PRISMS-PF

An Open-Source Phase Field Modeling Framework

PRISMS-PF User Guide (v2.0.2)

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February 1, 2018

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1 Overview

PRISMS-PF is an open-source finite element simulation framework with a focus on solving equations from phase field models. It is being developed as part of the PRISMS Center at the University of Michigan. PRISMS-PF is built on top of the popular and powerful deal.II finite element library. PRISMS-PF was developed to make high performance phase field simulation capabilities available to the wider scientific community with an easy-to-use and easy-to-learn interface. Benchmark tests show that even without its adaptive meshing capabilities PRISMS-PF is competitive with specialized finite difference codes written in Fortran with MPI parallelization in terms performance, and in some cases runs several times faster. PRISMS-PF can be used to solve a wide variety of systems of coupled parabolic partial differential equations (e.g. the diffusion equation) and elliptic partial differential equations (e.g. Poisson's equation). With PRISMS-PF, you have access to adaptive meshing and parallelization that has been demonstrated on over a thousand processors. Moreover, the matrix-free framework from deal.II allows much larger than typical finite element programs – PRISMS-PF has been used for calculations with over one *billion* degrees of freedom.

This user guide starts with instructions for downloading PRISMS-PF and install the necessary prerequisites. Next are instructions for running the built-in example applications and visualizing the results. A detailed look at the input files follows, and the guide finishes with some instructions on how to create your own PRISMS-PF applications.

If you run into any issues not covered by this guide, or have any questions, please send an email to the PRISMS-PF email list: prisms-pf-users@googlegroups.com. If you'd like to contact the PRISMS-PF developers directly, send an email to: prismsphaseField.dev@umich.edu.

PRISMS-PF was developed as part of the PRedictive Integrated Structural Materials Science (PRISMS) Center at University of Michigan which is supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award #DE-SC0008637.

2 Downloading deal.II and PRISMS-PF

Before downloading PRISMS-PF itself, one should install CMake and deal.II. CMake can be downloaded at: https://cmake.org/download, which also has installation instructions. Be sure to add CMake to your path by entering:

```
$ $ PATH="/path/to/cmake/Contents/bin":"$PATH"
```

filling in the path to the installation of CMake (for example, on Mac OS, the default installation path is /Applications/CMake.app/Contents/bin). For convience, we recommend adding this line to your bash profile. Your bash profile can be opened via the following terminal command

```
$ vi ~/.profile
```

Deal.II can be downloaded at https://www.dealii.org/download.html, which also has instructions. The deal.II installation process depends on your operating system. PRISMS-PF has been tested with Deal.II versions 8.3.0 through 8.5.0. We recommend using deal.II 8.4.2, if possible. If you use deal.II 8.5.0, expect to recieve a number of warnings during compilation (discussed in Sec. 3) about functions used in PRISMS-PF that are deprecated in deal.II 8.5.0.

2.1 Installing deal.II for Mac OS X

A binary package for version 8.4.2 (and other versions) is available at https://github.com/dealii/dealii/releases. The binary package includes all the libraries that you need (excluding CMake). To install deal.II open the .dmg file and drag “deal.II.app” into your Applications folder. Then, open “deal.II.app”, which will open a Terminal window and set the necessary environment variables. You may need to modify your security settings so that your operating system will let you open the application (in System Preferences, select Security & Privacy, then under the general tab choose to allow apps downloaded from anywhere; don’t click “Open deal.II.app anyway”, we have found that doing so doesn’t actually launch deal.II.app).

In some cases, deal.II.app will not open, possibly freezing at the “Verifying...” stage. If this happens, right click on it and select “Show Package Contents”. Then go to “/Contents/Resources/bin/” and launch “dealii-terminal”. This should launch the Terminal window that sets the environment variables.

We have found that for some older versions of Mac OS are incompatible with deal.II version 8.4.2 (due to the version of the Clang compiler that is installed by default). In those cases we recommend downloading this version 8.3.0 package:
https://github.com/dealii/dealii/releases/download/v8.3.0/dealii-8.3.0.nocxx14.dmg.

2.2 Installing deal.II for Linux

Unfortunately, on a Linux machine you will likely have to compile and install deal.II from the source. The source code for version 8.4.2 can be downloaded at https://github.com/dealii/dealii/releases. Detailed installation directions can be found at https://www.dealii.org/8.5.0/readme.html. For some versions of Linux, packages are available (Gentoo, Debian testing (stretch), and Ubuntu 16.10+). See https://www.dealii.org/download.html for details.

Below we list instructions for installing deal.II and its prerequisites both manually and using candi, an automatic deal.II installation script. For now, we recomend the traditional route, because we haven’t been able to get candi to consistently work. Recently, deal.II has been made available on Linuxbrew. We have not tried this yet, but it may be a good option. Details can be found at https://github.com/dealii/dealii/wiki/deal.II-on-Homebrew—Linuxbrew.

2.2.1 Traditional Installation (Recommended assuming no package is available)

Before building deal.II, you will need to install two libraries, MPI and p4est. Make sure you have both libraries installed before installing deal.II, or else you will have to reinstall deal.II! Many computing clusters already have these libraries installed. MPI libraries (such as MPICH2) are often available through package managers (e.g. yum, apt, pkg_add, port, brew), installing it using your package manager of choice is likely the simplest option. If not, you can find binaries and the source code at http://www.mpich.org/downloads/, as well as instructions for installation. The p4est library may also be available through your package manager. If not, you can download the latest release tarball at http://www.p4est.org/. To install, unzip the archive, move to the p4est root directory and enter the following commands at the command line:

```
$ ./configure --enable-mpi; make; make install
```

Users have found that this approach works better than the setup script "p4est-setup.sh" that is on the deal.ii website. More detailed installation instructions can be found in the "INSTALL" and "README" files in the p4est root directory.

With MPI and p4est installed, you are ready to install deal.II. Open the archive you downloaded from the deal.II website. From the root deal.II directory enter the following commands:

```
$ mkdir build
$ cd build
$ cmake -DP4EST_DIR=/path/to/installation/dir -DDEAL_II_WITH_P4EST=ON
-DDEAL_II_WITH_MPI=ON -DCMAKE_INSTALL_PREFIX=/path/to/install/dir
$ make install
```

where "/path/to/install/dir" is the path to where you want to install deal.II. After installation is complete (which can take take up to an hour), open the file "summary.log". The second section of the log file lists the configured features. Ensure that DEAL_II_WITH_MPI and DEAL_II_WITH_P4EST say either "set up with bundled packages" or "set up with external dependences". If either is listed as "OFF", then deal.II was unable to find MPI or p4est. If this is the case, double check that MPI and p4est were installed correctly.

2.2.2 Using candi

An alternative route is to use the following candi (compile and install) script to install deal.II and its prerequisites:
https://github.com/koecher/candi

If it works, it should be much simpler than the traditional route described above. However in limited attempts, we have not been able to successfully install deal.II with candi. After more testing and/or consultation with the developer, we hope to make this a plausible option.

2.3 Downloading PRISMS-PF

PRISMS-PF is available for download at our GitHub site: https://github.com/prisms-center/phaseField. The recommended method for downloading the PRISMS-PF source code is through git. Using a Linux/Unix terminal, go to the directory where you want PRISMS-PF to be located. To clone the repository, type:

```
$ git clone https://github.com/prisms-center/phaseField.git
```

Git will then download the PRISMS-PF source code into a directory entitled "phaseField". A resource for learning to use Git can be found at:
https://git-scm.com/book.

If you prefer not to use Git, a zip file containing the PRISMS-PF source code can be downloaded at:
https://github.com/prisms-center/phaseField/releases.

3 Running the Example Applications

3.1 The Example Applications

After deal.II and PRISMS-PF are downloaded, you can run the pre-built PRISMS-PF example applications. At this time, the example applications include:

- allenCahn: An implementation of the Allen-Cahn equation for two phases. (2D)
- allenCahn_pfield: Like allenCahn, but loads in initial conditions using PRISMS IntegrationTools. (2D)
- cahnHilliard: An implementation of the Cahn-Hilliard equation for two phases. (2D)
- cahnHilliardWithAdaptivity: Like cahnHilliard, but with adaptive meshing enabled. (2D)
- coupledCahnHilliardAllenCahn: An implementation of the coupled Cahn-Hilliard/Allen-Cahn set of equations. (2D)
- CHAC_anisotropy: Coupled Cahn-Hilliard/Allen-Cahn equations with weakly anisotropic interfacial energy. (2D)
- CHAC_anisotropyRegularized: Like CHAC_anisotropy, but with a regularization term to permit strongly anisotropic interfacial energy. (2D)
- anisotropyFacet: A different strong anisotropy formation than in CHAC_anisotropyRegularized that is easier to specify particular facets in the Wulff shape. (2D)
- fickianDiffusion: An implementation of the diffusion equation with a time-dependent source term. (2D)
- mechanics: An implementation of linear elasticity for a material in uniaxial tension. (3D)
- CHiMaD_benchmark1a: An implementation of the CHiMaD spinodal decomposition benchmark problem. (2D)
- CHiMaD_benchmark2a: An implementation of the CHiMaD Ostwald ripening benchmark problem. (2D)
- CHiMaD_benchmark6a: An implementation of the CHiMaD electrochemistry benchmark problem. (2D)
- CHiMaD_benchmark6b: An implementation of the CHiMaD electrochemistry benchmark problem with a curved domain. (2D)
- dendriticSolidification: An implementation of a solidification model for a pure material resulting in the growth of a dendrite. (2D)
- eshelbyInclusion: An implementation of linear elasticity for a spherical inclusion. (3D)
- grainGrowth: An implementation of ten coupled Allen-Cahn equations simulating grain growth in two dimensions. (2D)
- precipiateEvolution: An implementation of the coupled Cahn-Hilliard/Allen-Cahn/Linear Elasticity equations often used in phase field simulation of precipitate evolution. (2D)
- precipiateEvolution_pfunction: Like precipitateEvolution, but loads inputs using PRISMS IntegrationTools. (2D)

- singlePrecipitateKKS: Similar to precipiateEvolution, but uses the KKS model rather than the WBM model for the free energy functional. (3D)
- nucleationModel: KKS precipitation model that makes use of the PRISMS-PF explicit nucleation capabilities. (2D)
- preferential_nucleationModel: Like nucleationModel, but with a zone with an increased nucleation rate to simulate a grain boundary. (2D)

A directory for each of these applications can be found in the applications directory (i.e. phaseField/applications). The applications contain a formulation file giving the governing equations. In addition to the 21 applications listed above, some application names may be preceded by an underscore. The underscore is used to denote applications that are still under active development.

3.2 Compiling the Core PRISMS-PF Library

After downloading PRISMS-PF, we recommend that you compile the core library (see note at the end of this section). To do so, enter the root PRISMS-PF directory from the directory where you downloaded it to, run CMake, and then compile the library:

```
$ cd phaseField
$ cmake .
$ make -j 8
```

In the last command, the number following "-j" is the number of threads used during compilation. The general rule of thumb is to pick a number 1.5× the number of processors available. This process should take a minute or two and will compile both the "debug" and "release" versions of the core PRISMS-PF library (see 3.7).

