1. **Lennard-Jones fluid**
   Simulate a LJ fluid with MD, under periodic boundary conditions. Choose a reduced temperature of T^*=1.2 and density rho^*=0.8. Measure the virial pressure.

2. **Crystalization**
   Simulate with MD a system of *N* atoms interacting with an exp-6 potential

$$u(r) = \epsilon \left\{ \frac{6}{\alpha - 6} \exp\left[\alpha\left(1 - \frac{r}{r_\mathrm{m}}\right)\right] - \frac{\alpha}{\alpha - 6}\left(\frac{r_\mathrm{m}}{r}\right)^6 \right\}$$

   with *alpha* = 12, *epsilon*=r_m=1, or with a LJ potential. The system is enclosed in a spherical vessel with repulsive walls characterized by an additional potential

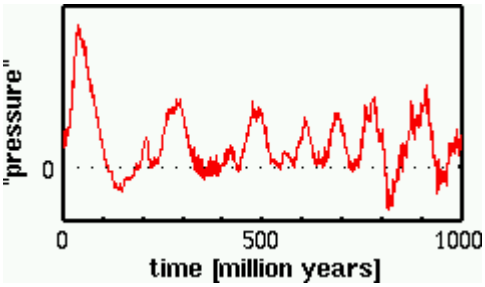
$$u(r) = \begin{cases} 0 & \text{pro } r \le R, \\ (r - R)^2 & \text{pro } r > R, \end{cases}$$

   where *r* is the distance from the center of the vessel ("pro" = for). Choose the initial density of around 0.5. Implement a thermostat (Berendsen) and decrease the temperature slowly to zero (this is actually simulated annealing). What do you observe?

3. **Globular star cluster**
   Simulate with MD a system of *N* massive points interacting with the Newton gravitation potential. As the initial conditions, choose a 3D-Gaussian distribution of distances as well as velocities, and determine the "temperature" from the virial theorem (*2Ekin=-Epot*). Will you obtain a stable globular cluster?
   Note: It is necessary to solve the problem of close passes. It is possible to use the Runge-Kutta integration method with a variable time step – for example, the fastest star passes at most one tenth of the shortest interstellar separation within one time step, or the trick described at http://www.volny.cz/kolafa/jiri/movies/stars.htm

Star cluster

The dynamic evolution of a globular cluster of 300 stars during 1 billion (10^9) years. The size of the sky window is 20 × 20 pc, masses of all stars are equal to the mass of the Sun. The final star density in the center is about 50/pc^3.



The inital configuration of the MD was a cloud with normal distribution of star positions. The inital velocities were drawn from the Maxwell–Boltzmann distribution with "temperat." chosen so that the initial "pressure" = 2×Ekin + Epot = 0. This condition is far from equilibrium and so the time evolution of "pressure" exhibits an increase in the first about 50 M years during which 8 stars escape ("evaporate") from the cluster. The remaining cluster of 292 stars seems to be stable (escape rate less than a few/G years) although the "pressure" still oscillates.

The simulation was performed with MACSIMUS (http://www.vscht.cz/fch/software/macsimus) with a simple sign change transforming electrostatic repulsion of ions into gravitational attraction of stars. The time step was 250 years. To avoid close collisions, a Lennard-Jones potential was added to the star-star gravitational force; an apparent artifact of this approach is the occurence of about 1% of "double stars" kept together by this additional attraction (equilibrium distance about 0.018 pc). The max. relative error of total energy conservation during the run was 1.2×10^{-5}, st. dev. 3.5×10^{-7}.

