script after reading the data file, by specifying additional pair_coeff commands for any desired I,J pairs.

If the value is specified as *ij*, then one line of coefficients is written for all I,J pairs where I <= J. These coefficients will include any specific settings made in the input script up to that point. The presence of these I != J coefficients in the data file will effectively turn off the default mixing rule for the pair style. Again, the coefficient values in the data file can can be overridden in the input script after reading the data file, by specifying additional pair_coeff commands for any desired I,J pairs.

Restrictions:

This command requires inter-processor communication to migrate atoms before the data file is written. This means that your system must be ready to perform a simulation before using this command (force fields setup, atom masses initialized, etc).

Related commands:

read_data, write_restart

Default:

The option defaults are pair = ii.

write_dump command

Syntax:

```
write_dump group-ID style file dump-args modify dump_modify-args
```

- group-ID = ID of the group of atoms to be dumped
- style = any of the supported dump styles
- file = name of file to write dump info to
- dump-args = any additional args needed for a particular dump style
- modify = all args after this keyword are passed to dump_modify (optional)
- dump-modify-args = args for dump_modify (optional)

Examples:

```
write_dump all atom dump.atom
write_dump subgroup atom dump.run.bin
write_dump all custom dump.myforce.* id type x y vx fx
write_dump flow custom dump.%.myforce id type c_myF[3] v_ke modify sort id
write_dump all xyz system.xyz modify sort id elements O H
write_dump all image snap*.jpg type type size 960 960 modify backcolor white
write_dump all image snap*.jpg element element &
   bond atom 0.3 shiny 0.1 ssao yes 6345 0.2 size 1600 1600  &
   modify backcolor white element C C O H N C C C O H H S O H
```

Description:

Dump a single snapshot of atom quantities to one or more files for the current state of the system. This is a one-time immediate operation, in contrast to the dump command which will will set up a dump style to write out snapshots periodically during a running simulation.

The syntax for this command is mostly identical to that of the dump and dump_modify commands as if they were concatenated together, with the following exceptions: There is no need for a dump ID or dump frequency and the keyword *modify* is added. The latter is so that the full range of dump_modify options can be specified for the single snapshot, just as they can be for multiple snapshots. The *modify* keyword separates the arguments that would normally be passed to the *dump* command from those that would be given the *dump_modify*. Both support optional arguments and thus LAMMPS needs to be able to cleanly separate the two sets of args.

Note that if the specified filename uses wildcard characters "*" or "%", as supported by the dump commmand, they will operate in the same fashion to create the new filename(s). Normally, dump image files require a filename with a "*" character for the timestep. That is not the case for the write_dump command; no wildcard "*" character is necessary.

Restrictions:

All restrictions for the dump and dump_modify commands apply to this command as well, with the exception of the dump image filename not requiring a wildcard "*" character, as noted above.

Since dumps are normally written during a run or energy minimization, the simulation has to be ready to run before this command can be used. Similarly, if the dump requires information from a compute, fix, or variable, the information needs to have been calculated for the current timestep (e.g. by a prior run), else LAMMPS will generate an error message.

For example, it is not possible to dump per-atom energy with this command before a run has been performed, since no energies and forces have yet been calculated. See the variable doc page sectinn on Variable Accuracy for more information on this topic.

Related commands:

dump, dump image, dump_modify

Default:

The defaults are listed on the doc pages for the dump and dump image and dump_modify commands.

write_restart command

Syntax:

```
write_restart file keyword value ...
```

- file = name of file to write restart information to
- zero or more keyword/value pairs may be appended
- keyword = *fileper* or *nfile*

```
  fileper arg = Np
      Np = write one file for every this many processors
    nfile arg = Nf
      Nf = write this many files, one from each of Nf processors
```

Examples:

```
write_restart restart.equil
write_restart restart.equil.mpiio
write_restart poly.%.* nfile 10
```

Description:

Write a binary restart file of the current state of the simulation.

During a long simulation, the restart command is typically used to output restart files periodically. The write_restart command is useful after a minimization or whenever you wish to write out a single current restart file.

Similar to dump files, the restart filename can contain two wild-card characters. If a "*" appears in the filename, it is replaced with the current timestep value. If a "%" character appears in the filename, then one file is written by each processor and the "%" character is replaced with the processor ID from 0 to P-1. An additional file with the "%" replaced by "base" is also written, which contains global information. For example, the files written for filename restart.% would be restart.base, restart.0, restart.1, ... restart.P-1. This creates smaller files and can be a fast mode of output and subsequent input on parallel machines that support parallel I/O. The optional *fileper* and *nfile* keywords discussed below can alter the number of files written.

The restart file can also be written in parallel as one large binary file via the MPI-IO library, which is part of the MPI standard for versions 2.0 and above. Using MPI-IO requires two steps. First, build LAMMPS with its MPIIO package installed, e.g.

```
make yes-mpiio    # installs the MPIIO package
make g++          # build LAMMPS for your platform
```

Second, use a restart filename which contains ".mpiio". Note that it does not have to end in ".mpiio", just contain those characters. Unlike MPI-IO dump files, a particular restart file must be both written and read using MPI-IO.

Restart files can be read by a read_restart command to restart a simulation from a particular state. Because the file is binary (to enable exact restarts), it may not be readable on another machine. In this case, you can use the -r command-line switch to convert a restart file to a data file.

NOTE: Although the purpose of restart files is to enable restarting a simulation from where it left off, not all information about a simulation is stored in the file. For example, the list of fixes that were specified during the initial run is not stored, which means the new input script must specify any fixes you want to use. Even when restart information is stored in the file, as it is for some fixes, commands may need to be re-specified in the new input script, in order to re-use that information. Details are usually given in the documentation of the respective command. Also, see the read_restart command for general information about what is stored in a restart file.

The optional *nfile* or *fileper* keywords can be used in conjunction with the "%" wildcard character in the specified restart file name. As explained above, the "%" character causes the restart file to be written in pieces, one piece for each of P processors. By default P = the number of processors the simulation is running on. The *nfile* or *fileper* keyword can be used to set P to a smaller value, which can be more efficient when running on a large number of processors.

The *nfile* keyword sets P to the specified Nf value. For example, if Nf = 4, and the simulation is running on 100 processors, 4 files will be written, by processors 0,25,50,75. Each will collect information from itself and the next 24 processors and write it to a restart file.

For the *fileper* keyword, the specified value of Np means write one file for every Np processors. For example, if Np = 4, every 4th processor (0,4,8,12,etc) will collect information from itself and the next 3 processors and write it to a restart file.

Restrictions:

This command requires inter-processor communication to migrate atoms before the restart file is written. This means that your system must be ready to perform a simulation before using this command (force fields setup, atom masses initialized, etc).

To write and read restart files in parallel with MPI-IO, the MPIIO package must be installed.

Related commands:

restart, read_restart, write_data

Default: none