Note: This step can be skipped and the core library will be compiled the first time that you compile one of the applications. However, the compilation will be on a single thread and thus will take much longer than if you follow the instructions above and use multiple threads.

3.3 Running the Allen-Cahn Example Application

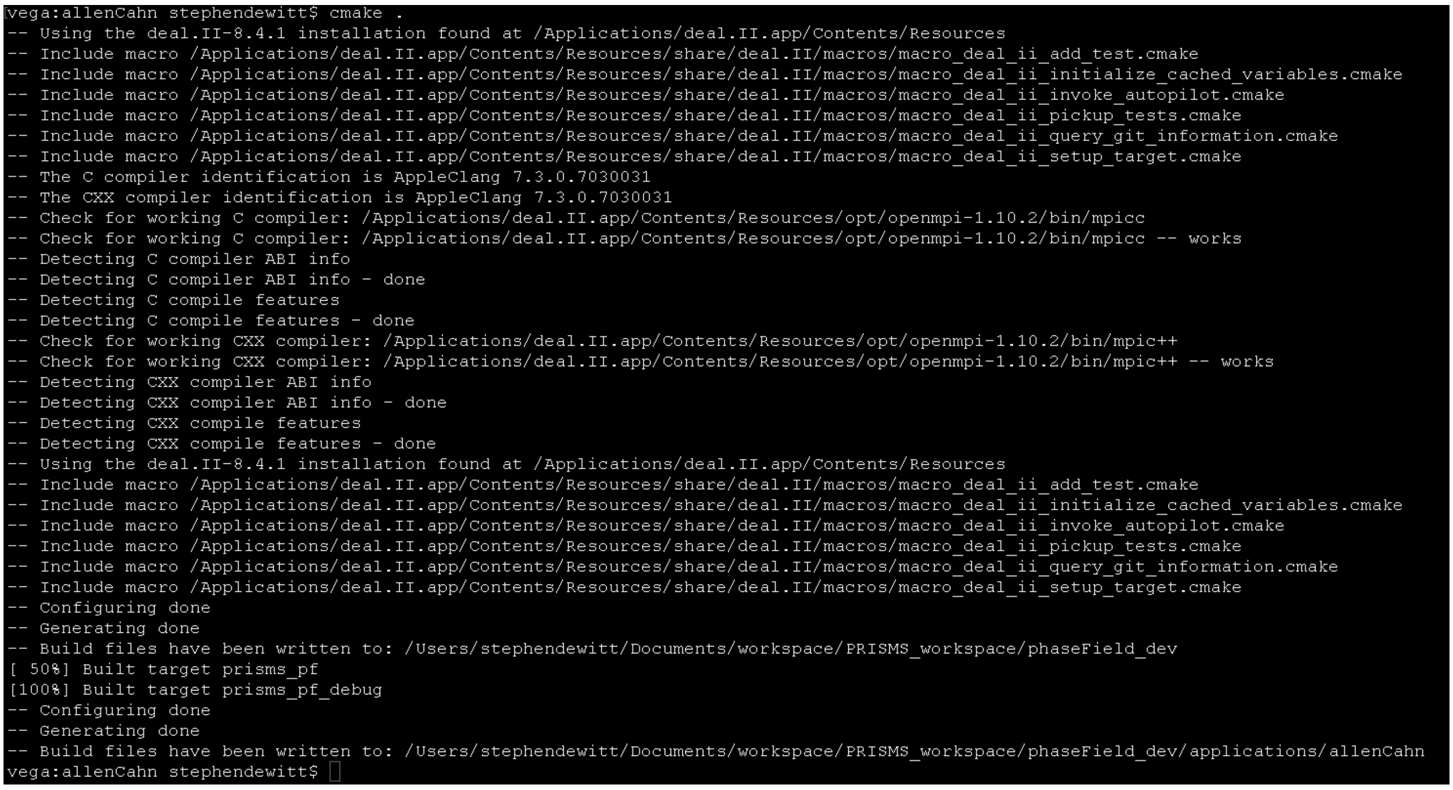
From the "phaseField" directory one can run the Allen-Cahn example application through to following terminal commands:

```
$ cd applications/allenCahn/
$ cmake .
$ make debug
$ mpirun -n 1 main
```

The first command moves from the "phaseField" directory to the directory of the Allen-Cahn example. The second command checks that core PRISMS-PF library has been compiled, (re-)compiles it if necessary, and creates a *makefile* using CMake. The third command compiles the executable in "debug" mode, which enables a number of exception checks in the code and adds debugging information that can be used by a debugger (e.g. gdb). The fourth command runs the program using a single processor.

As the program runs, information from each time step outputs to the terminal window. After the simulation is complete, a summary the time taken in a few major sections of the code and the total wall time is printed to the terminal window.

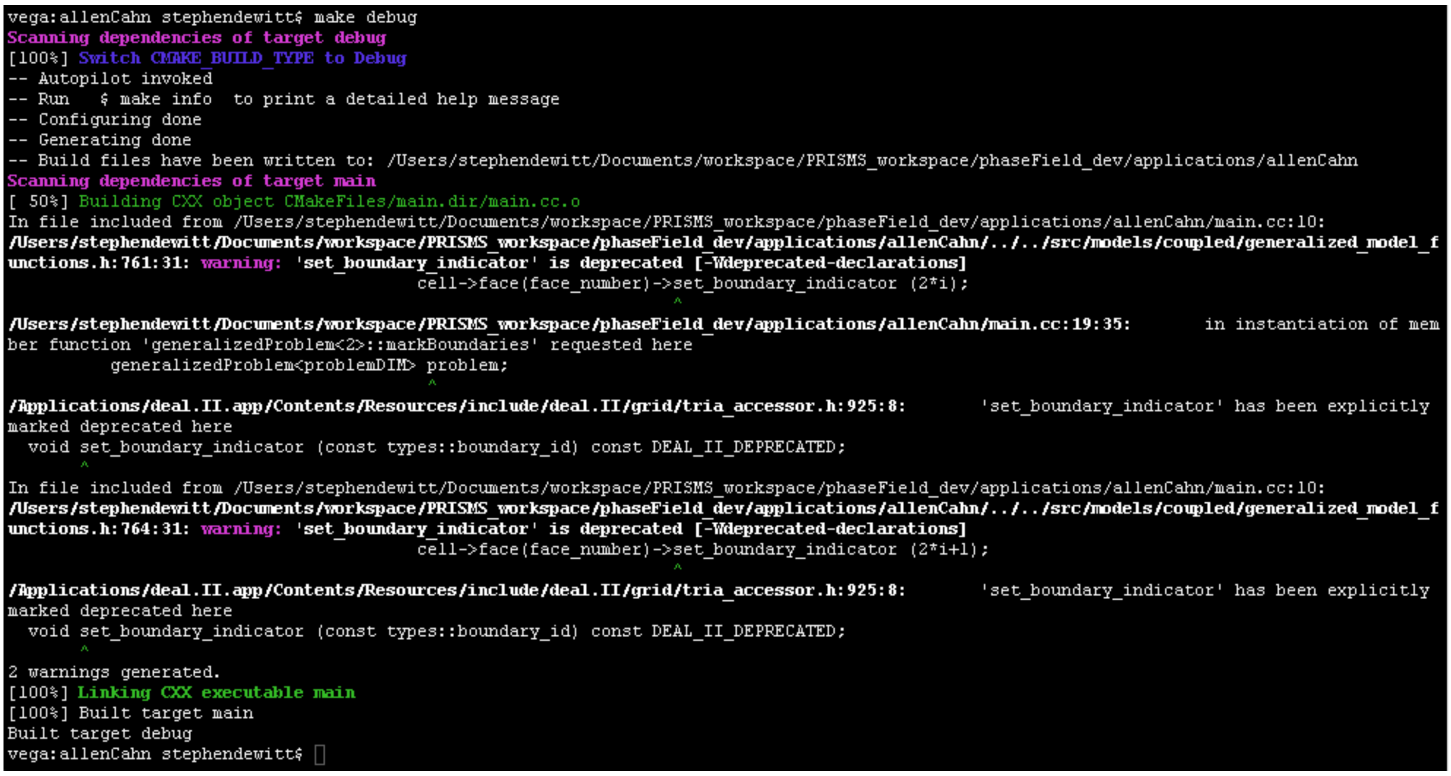
Here is a screenshot of typical output from CMake as you create the *makefile*:



```
vega:allenCahn stephendewitt$ cmake .
-- Using the deal.II-8.4.1 installation found at /Applications/deal.II.app/Contents/Resources
-- Include macro /Applications/deal.II.app/Contents/Resources/share/deal.II/macros/macro_deal_ii_add_test.cmake
-- Include macro /Applications/deal.II.app/Contents/Resources/share/deal.II/macros/macro_deal_ii_initialize_cached_variables.cmake
-- Include macro /Applications/deal.II.app/Contents/Resources/share/deal.II/macros/macro_deal_ii_invoke_autopilot.cmake
-- Include macro /Applications/deal.II.app/Contents/Resources/share/deal.II/macros/macro_deal_ii_pickup_tests.cmake
-- Include macro /Applications/deal.II.app/Contents/Resources/share/deal.II/macros/macro_deal_ii_query_git_information.cmake
-- Include macro /Applications/deal.II.app/Contents/Resources/share/deal.II/macros/macro_deal_ii_setup_target.cmake
-- The C compiler identification is AppleClang 7.3.0.7030031
-- The CXX compiler identification is AppleClang 7.3.0.7030031
-- Check for working C compiler: /Applications/deal.II.app/Contents/Resources/opt/openmpi-1.10.2/bin/mpicc
-- Check for working C compiler: /Applications/deal.II.app/Contents/Resources/opt/openmpi-1.10.2/bin/mpicc -- works
-- Detecting C compiler ABI info
-- Detecting C compiler ABI info - done
-- Detecting C compile features
-- Detecting C compile features - done
-- Check for working CXX compiler: /Applications/deal.II.app/Contents/Resources/opt/openmpi-1.10.2/bin/mpic++
-- Check for working CXX compiler: /Applications/deal.II.app/Contents/Resources/opt/openmpi-1.10.2/bin/mpic++ -- works
-- Detecting CXX compiler ABI info
-- Detecting CXX compiler ABI info - done
-- Detecting CXX compile features
-- Detecting CXX compile features - done
-- Using the deal.II-8.4.1 installation found at /Applications/deal.II.app/Contents/Resources
-- Include macro /Applications/deal.II.app/Contents/Resources/share/deal.II/macros/macro_deal_ii_add_test.cmake
-- Include macro /Applications/deal.II.app/Contents/Resources/share/deal.II/macros/macro_deal_ii_initialize_cached_variables.cmake
-- Include macro /Applications/deal.II.app/Contents/Resources/share/deal.II/macros/macro_deal_ii_invoke_autopilot.cmake
-- Include macro /Applications/deal.II.app/Contents/Resources/share/deal.II/macros/macro_deal_ii_pickup_tests.cmake
-- Include macro /Applications/deal.II.app/Contents/Resources/share/deal.II/macros/macro_deal_ii_query_git_information.cmake
-- Include macro /Applications/deal.II.app/Contents/Resources/share/deal.II/macros/macro_deal_ii_setup_target.cmake
-- Configuring done
-- Generating done
-- Build files have been written to: /Users/stephendewitt/Documents/workspace/PRISMS_workspace/phaseField_dev
[ 50%] Built target prisms_pf
[100%] Built target prisms_pf_debug
-- Configuring done
-- Generating done
-- Build files have been written to: /Users/stephendewitt/Documents/workspace/PRISMS_workspace/phaseField_dev/applications/allenCahn
vega:allenCahn stephendewitt$ 
```

Don't worry if the output isn't exactly the same as what you see, the details of some of the messages depend on your operating system and which compilers you have installed. The important part is that the bottom three messages are “Configuring done”, “Generating done”, and “Build files have been written to: ...”. In the future, entering “$ cmake .” will result in a shorter set of messages because CMake caches some variables from the last time it was run. As a result, you can omit the CMake step for future simulations as long as the path name to your current directory is unchanged and your installation of deal.II is unchanged.