4. **A simple model of polymer chain**

   Consider a chain of *N* atoms. The neighboring atoms interact with the potential

   $$U(\mathbf{r}_i,\mathbf{r}_{i+1}) = 100\ [|\mathbf{r}_i\text{-}\mathbf{r}_{i+1}|^2 - 1]^2$$

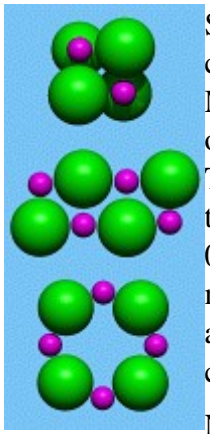
   and all non-neighboring atoms interact with a Lennard-Jones potential with *epsilon = sigma = 1*. Simulate with MD. Monitor the distance of the ends of the chain and the gyration radius r_g

   $$r_g^2 = \sum_{i=1}^{N} m_i(\mathbf{r}_i - \mathbf{r}^{\mathrm{CM}})^2 / \sum_{i=1}^{N} m_i, \qquad \mathbf{r}^{\mathrm{CM}} = \sum_{i=1}^{N} m_i\mathbf{r}_i / \sum_{i=1}^{N} m_i$$

5. *Vibrational spectrum of molecules*

Simulate with MD a cluster of four anions Cl^- and four cations Na^+. The ions interact, apart from the electrostatic forces, with the Lennard-Jones potential with parameters given in the table (1 kcal=4.184 kJ, 1 A=10^{-10} m). The parameters E_{min}, R_{min} for Na^+–Cl^- are given as geometrical mean of both components.

ion	at. mass [g/mol]	$-E_{min}$ [kcal/mol]	R_{min} [Angstrom]
Na^+	22.9898	1.607143	1.0649016
Cl^-	35.4530	0.1177885	2.4790916



Start with a random initial configuration with the distances of ions of 3 to 5 A (take care to avoid any overlap of ions!) First, find an approximate local minimum with an MD simulation with decreasing temperature (use the method of re-scaling velocities or frictional thermostat) to the target of ca. 0.1 K. A suitable integration step is 2 fs. Then, set the velocities randomly, corresponding to ca. 1 K, and simulate without thermostat (in microcanonic ensemble) for at least several tens ps. Measure every 0.01 ps the kinetic energy, optionally the coordinates of the atoms, the dipole moment etc. and perform the Fourier transform. Visualize the resulting spectrum and try to assign the frequencies of normal modes, higher harmonics and combination bands.

Note: there are (at least) three local minima (the figures in parentheses are three lowest frequencies in cm^{-1} obtained with the diagonalization of the Hessian):

- a cube with ions as in the primitive cell of NaCl crystal (138.514, 139.069, 237.569)
- a band 2x4 with chessboard-like distributed ions (17.975, 47.379, 96.634)
- a circle (octagon) with alternating ions (26.462, 31.439, 34.348)

6. *Hard spheres*

Write a program for the MD of hard elastic spheres in periodic boundary conditions. A possible algorithm is as follows:

1. Start with a simple cubic grid of dimensions 5^3 or 6^3. Adjust the grid constant (length of the edge) so that the packing fraction y=(volume of spheres)/(volume of space)=0.4. Assign random initial velocities to the spheres; the system will introduce chaos itself.
2. For every pair, find the time at which the next collision occurs (if it will). For sufficiently dense systems, it is enough to consider the nearest neighbors in PBC. Store the times of collision in a table.
3. Find the time of the next collision. Calculate new velocities after the collision.
4. Redo steps 2 and 3 in a loop. (Re-calculate the times of collisions, perform collision...)

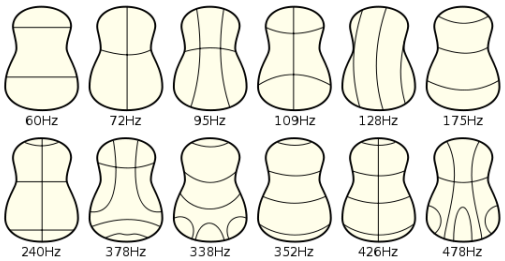
As soon as the equilibrium is reached, obtain the compressibility factor as