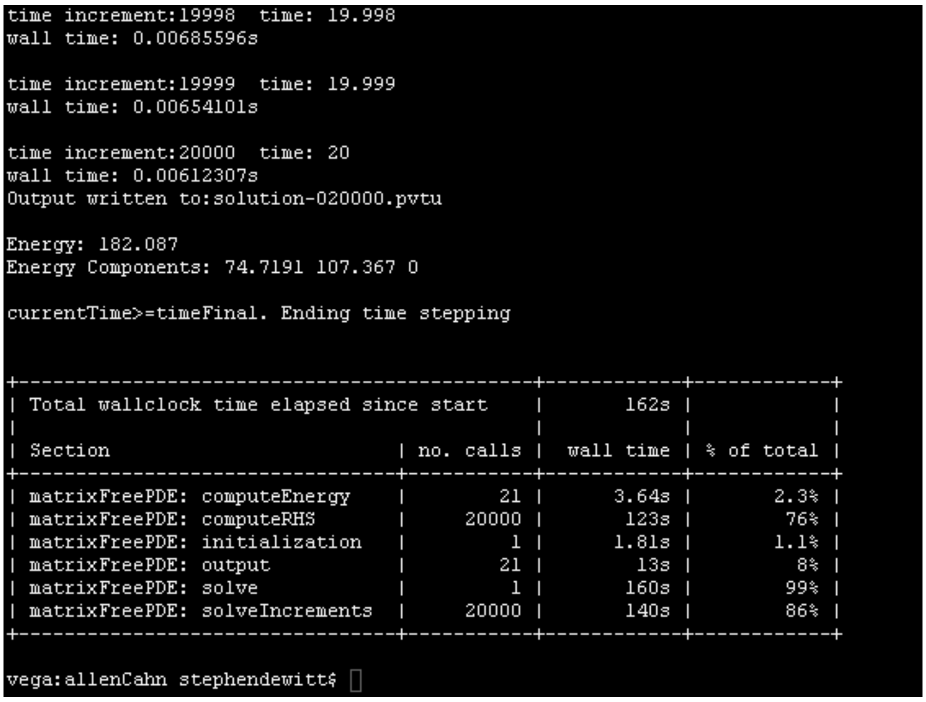
Here is a screenshot of typical output from the compiler as you compile the executable:



```
vega:allenCahn stephendewitt$ make debug
Scanning dependencies of target debug
[100%] Switch CMAKE_BUILD_TYPE to Debug
-- Autopilot invoked
-- Run   $ make info  to print a detailed help message
-- Configuring done
-- Generating done
-- Build files have been written to: /Users/stephendewitt/Documents/workspace/PRISMS_workspace/phaseField_dev/applications/allenCahn
Scanning dependencies of target main
[ 50%] Building CXX object CMakeFiles/main.dir/main.cc.o
In file included from /Users/stephendewitt/Documents/workspace/PRISMS_workspace/phaseField_dev/applications/allenCahn/main.cc:10:
/Users/stephendewitt/Documents/workspace/PRISMS_workspace/phaseField_dev/applications/allenCahn/../../src/models/coupled/generalized_model_f
unctions.h:761:31: warning: 'set_boundary_indicator' is deprecated [-Wdeprecated-declarations]
                                        cell->face(face_number)->set_boundary_indicator (2*i);
                                                                 ^
/Users/stephendewitt/Documents/workspace/PRISMS_workspace/phaseField_dev/applications/allenCahn/main.cc:19:35:       in instantiation of mem
ber function 'generalizedProblem<2>::markBoundaries' requested here
          generalizedProblem<problemDIM> problem;
                                         ^
/Applications/deal.II.app/Contents/Resources/include/deal.II/grid/tria_accessor.h:925:8:       'set_boundary_indicator' has been explicitly
marked deprecated here
  void set_boundary_indicator (const types::boundary_id) const DEAL_II_DEPRECATED;
       ^
In file included from /Users/stephendewitt/Documents/workspace/PRISMS_workspace/phaseField_dev/applications/allenCahn/main.cc:10:
/Users/stephendewitt/Documents/workspace/PRISMS_workspace/phaseField_dev/applications/allenCahn/../../src/models/coupled/generalized_model_f
unctions.h:764:31: warning: 'set_boundary_indicator' is deprecated [-Wdeprecated-declarations]
                                        cell->face(face_number)->set_boundary_indicator (2*i+1);
                                                                 ^
/Applications/deal.II.app/Contents/Resources/include/deal.II/grid/tria_accessor.h:925:8:       'set_boundary_indicator' has been explicitly
marked deprecated here
  void set_boundary_indicator (const types::boundary_id) const DEAL_II_DEPRECATED;
       ^
2 warnings generated.
[100%] Linking CXX executable main
[100%] Built target main
Built target debug
vega:allenCahn stephendewitt$ 
```

Depending on your version of deal.II, different warnings may appear as you compile. Common warnings include the use of functions that deal.II has marked as depricated (as in the screenshot above) and unused type definitions. In this case, PRISMS-PF uses these functions for backward compatability with deal.II version 8.4.x. We will switch to the updated functions in the near future.

Once the simultation is complete, the terminal output at the end of the simulation should look like:

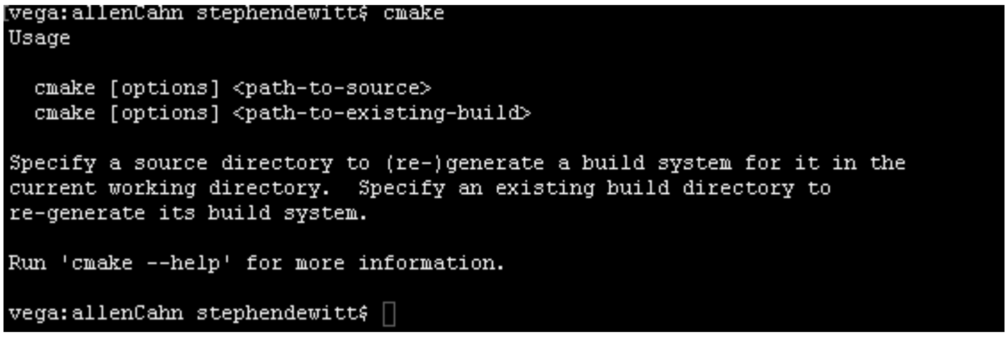


```
time increment:19998  time: 19.998
wall time: 0.00685596s

time increment:19999  time: 19.999
wall time: 0.00654101s

time increment:20000  time: 20
wall time: 0.00612307s
Output written to:solution-020000.pvtu

Energy: 182.087
Energy Components: 74.7191 107.367 0

currentTime>=timeFinal. Ending time stepping


+---------------------------------------------+------------+------------+
| Total wallclock time elapsed since start    |       162s |            |
|                                             |            |            |
| Section                         | no. calls |  wall time | % of total |
+---------------------------------+-----------+------------+------------+
| matrixFreePDE: computeEnergy    |        21 |      3.64s |       2.3% |
| matrixFreePDE: computeRHS       |     20000 |       123s |        76% |
| matrixFreePDE: initialization   |         1 |      1.81s |       1.1% |
| matrixFreePDE: output           |        21 |        13s |         8% |
| matrixFreePDE: solve            |         1 |       160s |        99% |
| matrixFreePDE: solveIncrements  |     20000 |       140s |        86% |
+---------------------------------+-----------+------------+------------+

vega:allenCahn stephendewitt$
```

3.4 What Can Go Wrong

If you were able to enter all of the commands in the previous section and get output similar to the screenshots, congratulations! you just ran your first PRISMS-PF simulation. If not, you may be experiencing one of the common issues listed below.

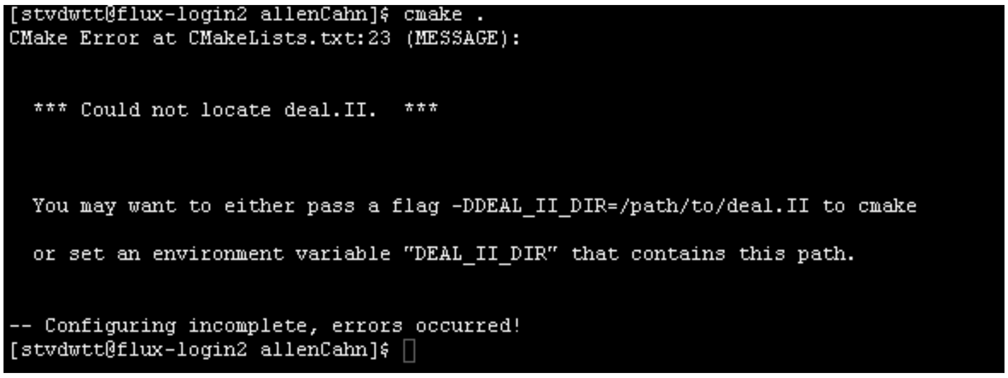
If CMake gives an error message like this:



```
vega:allenCahn stephendewitt$ cmake
Usage

  cmake [options] <path-to-source>
  cmake [options] <path-to-existing-build>

Specify a source directory to (re-)generate a build system for it in the
current working directory.  Specify an existing build directory to
re-generate its build system.

Run 'cmake --help' for more information.

vega:allenCahn stephendewitt$ 
```

Then you likely forgot the period at the end of the command "$ cmake .".

If CMake gives an error message like this:



```
[stvdwtt@flux-login2 allenCahn]$ cmake .
CMake Error at CMakeLists.txt:23 (MESSAGE):


  *** Could not locate deal.II.  ***


  You may want to either pass a flag -DDEAL_II_DIR=/path/to/deal.II to cmake

  or set an environment variable "DEAL_II_DIR" that contains this path.


-- Configuring incomplete, errors occurred!
[stvdwtt@flux-login2 allenCahn]$ 
```

CMake cannot find your installation of deal.ii. This issue is probably caused by the lack of an environment variable pointing to the directory containing your deal.II library. You can check this with the following command:

```
$ echo $DEAL_II_DIR
```

The terminal should then output the path to the deal.II library. For example in Mac OS, the deal.II directory may be "/Applications/deal.II.app/Resources". If DEAL_II_DIR contains a path, go there to see if deal.II is actually installed there. If DEAL_II_DIR is incorrect or empty, you should set it to the directory of the correct path of your deal.II installation with the following command:

```
$ export DEAL_II_DIR=/path/to/dealii
```

Environment variables are erased when you close your shell. To have this path set every time you open a shell (i.e. every time you open a new terminal window), you can add the command above to your shell profile (e.g. .bashrc if you use a bash shell). If you are still having problems, there may be an issue with your deal.II installation. Please consult the deal.II website for instructions.