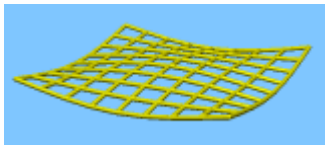
$$z = P\,V / R\,T = 1 + CR\ \mathrm{sqrt}[(PI/3)\ (N/E_{kin})]$$

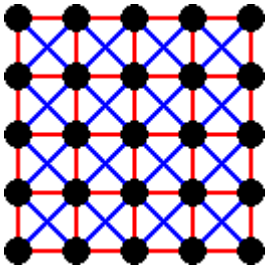
with CR = collision rate = number of collisions per unit of time

7. *Chladni plates*

Certain patterns are observed when a mechanical surface vibrates after being covered with a fine powder. The powder then accumulates on the nodal lines. Chladni, *Entdeckungen über die Theorie des Klanges ("Discoveries in the Theory of Sound")*, 1787. http://wn.com/Chladni's_figures



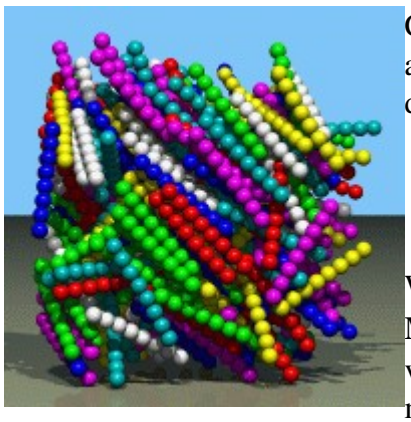


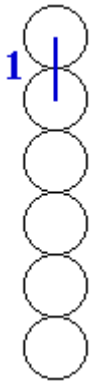


Consider a discrete model of a square plate composed of *N*x*N* "atoms" in a plane; an appropriate *N* is odd. Let the nearest neighbors interact with a potential $U=r^2-1$, and the second-nearest neighbors with $U=r^2-2$. In case of a 3D model (including transversal oscillations), it is necessary to include an additional potential holding the atoms in the plane). Implement the equations of motion, e.g. with the Verlet method.

Does the energy remain constant? Add moderate damping, e.g. in a similar manner like used with velocity rescaling. Add an excitation force to a selected atom, of the form const x cos(t.*omega(t)), where omega* is a slowly varying function of time. Observe the oscillations. Try a plate supported in the center – the central atom has a much larger mass than the others.

8. Liquid crystal





Consider hard rod-like molecules composed of six to ten atoms with a distance of 1 (reduced unit). The atoms in different molecules interact with a WCA LJ potential:

$$u(r) = 4r^{-12} - 4r^{-6} + 1, \quad r<2^{1/6}$$
$$u(r) = 0, \quad r>2^{1/6}$$

Write a program for a Monte Carlo simulation (**you can try MD as well**) in PBC in isobaric ensemble (NPT). Choose a very dilute initial configuration with randomly oriented molecules. The number of molecules should be 200 at least. Perform a simulation with increasing pressure and reduced temperature of T=1. The final pressure should be quite large because the model has no attractive forces. Monitor the parameter of orientation order. What kind of structure do you obtain?

Note: It may take even a couple of days until an ordered structure has established, depending on the efficiency of the code.

The figure shows one periodic simulation cell from a MD simulation with 343 molecules.

9. Traffic jam

Simulate the behavior of cars at a rush hour. Consider a “free” car to move with a constant acceleration (e.g. 2 m/s^2) until it reaches a maximum speed (of e.g. 36 m/s). If the driver sees another car in front of him, he starts to decelerate. The safe distance between cars depends on the speed (e.g. the distance that the car goes within 1 s). The intensity of deceleration should depend on the distance as well (if it is very short, the driver has to kick the brake). The model should contain the element of randomness (decent small acceleration or deceleration, different safe distances held by the individual drivers etc.).

Perform the simulation with PBC – a circular road, with all the cars standing still at the beginning.

An appropriate set of parameters leads to the onset of a traffic jam. The location of the jam is moving in the opposite direction relative to the movement of the cars (backwards).