If CMake cannot successfully detect a C++ compiler, it will generate an error message. The most common cause for this is that the machine runs the Mac OS operating system with an outdated version of the Clang compiler. Upgrading your OS to version 10.11 or newer, updating Xcode, and (re)installing the Xcode command line tools may help. Alternatively, you can install a certain version of the deal.II package that was developed to sidestep this issue:
https://github.com/dealii/dealii/releases/download/v8.3.0/dealii-8.3.0.nocxx14.dmg

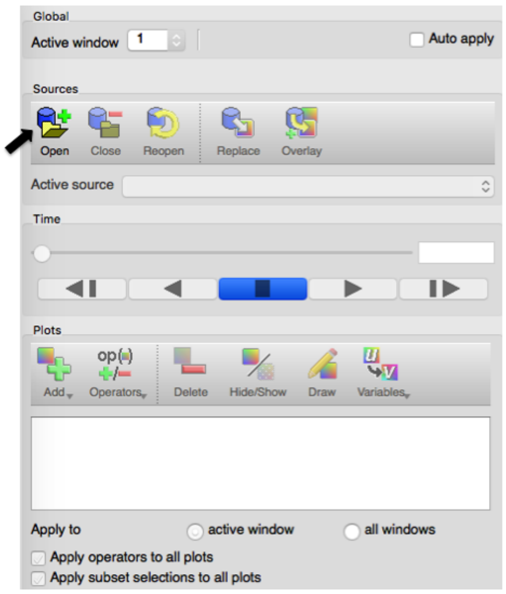
Most of issues users have had are during the CMake step. If the fixes suggested above don't work for your or you have an issue not covered by this list, please contact the PRISMS-PF users list: prisms-pf-users@googlegroups.com. If you are not already on the list, please submit a join request through Google Groups or send an email with "SUBSCRIBE" in the subject line to prismsphasefield.dev@umich.edu. As users come across new issues, we will add them (and suggested fixes) to this section.

3.5 Visualizing the Results of the Simulation

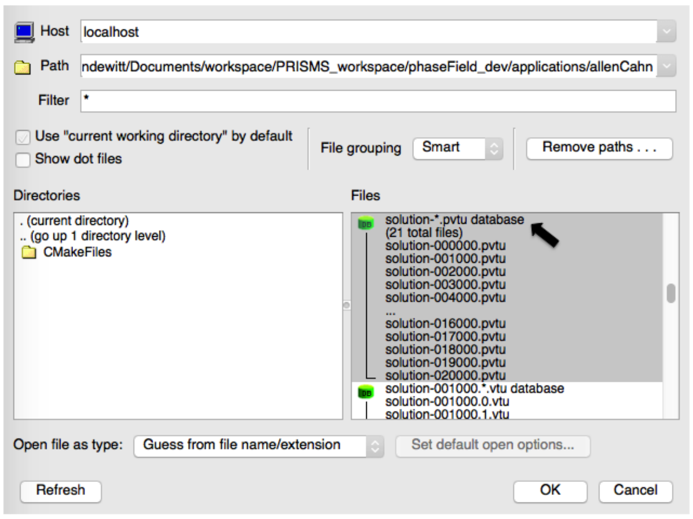
Once you have successfully run a simulation, you will likely want to visualize the results. PRISMS-PF output files are generated in the popular VTK format, as a series of *.vtu and *.pvtu files. Two common open-soure, multi-platform visualization tools for these types of files are VisIt and ParaView. Instructions for downloading this software can be found at their respective websites:
VisIt: https://wci.llnl.gov/simulation/computer-codes/visit/
ParaView: http://www.paraview.org/

To get you started, here is a brief tutorial on how to use VisIt to visualize your simulation results. For more detailed instructions, please consult the VisIt manual:
https://wci.llnl.gov/simulation/computer-codes/visit/manuals

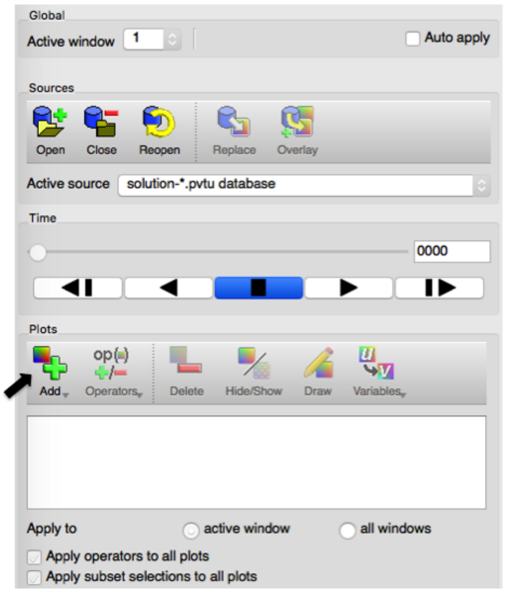
After launching the VisIt application, click "Open" and find the directory for the Allen Cahn example:



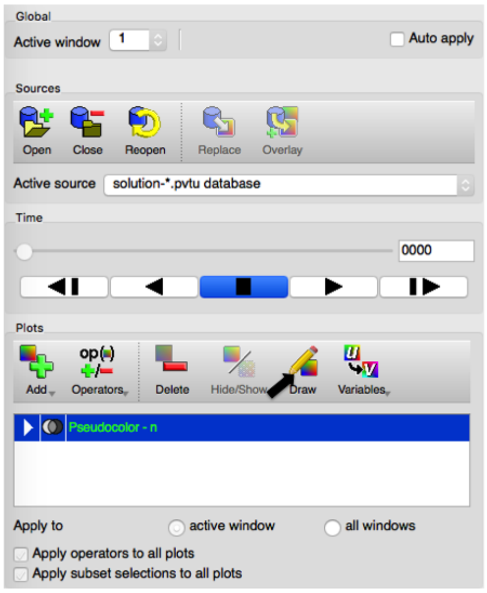
and select "solution-*.pvtu:



Next, click "Add", hover over "Pseudocolor", and select "n":



Next, click "Draw" to make a plot:



Active window 1

Auto apply

Sources

Active source solution-*.pvtu database

0000

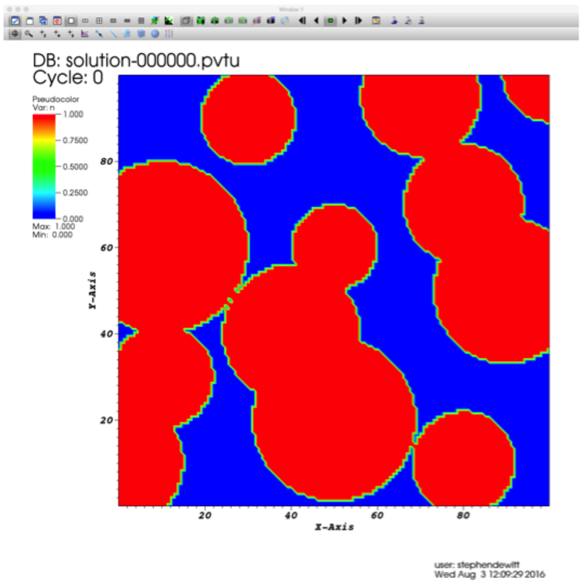
Pseudocolor - n

Apply to active window all windows

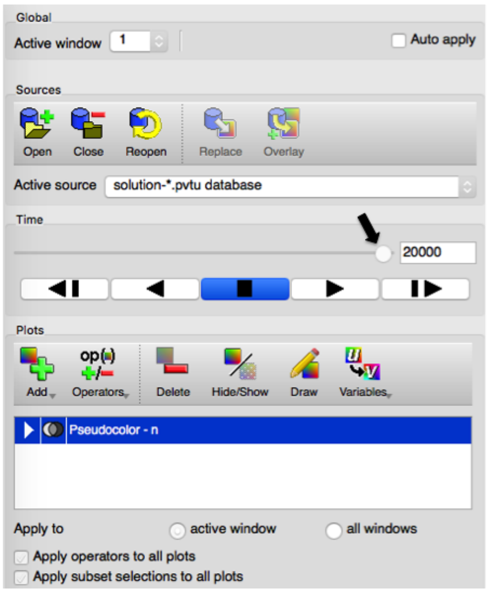
Apply operators to all plots

Apply subset selections to all plots

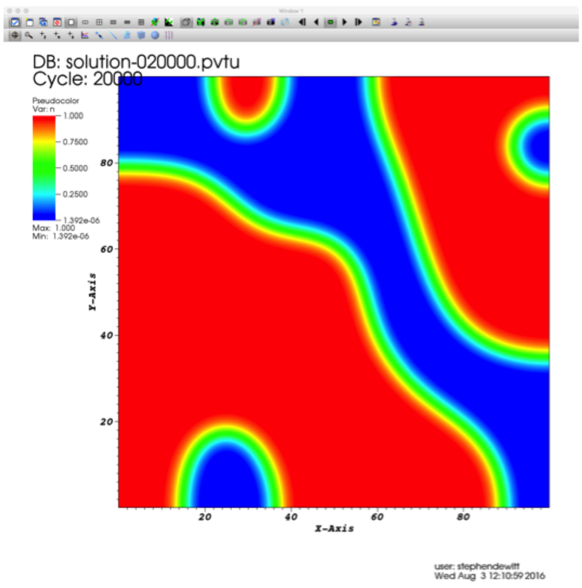
The VisIt window will now have a plot of the initial condition of the order parameter:



The result at other time steps can be visualized by dragging the time bar, or using the controls directly below the time bar. Dragging the time bar to the end will display the final result of the simulation:



Active window 1
Auto apply
Active source solution-*.pvtu database
20000
Pseudocolor - n
Apply to active window all windows
Apply operators to all plots
Apply subset selections to all plots


DB: solution-020000.pvtu
Cycle: 20000

VisIt has a wide variety of capabilities for visualizing 1D, 2D, and 3D data, including postprocessing of output fields (e.g. to obtain derivatives of output fields or the result of mathematical expressions involving one or more output field). VisIt also has a powerful Python interface to provide scripting capabilities. More more instructions on how to use these, and other, features of VisIt, please consult the VisIt manual.

3.6 Running the Other Example Applications

Running the other example applications is as simple as going to the directory for the application of interest and repeating the steps in Section 3.3. For example, to run the Cahn-Hilliard example application, when you are currently in the directory for the Allen-Cahn example application, you would type the following commands:

```
$ cd ../cahnHilliard/
$ cmake .
$ make debug
$ mpirun -n 1 main
```

3.7 Running in Release Mode and with Multple Processors

Once you are sure that your code works as expected, you can compile it in "Release Mode", which is approximately 10x faster than "Debug Mode". However, no exceptions are checked in Release Mode and therefore the code may compile and run even if it contains several errors. Therefore, we strongly recommend that all new code is tested in Debug Mode before switching to Release Mode. To compile in Release mode, replace "$ make debug" with "$ make release".

One of the strengths of PRISMS-PF is that it can be run in parallel with almost no extra effort from the user. To run a simulation in parallel, replace the "1" in the "mpirun" command with the desired number of processor cores. The deal.II packages on their website already contain the MPI library, so no extra software has to be downloaded to use multiple cores.

From the directory of an example application, a simulation can be run in Release Mode on 4 cores using the following commands:

```
$ cmake .
$ make release
$ mpirun -n 4 main
```

4 Structure of a PRISMS-PF Application

4.1 Files in the Application Directories

Each of the example application directories should contain at least eight files:

- parameters.in
- equations.h
- ICs_and_BCs.h
- postprocess.h
- customPDE.h
- main.cc
- formulation.pdf

- CMakeLists.txt

It may contain two other files:

- postprocess.h
- nucleation.h

The following section (Sec. 5) will discuss the structure and options for the input file, parameters.h. Users who do not need to change the governing equations or make other fundamental changes to the application will only need to modify this file.

Section 6 discusses the structure of the files that define an application: equations.h, ICs_and_BCs.h, postprocess.h, nucleation.h, customPDE.h, and main.cc. Users who want to substantially modify existing PRISMS-PF applications or create their own will find this section useful.

The final two files in each application directory are formulation.pdf and CMakeLists.txt. The file formulation.pdf describes the mathematical formulation of the problem solved by the application. Finally, the file CMakeLists.txt is used by CMake to generate the makefile. Most users will not have any reason to change CMakeLists.txt.

5 The Input File: parameters.in

Most PRISMS-PF users will spend the majority of their time interacting with the input file, parameters.h. This file allows users to specify the computational domain, the mesh, the time step parameters, the boundary conditions, the output, and model constants (and more). This file is read as a text file, so modifications to it do not require recompilation of the application.

Here is an example of an input file from the allenCahn application:

```
# Parameter list for the Allen-Cahn example application
# Refer to the PRISMS-PF manual for use of these parameters in the source code.

# =================================================================================
# Set the number of dimensions (2 or 3 for a 2D or 3D calculation)
# =================================================================================
set Number of dimensions = 2

# =================================================================================
# Set the length of the domain in all three dimensions
# (Domain size Z ignored in 2D)
# =================================================================================
# Each axes spans from zero to the specified length
set Domain size X = 100
set Domain size Y = 100
set Domain size Z = 100

# =================================================================================
# Set the element parameters
# =================================================================================
# The number of elements in each direction is 2^(refineFactor) * subdivisions
# Subdivisions Z ignored in 2D
# For optimal performance, use refineFactor primarily to determine the element size
set Subdivisions X = 1
set Subdivisions Y = 1
set Subdivisions Z = 1

set Refine factor = 8

# Set the polynomial degree of the element (allowed values: 1, 2, or 3)
set Element degree = 1

# =================================================================================
# Set the time step parameters
# =================================================================================
# The size of the time step
set Time step = 1.0e-2

# The simulation ends when either the number of time steps is reached or the
# simulation time is reached.
set Number of time steps = 5000

# =================================================================================
# Set the boundary conditions
# =================================================================================
# Set the boundary condition for each variable, where each variable is given by
# its name, as defined in equations.h. The four boundary condition
# types are NATURAL, DIRICHLET, NON_UNIFORM_DIRICHLET and PERIODIC. If all
# of the boundaries have the same boundary condition, only one boundary condition
# type needs to be given. If multiple boundary condition types are needed, give a
# comma-separated list of the types. The order is the miniumum of x, maximum of x,
# minimum of y, maximum of y, minimum of z, maximum of z (i.e left, right, bottom,
# top in 2D and left, right, bottom, top, front, back in 3D). The value of a
# Dirichlet BC is specfied in the following way -- DIRCHILET: val -- where 'val' is
# the desired value. If the boundary condition is NON_UNIFORM_DIRICHLET, the
# boundary condition should be specified in the appropriate function in 'ICs_and_BCs.h'.
# Example 1: All periodic BCs for variable 'c'
# set Boundary condition for variable c = PERIODIC
# Example 2: Zero-derivative BCs on the left and right, Dirichlet BCs with value
# 1.5 on the top and bottom for variable 'n' in 2D
# set Boundary condition for variable n = NATURAL, NATURAL, DIRICHLET: 1.5, DIRICHLET: 1.5

set Boundary condition for variable n = NATURAL

# =================================================================================
# Set the model constants
# =================================================================================
# Set the user-defined model constants, which must have a counter-part given in
# customPDE.h. These are most often used in the residual equations in equations.h,
# but may also be used for initial conditions and nucleation calculations. The type
# options currently are DOUBLE, INT, BOOL, TENSOR, and [symmetry] ELASTIC CONSTANTS
# where [symmetry] is ISOTROPIC, TRANSVERSE, ORTHOTROPIC, or ANISOTROPIC.

# The mobility, MnV in equations.h
set Model constant MnV = 1.0, DOUBLE

# The gradient energy coefficient, KnV in equations.h
set Model constant KnV = 2.0, DOUBLE

# =================================================================================
# Set the output parameters
# =================================================================================
# Type of spacing between outputs ("EQUAL_SPACING", "LOG_SPACING", "N_PER_DECADE",
# or "LIST")
set Output condition = EQUAL_SPACING

# Number of times the program outputs the fields (total number for "EQUAL_SPACING"
# and "LOG_SPACING", number per decade for "N_PER_DECADE", ignored for "LIST")
set Number of outputs = 5

# The number of time steps between updates being printed to the screen
set Skip print steps = 1000
```

The syntax for setting each input parameter is:

```
set [parameter name] = [parameter value]
```

The pound symbol (#) is used for comments, and any text after it is ignored by the file parser.

The following table lists all of the input parameters, seperated into the same groupings in the input file above:

Dimensionality

Name	*Options*	*Required*	*Default*	*Description*
Number of dimensions	2, 3	yes	n/a	The number of dimensions for the simulation.

Compuational Domain

Name	*Options*	*Required*	*Default*	*Description*
Domain size X	Any positive real number	yes	n/a	The size of the domain in the x direction.
Domain size Y	Any positive real number	yes	n/a	The size of the domain in the y direction.
Domain size Z	Any positive real number	yes	n/a	The size of the domain in the z direction.

Element Parameters

Name	*Options*	*Required*	*Default*	*Description*
Subdivisions X	Any positive integer	no	1	The number of mesh subdivisions in the x direction to control the element aspect ratio. The mesh size is $2^{(RefineFactor)}$ × Subdivisions in each direction.
Subdivisions Y	Any positive integer	no	1	The number of mesh subdivisions in the y direction to control the element aspect ratio.The mesh size is $2^{(RefineFactor)}$ × Subdivisions in each direction.
Subdivisions Z	Any positive integer	no	1	The number of mesh subdivisions in the z direction to control the element aspect ratio. The mesh size is $2^{(RefineFactor)}$ × Subdivisions in each direction.
Refine factor	Any non-negative integer	yes	n/a	The number of initial refinements of the mesh. The mesh size is $2^{(RefineFactor)}$ × Subdivisions in each direction. While in principle the mesh could be entirely controlled by the number of subdivisons, computational performance is best when the majority of the refinement is done via the Refine factor.
Element degree	1, 2, 3	no	1	The polynomial order of the elements. The spatial order of accuracy is one plus the degree.

Mesh Adaptivity (Optional)				
Name	*Options*	*Required*	*Default*	*Description*
Mesh adaptivity	Boolean	no	false	Controls whether mesh adaptivity is enabled.
Max refinement level	Any non-negative integer	no	-1	The maximum number of local refinements during adaptive meshing. This parameter does not need to be specified if mesh adaptivity is disabled, but the default value will cause an error if mesh adaptivity is enabled.
Min refinement level	Any non-negative integer	no	-1	The minimum number of local refinements during adaptive meshing. This parameter does not need to be specified if mesh adaptivity is disabled, but the default value will cause an error if mesh adaptivity is enabled.
Refinement criteria fields	Comma separated list of variable names	no	0	The indices of the variables that will determine the mesh refinement. The variable names are determined by the names given in equations.h.
Refinement window max	Comma separated list of real numbers	no		The mesh refines where the specified variables are between an upper and lower bound. This specifies the upper bound.
Refinement window min	Comma separated list of real numbers	no		The mesh refines where the specified variables are between an upper and lower bound. This specifies the lower bound.
Steps between remeshing operations	Positive integer	no	1	The number of time steps between mesh refinement operations.

Time Stepping				
Name	*Options*	*Required*	*Default*	*Description*
Time step	Any positive real number	yes	n/a	The time step size for the simulation.
Number of time steps	Any non-negative integer	no	-1	The number of time steps until the simulation stops. Either this or the simulation end time must be specified. If both are specified, the simulation will end when the first condition is reached.
Simulation end time	Any non-negative real number	no	-0.1	The simulated time when until the simulation stops. Either this or the number of time steps must be specified. If both are specified, the simulation will end when the first condition is reached.

Elliptic Solver Parameters (Optional)				
Name	*Options*	*Required*	*Default*	*Description*
Linear solver	SolverCG	no	SolverCG	Currently the only option is the deal.II conjugate gradient solver.
Use absolute convergence tolerance	Boolean	no	false	Sets whether to use an absolute tolerance for the linear solver (versus a relative tolerance).
Solver tolerance value	Any positive real number	no	1e-3	The tolerance for the linear solver. If an absolute tolerance is used, the iterative solver stops when the L2 norm of the residual drops below the tolerance. If a relative tolerance is used, the iterative solver stops when the L2 norm of the residual has dropped by a factor equal to the tolerance.
Maximum allowed solver iterations	Any positive integer	no	10000	The maximum number of iterations for the linear solver, if this number of iterations is reached, the solver stops regardless of the tolerance value.

Output (Optional)				
Name	*Options*	*Required*	*Default*	*Description*
Output condition	EQUAL_SPACING, LOG_SPACING, N_PER_DECADE, LIST	no	EQUAL _SPACING	This sets the spacing between the times the simulation outputs the model variables. EQUAL_SPACING spaces them equally, LOG_SPACING spaces them $10^{n/(outputs)\log(timesteps)}$, N_PER_DECADE allows the user to set how many times the simulation outputs per power of ten iterations, and LIST outputs at a user-given list of time step numbers.
Number of outputs	Any non-negative integer	no	10	The number of inputs if the output condition is EQUAL_SPACING. The number of outputs if the output condition is N_PER_DECADE. Ignored for the other output conditions.
List of time steps to output	Comma-separated list of non-negative integers	no	0	The list of time steps to output, used for the LIST output condition and ignored for the others.
Output file name (base)	String	no	solution	The name for the output file, before the time step and processor info are added.
Output file type	vtu, vtk	no	vtu	The output file type (currently limited to either vtu or vtk).
Output separate files per process	Boolean	no	false	Whether to output separate vtu files for each process in a parallel calculation (automatically set to true for vtk files). Separate files may decrease the time spent outputting results but may increase file tranfer times, as well as cluttering directories.
Skip print steps	Any positive integer	no	1	The number of time steps between updates to the terminal window (1 is every time step).

Checkpoints (Optional)				
Name	*Options*	*Required*	*Default*	*Description*
Load from a checkpoint	Boolean	no	false	Whether to start the simulation from the checkpoint of another simulation. See Note 2 below for the details of the checkpoint/restart system.
Checkpoint condition	EQUAL_SPACING, LOG_SPACING, N_PER_DECADE, LIST	no	EQUAL _SPACING	This sets the spacing between the times the simulation outputs the model variables. EQUAL_SPACING spaces them equally, LOG_SPACING spaces them $10^{n/(outputs)\log(timesteps)}$, N_PER_DECADE allows the user to set how many times the simulation outputs per power of ten iterations, and LIST outputs at a user-given list of time step numbers.
Number of checkpoints	Any non-negative integer	no	1	The number of inputs if the output condition is EQUAL_SPACING. The number of outputs if the output condition is N_PER_DECADE. Ignored for the other output conditions.
List of time steps to save checkpoints	Comma-separated list of non-negative integers	no	0	The list of time steps to create checkpoints, used for the LIST output condition and ignored for the others.

Boundary Conditions				
Name	*Options*	*Required*	*Default*	*Description*
Boundary condition for variable [variable name]	NATURAL, DIRICHLET, NON_UNIFORM _DIRICHLET, PERIODIC	yes	n/a	Sets the boundary condition for each scalar variable, using the variable name from equations.h. One line is required for each scalar variable. See Note 1 below for details.
Boundary condition for variable [variable name], component [direction]	NATURAL, DIRICHLET, NON_UNIFORM _DIRICHLET, PERIODIC	yes	n/a	Sets the boundary condition for each vector variable, using the variable name from equations.h. One line is required for each vector variable. See Note 1 below for details.

Loading Initial Conditions from File (Optional)

Name	*Options*	*Required*	*Default*	*Description*
Load initial conditions	Comma-separated list of booleans	no	false	One true/false flag for each variable for whether the initial condition should be loaded from a vtk file. Currently, only scalar fields can be read in. See Note 3 below for details.
Load parallel file	Comma-separated list of booleans	no	false	One true/false flag for each variable for whether each processor should read the initial conditions from a seperate file. See Note 3 below for details.
File names	Comma-separated list of strings	no		The name of the vtk file to be read for each variable, ignored for variables where the initial conditions isn't read in from a file. Often, all of the variables will read from the same vtk file. See Note 3 below for details.
Variable names in the files	Comma-separated list of strings	no		What each variable is named in the file being loaded. See Note 3 below for details.

Shared Nucleation Parameters (Optional)

Name	*Options*	*Required*	*Default*	*Description*
Time steps between nucleation attempts	Any positive integer	no	100	The number of time steps between nucleation attempts. This parameter is shared among all nucleating variables. See Note 4 below for details.
Minimum allowed distance between nuclei	Any non-negative real number	no	2× the largest nucleus semiaxis	The minimum allowed distance between nuclei centers during a single nucleation attempt. This parameter is shared among all nucleating variables. See Note 4 below for details.
Order parameter cutoff value	Any non-negative real number	no	0.01	The minimum allowed value of the sum of all nucleating variable fields where nucleation is allowed to occur. Implemented to prevent nucleation inside existing particles. This parameter is shared among all nucleating variables. See Note 4 below for details.
	Any positive integer	no	100	The number of time steps between nucleation attempts. This parameter is shared among all nucleating variables. See Note 4 below for details.

Nucleation Parameters for Each Nucleating Variable (Optional)				
Name	*Options*	*Required*	*Default*	*Description*
Nucleus semiaxes (x, y ,z)	Three positive real numbers	no		The semiaxes of the ellipsoidal nuclei to be seeded. See Note 4 below for details.
Nucleus rotation in degrees (x, y, z)	Three real numbers	no		The rotation of the nuclei placed with the explicit nucleation algorithm. The rotations are given with respect to the normal direction using intrinsic Tait-Bryan angles. Positive rotations correspond to a counter-clockwise rotation when looking along the positive axis of interest. All three angles must be specified regardless of problem dimension.
Freeze zone semiaxes (x, y ,z)	Three positive real numbers	no		The semiaxes for the ellipsoidal region where the nucleus is frozen after seeding. See Note 4 below for details.
Freeze time following nucleation	Any non-negative real number	no	0	The amount of time the nucleus is frozen after seeding. See Note 4 below for details.
Nucleation-free border thickness	Any non-negative real number	no	0	The size of the buffer region where nucleation is not allowed unless the boundary conditions are periodic. See Note 4 below for details.

Model constants (Optional)				
Name	*Options*	*Required*	*Default*	*Description*
Model constant [constant name]	value followed by a comma then a type	no		Sets the value of a constant defined for that particular application. The allowed types are DOUBLE, INT, BOOL, TENSOR, and [symmetry] ELASTIC CONSTANTS where [symmetry] is ISOTROPIC, TRANSVERSE, ORTHOTROPIC, or ANISOTROPIC. See Note 5 below for details.

Note 1 (Boundary Conditions):
The boundary condition must be set for each variable, where each variable is given by its name, as defined in equations.h. The four boundary condition types are NATURAL, DIRICHLET, NON_UNIFORM_DIRICHLET and PERIODIC. If all of the boundaries have the same boundary condition, only one boundary condition type needs to be given. If multiple boundary condition types are needed, give a comma-separated list of the types. The order is the miniumum of x, maximum of x, minimum of y, maximum of y, minimum of z, maximum of z (i.e left, right, bottom, top in 2D and left, right, bottom, top, front, back in 3D). The value of a Dirichlet BC is specfied in the following way – DIRCHILET: val – where 'val' is the desired value. If the boundary condition is NON_UNIFORM_DIRICHLET, the boundary condition should be specified in the appropriate function in 'ICs_and_BCs.h'. For vector variables, one boundary condition should be specified for each component.

Example 1: All periodic BCs for variable 'c'

```
set Boundary condition for variable c = PERIODIC
```

Example 2: Zero-derivative BCs on the left and right, Dirichlet BCs with value 1.5 on the top and bottom for variable 'n' in 2D

```
set Boundary condition for variable n = NATURAL, NATURAL, DIRICHLET: 1.5,
 DIRICHLET: 1.5
```

Example 3: All periodic BCs for the y component of the vector variable 'u'

```
set Boundary condition for variable u, component y = PERIODIC
```

Note 2 (Checkpoint/Restart):
The checkpoint/restart simulation allows one to continue from a previous simulation by loading the mesh and variable values from that previous simulation. One use of this system is to continue a simulation that stopped part of the way through, due to a hardware failure, running out of the allotted time on a cluster, etc. A second use is to use one simulation as the initial condition for another. Note that the simulated time carries over from the checkpoint. Thus if one ran a simulation to completion but wanted to see further evolution, one could load from the checkpoint created at the end of that simulation, but the desired number of time steps or simulation end time would have to be increased. Currently, the checkpoint system always read from files named "restart.mesh", "restart.mesh.info", and "restart.time.info". When a checkpoint is created, the previous checkpoint files have ".old" appended to their file names. To load from these older checkpoint files, the newer ones should be deleted (or moved) and the ".old" should be deleted from the names of the older files. An example of using the checkpoint/restart system can be seen in the 'dendriticSolidification' application.

Note 3 (Loading Initial Conditions from File):
Currently, initial conditions can only be read from vtk files (*not* vtu files). Some variables can have initial conditions read from file and others can be specified in ICs_and_BCs.h in the same application. For each variable, the user must set whether the file(s) to be read are in serial format, where all processors read from the same file, or parallel format, where all processors read from different files. If parallel format is selected, the desired domain decomposition must between the files and the simulation to be run. For non-adaptive meshes this will be true if the same number of cores is the same between the simulation that generated the vtk files and the simulation reading the vtk files. For adaptive meshes, obtaining the same domain decomposition may be difficult and merging parallel vtk files into a single file is likely the best approach. This process is planned to be cleaner in future versions of PRISMS-PF. An example of loading inital conditions from file can be seen in the 'allenCahn_pfield' application.

Note 4 (Nucleation):
PRISMS-PF includes the capability for explicitly placing nuclei over the course of a simulation using an approach similar to the one described in the following publication:
Jokisaari, Permann, and Thornton, A nucleation algorithm for the coupled conserved-nonconserved phase field model, *Computational Materials Science*, 112, (2016).
A nucleus of an non-conserved order parameter is placed within the computational domain determined by a probability given by the 'getNucleationProbability' function in the 'nucleation.h' file. The variables that are allowed to nucleate are specified in the 'loadVariableAttributes' function in the 'equations.h' file, as are the variable values needed to calculate the nucleation probability. The determination of when and where a nucleus should be seeded is determined in the core

PRISMS-PF library, but the actual placement of the nucleus by modifying one of the model fields is expected to be performed in the 'residualRHS' function in the 'equations.h' file. The placement of the nucleus is aided by the 'weightedDistanceFromNucleusCenter' function in the core library. The mobility for the nucleated field should be set to zero in the region surrounding the nucleus (the "freeze zone") for a specified amount of time (the "freeze time"). Examples of nucleating particles can be found in the nucleationModel and preferential_nucleationModel applications.

Currently, the nucleation parameters are the only place where the 'subsection' command is used in 'parameters.in'. This command is used to set nucleation parameters seperately for each nucleating variable. Each subsection is opened by "subsection Nucleation parameters:" followed by the variable name as set in 'equations.h'. The end of each subsection block is concluded with the 'end' command. For example, if there are two nucleating order parameters *n1* and *n2*, the nucleation parameters section could look as follows:

```
# ==========================================================================
# Set the nucleation parameters
# ==========================================================================

set Time steps between nucleation attempts = 30
set Minimum allowed distance between nuclei = 50.0
set Order parameter cutoff value = 0.01

subsection Nucleation parameters: n1
    set Nucleus semiaxes (x, y, z) = 10, 5, 5
    set Nucleus rotation in degrees (x, y, z) = 0, 0, 60
    set Freeze zone semiaxes (x, y, z) = 15, 7.5, 7.5
    set Freeze time following nucleation = 20
    set Nucleation-free border thickness = 15
end

subsection Nucleation parameters: n2
    set Nucleus semiaxes (x, y, z) = 20, 10, 10
    set Nucleus rotation in degrees (x, y, z) = 0, 0, 0
    set Freeze zone semiaxes (x, y, z) = 30, 15, 15
    set Freeze time following nucleation = 40
    set Nucleation-free border thickness = 30
end
```

The first three lines set the shared nucleation parameters. Next comes the subsection block for the variable *n1* and the subsection block for the variable *n2*.

Note 5 (Model constants):
Each application specifies its own set of model constants. These are most often used in the residual equations in the 'equations.h' file, although they may also be used to specify initial conditions, non-uniform Dirichlet boundary conditions, nucleation probabilties, etc. Currently, five types of model constants are accepted: DOUBLE, INT, BOOL, TENSOR, and ELASTIC CONSTANTS. The use of these different types is as follows:

- DOUBLE: For individual real numbers
- INT: For individual integers
- BOOL: For individual booleans (true/false)
- TENSOR: For either rank 1 tensors (i.e. vectors) or rank 2 tensors (i.e. matrices) with a size of the number of dimensions. These are assumed to be real numbers. Each row should be given by a comma-separated list in parentheses. For example, a 3D vector would be given as "(2.5, 1.2, 0.1)" and a 2D matrix would be given as: "((4.1, 2.0),(1.6, 5.2))".
- [symmetry] ELASTIC CONSTANTS: For sets of elastic constants, given as a vector. The symmetry options are ISOTROPIC, TRANSVERSE, ORTHOTROPIC, or ANISOTROPIC.

The number of entries for the different symmetries are given below. PRISMS-PF converts these sets of elastic constants into a stiffness matrix.

The number and order of the entries for the elastic constants are (where C_{ij} are entries in the stiffness matrix):

- ISOTROPIC (2D/3D): 2 constants (Young's Modulus, Poisson's Ratio)
- TRANSVERSE (3D): 5 constants (C_{11}, C_{33}, C_{44}, C_{12}, C_{13})
- ORTHOTROPIC (3D): 9 constants (C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}, C_{12}, C_{13}, C_{23})
- ANISOTROPIC (2D/3D): 21 constants (C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}, C_{12}, C_{13}, C_{14}, C_{15}, C_{16}, C_{23}, C_{24}, C_{25}, C_{26}, C_{34}, C_{35}, C_{36}, C_{45}, C_{46}, C_{56})

Each model constant in 'parameters.in' must have a counterpart in the appropriate section of the 'customPDE.h' file.

6 The Application Files: equations.h, ICs_and_BCs.h, postprocess.h, nucleation.h, customPDE.h, and main.cc

This section details the files that define each application. The norm is that substantial modifications to these files consistute a new application (in contrast to simply making changes to 'parameters.in'. Modifying these files may require some knowledge of C++.

A very brief description of the purpose of each of these files is below, an in-depth discussion can be found in the following subsections:

- equations.h: Specifies the attributes of the model variables and the model's residual equations
- ICs_and_BCs.h: Specifies the initial conditions for each variable (unless the initial condition is read from file) and non-uniform Dirichlet boundary conditions, if applicable.
- postprocess.h: Specifies variable other than the primary model variables to output, as well as the expressions to derive these variables.
- nucleation.h: Contains the function that determines the probability density of nucleation.
- customPDE.h: Contains the prototypes of the functions for the application, also contains declarations of the model constants given in 'parameters.h'.
- main.cc: Main C++ function that controls the flow of the simulation. Identical for all the example applications and it is unlikely that users will need to modify it.

In all of these files, the user can access user inputs from parameters.in via the "userInputs" object (e.g. the domain size, the time step size). See Appendix I for a table of variable names inside "userInputs".

6.1 equations.h

The file "equations.h" contains a list of the variables in the model equations and their attributes as well as the residuals for the model equations. The file contains three functions: *loadVari-*

ableAttributes, *residualRHS*, and *residualLHS*.

To modify the functions in this file, one needs to be familar with the weak form of the governing equations (hereafter referred to as the residual equations). In PRISMS-PF, the residual equations are expressed in two terms. The first is the part of the integrand that is multiplied by the test function. The second is the part of the integrand that multipled by the gradient of the test function. For the coupled Cahn-Hilliard/Allen-Cahn system, the residual equations are

$$\int_\Omega w\eta^{n+1}\, dV = \int_\Omega w \left(\underbrace{\eta^n - \Delta t M_\eta\ ((f^n_{\beta,c} - f^n_{\alpha,c})H^n_{,\eta})}_{r_\eta} \right) + \nabla w \cdot \underbrace{(-\Delta t M_\eta \kappa)\nabla \eta^n}_{r_{\eta x}}\ dV \tag{1}$$

and

$$\int_\Omega wc^{n+1}\, dV = \int_\Omega w \underbrace{c^n}_{r_c} \tag{2}$$

$$+ \nabla w \underbrace{(-\Delta t M_c)\ [\ (f^n_{\alpha,cc}(1-H^{n+1}) + f^n_{\beta,cc}H^{n+1})\nabla c +\ \ ((f^n_{\beta,c} - f^n_{\alpha,c})H^{n+1}_{,\eta}\nabla\eta)]}_{r_{cx}}\ dV \tag{3}$$

for the Allen-Cahn and Cahn-Hilliard equation, respectively. Each of the residual terms is marked with an underbrace. The terms multiplied by the test function are referred to as the value residual terms and the terms multiplied by the gradient of the test function are referred to as the gradient residual terms.

6.1.1 loadVariableAttributes

Here is the *loadVariableAttributes* function for the coupled Allen-Cahn/Cahn-Hilliard example application:

```
// ================================================================================
// Set the attributes of the primary field variables
// ================================================================================
void variableAttributeLoader::loadVariableAttributes(){
	// Variable 0
	set_variable_name				(0,''c'');
	set_variable_type				(0,SCALAR);
	set_variable_equation_type		(0,PARABOLIC);

	set_need_value					(0,true);
	set_need_gradient				(0,true);
	set_need_hessian				(0,false);

	set_need_value_residual_term	(0,true);
	set_need_gradient_residual_term	(0,true);

	// Variable 1
	set_variable_name				(1,''n'');
	set_variable_type				(1,SCALAR);
	set_variable_equation_type		(1,PARABOLIC);

	set_need_value					(1,true);
	set_need_gradient				(1,true);
	set_need_hessian				(1,false);

	set_need_value_residual_term	(1,true);
	set_need_gradient_residual_term	(1,true);
}
```

This function specifies the model variables and their attributes. In this case, the two model variables are the concentration, “c”, and the order parameter, “n”. Here, “c” is listed as the zeroth variable and “n” is listed as the first. For each variable, a series of attributes are set using a series of C++ function calls. The following table lists the functions and a description of the attributes they set:

Function	*Options*	*Required*	*Default*	*Description*
set_variable_name	String	no	var	Sets the name of the variable. This name is used in ‘parameters.in’ as well as during output.
set_variable_type	SCALAR, VECTOR	no	SCALAR	Sets whether the variable is a scalar or a vector.
set_variable_equation_type	PARABOLIC, ELLIPTIC	no	PARABOLIC	Sets whether the govenring equation for the variable is a parabolic or ellpitic PDE.
set_need_value	Boolean	no	true	Sets whether the value of the variable is needed in the function *residualRHS* below.
set_need_gradient	Boolean	no	true	Sets whether the gradient of the variable is needed in the function *residualRHS* below.
set_need_hessian	Boolean	no	false	Sets whether the hessian of the variable is needed in the function *residualRHS* below.
set_need_need_value _residual_term	Boolean	no	false	Sets whether the residual equation has a value residual term.
set_need_need_gradient _residual_term	Boolean	no	false	Sets whether the residual equation has a gradient residual term.
set_need_value_LHS	Boolean	no	false	Sets whether the value of the variable is needed in the function *residualLHS* below. (Only needed for elliptic PDEs).
set_need_gradient_LHS	Boolean	no	false	Sets whether the gradient of the variable is needed in the function *residualLHS* below. (Only needed for elliptic PDEs).
set_need_hessian_LHS	Boolean	no	false	Sets whether the hessian of the variable is needed in the function *residualLHS* below. (Only needed for elliptic PDEs).
set_need_need_value _residual_term_LHS	Boolean	no	false	Sets whether the LHS residual equation has a value residual term. (Only needed for elliptic PDEs).
set_need_need_gradient _residual_term_LHS	Boolean	no	false	Sets whether the LHS residual equation has a gradient residual term. (Only needed for elliptic PDEs).
set_allowed_to_nucleate	Boolean	no	false	Sets whether the nucleation algorithms should be activated for this variable. (Only needed when nucleation is desired).
set_need_value_nucleation	Boolean	no	false	Sets whether the value of the variable is needed to calculate the nucleation probability in the ‘nucleation.h’ file. (Only needed when nucleation is desired).

Function	*Options*	*Required*	*Default*	*Description*
set_need_value_pp	Boolean	no	true	Sets whether the value of the variable is needed in the function *postProcessedFields* in 'postprocess.h'.
set_need_gradient_pp	Boolean	no	true	Sets whether the gradient of the variable is needed in the function *postProcessedFields* in 'postprocess.h'.
set_need_hessian_pp	Boolean	no	true	Sets whether the hessian of the variable is needed in the function *postProcessedFields* in 'postprocess.h'.

Some of these function calls are not present in the 'equations.h' file for the coupledCahnHilliardAllenCahn application. Use of the LHS function calls can be found in the preciptiateEvolution application (among others) and use the nucleation function calls can be found the nucleationModel and preferential_nucleationModel applications.

6.1.2 residualRHS

Here is the *residualRHS* function for the coupled Allen-Cahn/Cahn-Hilliard example application:

```
// ===========================================================================
// residualRHS
// ===========================================================================
// This function calculates the residual equations for each variable. It takes
// "variable_list" as an input, which is a list of the value and derivatives of
// each of the variables at a specific quadrature point. The (x,y,z) location of
// that quadrature point is given by "q_point_loc". The function outputs residuals
// to variable_list. The index for each variable in this list corresponds to
// the index given at the top of this file.
template <int dim, int degree>
void customPDE<dim,degree>::residualRHS(
                variableContainer<dim,degree,dealii::VectorizedArray<double> > & variable_list,
                 dealii::Point<dim, dealii::VectorizedArray<double> > q_point_loc) const {

//c
scalarvalueType c = variable_list.get_scalar_value(0);
scalargradType cx = variable_list.get_scalar_gradient(0);

//n
scalarvalueType n = variable_list.get_scalar_value(1);
scalargradType nx = variable_list.get_scalar_gradient(1);

// Free energy for each phase and their first and second derivatives
scalarvalueType faV = (-1.6704-4.776*c+5.1622*c*c-2.7375*c*c*c+1.3687*c*c*c*c);
scalarvalueType facV = (-4.776 + 10.3244*c - 8.2125*c*c + 5.4748*c*c*c);
scalarvalueType faccV = (10.3244-16.425*c+16.4244*c*c);
scalarvalueType fbV = (5.0*c*c-5.9746*c-1.5924);
scalarvalueType fbcV = (10.0*c-5.9746);
scalarvalueType fbccV = constV(10.0);

// Interpolation function and its derivative
scalarvalueType hV = (10.0*n*n*n-15.0*n*n*n*n+6.0*n*n*n*n*n);
scalarvalueType hnV = (30.0*n*n-60.0*n*n*n+30.0*n*n*n*n);

// Residual equations
scalargradType muxV = ( cx*((1.0-hV)*faccV+hV*fbccV) + nx*((fbcV-facV)*hnV) );
scalarvalueType rcV = c;
scalargradType rcxV = (constV(-McV*userInputs.dtValue)*muxV);
scalarvalueType rnV = (n-constV(userInputs.dtValue*MnV)*(fbV-faV)*hnV);
scalargradType rnxV = (constV(-userInputs.dtValue*KnV*MnV)*nx);

// Residuals for the equation to evolve the concentration
variable_list.set_scalar_value_residual_term(0,rcV);
variable_list.set_scalar_gradient_residual_term(0,rcxV);

// Residuals for the equation to evolve the order parameter
variable_list.set_scalar_value_residual_term(1,rnV);
variable_list.set_scalar_gradient_residual_term(1,rnxV);

}
```

In this function the residuals at a particular quadrature point are calculated. The inputs to this function are a list of the model variable values and derivatives, *variable_list* and a point giving access to (x,y,z) coordinates, *q_point_loc*. The residual terms are added to *variable_list* as the output. The first few lines of the function set more convienent names for the variables and their derivatives. By convention, the value of the variable is denoted by the variable name (c for the concentration and n for the structural order parameter in this case), the list of first derivatives is denoted by the variable name followed by an "x", and second derivatives are denoted by the variable name followed by "xx". Each variable in *variable* can be accessed by the index it was given in *loadVariableAttributes*. The variable value and the derivatives can be accessed through the *get_scalar_value*, *get_scalar_gradient*, and *get_scalar_hessian* object members for scalar variables and the *get_vector_value*, *get_vector_gradient*, and *get_vector_hessian* functions. The data type for the value of a scalar variable is *scalarvalueType* (a scalar), the data type for the first derivatives of a scalar variable is *scalargradType* (a vector with a length equal to the number of dimensions), and the data type for the second derivatives of a scalar variable is *scalarhessType* (a matrix with a size equal to the number of dimensions by the number of dimensions). For vector variables, the data types are *vectorvalueType* (a vector with length equal to the number of dimensions), *vectorgradType* (a matrix with a size equal to the number of dimensions by the number of dimensions), and *vectorgradType* (a rank-three tensor with a size in each direction equal to the number of dimensions).

After the nicknames for the field variables are set, the residual terms are calculated (including some intermediate variables, such as the free energies and the interpolation functions in the example above). These use the same six data types discussed in the preceding paragraph. The model variables given in 'parameters.h' can be used to define the residual terms.

Finally, the residuals for the governing equations are submitted to *variable_list*, using the functions *set_scalar_value_residual_term*, *set_scalar_gradient_residual_term*, *set_vector_value_residual_term*, and *set_vector_gradient_residual_term*, once again referring the variables by their index.

The nickname step can be skipped, if desired, although the code is generally more readable with nicknames (and the performance overhead is minimal). An example without nicknames for the fields can be found in the grainGrowth application, where loops over the ten variables are easier to construct when not declaring all of the variables at once. One word of caution, though: calling *set_scalar_value_residual_term* and *set_scalar_gradient_residual_term* overwrites the value and gradient of the variable, respectively (and same for the variants for vectors). Thus, either the residuals need to be cached and then set after all the residuals have been calculated (as is done in the grainGrowth application) or the values and gradients need to be cached before setting the residuals (as is done with the standard nicknaming approach).

A Note on Types: The deal.II library uses a data structure called a VectorizedArray to store the variable values and their derivatives. This data structured in optimized for modern vectorized processors, giving a substantial speedup in some cases. However, this data structure can complicate things slightly. One complicating factor is that VectorizedArrays can't always be added, subtracted, multiplied, or divided with more standard data types like doubles. For this reason, you will see the "constV(arguement)" function scattered throughout the code. This function turns a non-VectorizedArray into a VectorizedArray. To be safe, you can always encase non-VectorizedArrays with "constV()" when they share an operation with a VectorizedArray. A second complication is that not all of the standard mathematical operations are available for VectorizedArrays. The basic trigonometric functions are available, as are exponentials and square roots. However, hyperbolic tangents are not. If needed, they must be constructed from exponents. A third complication is that conditional statements involving VectorizedArrays are not allowed. VectorizedArrays contain data from multiple points that the processor operates on at once. Under normal conditions a conditional statement could only be applied to one of the points in the VectorizedArray. There are possible ways to break up the VectorizedArrays and work on the pieces of data individually, but this approach is not recommended for most users. Clever use of "max" and "min" functions (which do exist for VectorizedArrays) may be able to take the place of a conditional statement. For more details on the deal.II implementation of VectorizedArrays (including a list of mathematical operations that are allowed), please visit: https://www.dealii.org/8.4.0/doxygen/deal.II/classVectorizedArray.html

6.1.3 residualLHS

In the coupledCahnHilliardAllenCahn, the *residualLHS* function is empty because it is only needed for elliptic PDEs (or more specifically, when a non-trivial matrix inversion needs to be performed). Here is the *residualLHS* function from the precipitateEvolution application, where the equation for mechanical equilibrium is elliptic.

From the formulation file in the precipitateEvolution application, the residual equation for the mechanical displacement is:

$$R = \int_\Omega \nabla w : C(\eta_1, \eta_2, \eta_3) : \left(\epsilon - \epsilon^0(c, \eta_1, \eta_2, \eta_3)\right) \; dV = 0 \tag{4}$$

To turn this equation into a matrix inversion problem, we can linearize it with Newton's method. (It can also be directly written as a matrix inversion problem. For historical purposes we do the linearization and for some mundane reasons, non-zero Dirichlet boundary conditions do not currently work with that approach. Therefore, for the meantime, we recommend the approach below.) The solution u is found through the following expression, given an initial guess u_0:

$$0 = R(u) = R(u_0 + \Delta u) \tag{5}$$

where $\Delta u = u - u_0$. Then, applying the discretization that $u = \sum_i N^i U^i$, where N^i is the ith shape function, we can write the following linearization:

$$\frac{\delta R(u)}{\delta u} \Delta U = -R(u_0) \tag{6}$$

The discretized form of this equation can be written as a matrix inversion problem. However, in PRISMS-PF, we only care about the product $\frac{\delta R(u)}{\delta u} \Delta U$. Taking the variational derivative of

$R(u)$ yields:

$$\begin{aligned}
\frac{\delta R(u)}{\delta u} &= \frac{d}{d\alpha}\int_\Omega \nabla w : C : \left[\epsilon(u+\alpha w) - \epsilon^0\right]\ dV\Big|_{\alpha=0} && (7)\\
&= \int_\Omega \nabla w : C : \frac{1}{2}\frac{d}{d\alpha}\left[\nabla(u+\alpha w) + \nabla(u+\alpha w)^T - \epsilon^0\right]\ dV\Big|_{\alpha=0} && (8)\\
&= \int_\Omega \nabla w : C : \frac{d}{d\alpha}\left[\nabla(u+\alpha w) - \epsilon^0\right]\ dV\Big|_{\alpha=0} \quad \textit{(due to the symmetry of C)} && (9)\\
&= \int_\Omega \nabla w : C : \nabla w\ dV && (10)
\end{aligned}$$

In its discretized form $\frac{\delta R(u)}{\delta u}\Delta U$ is:

$$\frac{\delta R(u)}{\delta u}\Delta U = \sum_i \sum_j \int_\Omega \nabla N^i : C : \nabla N^j dV\ \Delta U^j \tag{11}$$

Moving back to the non-discretized form yields:

$$\frac{\delta R(u)}{\delta u}\Delta U = \int_\Omega \nabla w : C : \nabla(\Delta u) dV \tag{12}$$

Thus, the full equation relating u_0 and Δu is:

$$\int_\Omega \nabla w : \underbrace{C : \nabla(\Delta u)}_{r_{ux}^{LHS}} dV = -\int_\Omega \nabla w : \underbrace{(\epsilon - \epsilon^0)}_{r_{ux}}\ dV \tag{13}$$

The above values of r_{ux}^{LHS} and r_{ux} are used to define the residuals in the equations.h file. A similar process can be undertaken for other elliptic problems.

The *residualLHS* function from the preciptiateEvolution application is:

```
// =================================================================================
// residualLHS (needed only if at least one equation is elliptic)
// =================================================================================
// This function calculates the residual equations for the iterative solver for
// elliptic equations.for each variable. It takes "modelVariablesList" as an input,
// which is a list of the value and derivatives of each of the variables at a
// specific quadrature point. The (x,y,z) location of that quadrature point is given
// by "q_point_loc". The function outputs "modelRes", the value and gradient terms of
// for the left-hand-side of the residual equation for the iterative solver. The
// index for each variable in these lists corresponds to the order it is defined at
// the top of this file (starting at 0), not counting variables that have
// "need_val_LHS", "need_grad_LHS", and "need_hess_LHS" all set to "false". If there
// are multiple elliptic equations, conditional statements should be used to ensure
// that the correct residual is being submitted. The index of the field being solved
// can be accessed by "this->currentFieldIndex".
template <int dim, int degree>
void customPDE<dim,degree>::residualLHS(
        variableContainer<dim,degree,dealii::VectorizedArray<double> > & variable_list,
        dealii::Point<dim, dealii::VectorizedArray<double> > q_point_loc) const {

//n1
scalarvalueType n1 = variable_list.get_scalar_value(1);

//n2
scalarvalueType n2 = variable_list.get_scalar_value(2);

//n3
scalarvalueType n3 = variable_list.get_scalar_value(3);
//u
vectorgradType ux = variable_list.get_vector_gradient(4);
vectorgradType ruxV;

// Interpolation functions

scalarvalueType h1V = (10.0*n1*n1*n1-15.0*n1*n1*n1*n1+6.0*n1*n1*n1*n1*n1);
scalarvalueType h2V = (10.0*n2*n2*n2-15.0*n2*n2*n2*n2+6.0*n2*n2*n2*n2*n2);
scalarvalueType h3V = (10.0*n3*n3*n3-15.0*n3*n3*n3*n3+6.0*n3*n3*n3*n3*n3);

// Take advantage of E being simply 0.5*(ux + transpose(ux)) and use the dealii "symmetrize" function
dealii::Tensor<2, dim, dealii::VectorizedArray<double> > E;
E = symmetrize(ux);

// Compute stress tensor (which is equal to the residual, Rux)
if (n_dependent_stiffness == true){
        dealii::Tensor<2, CIJ_tensor_size, dealii::VectorizedArray<double> > CIJ_combined;
        CIJ_combined = CIJ_Mg*(constV(1.0)-h1V-h2V-h3V) + CIJ_Beta*(h1V+h2V+h3V);

        computeStress<dim>(CIJ_combined, E, ruxV);
}
else{
        computeStress<dim>(CIJ_Mg, E, ruxV);
}

variable_list.set_vector_gradient_residual_term(4,ruxV);

}
```

Like *residualRHS*, *residualLHS* takes *variables_list* and *q_point_loc* as inputs. However, because only one elliptic equation is solved at a time, the output are the residual terms for a single residual. As in *residualRHS*, the model variable values and derivatives are given convienent names at the start of the file. Similar to *residualRHS*, the value of *ruxV* is set and then used to set the appropriate residual for *variables_list* (in this case the vector residual term for the fourth variable).

If multiple elliptic equations need to be solved, you will need to use conditional statements to calculate the proper residual depending on the elliptic equation being solved. The index of the field being solved can be accessed using the "this->currentFieldIndex" statement.

6.2 IC_and_BCs.h

The 'ICs_and_BCs.h' file contains four functions: *InitialCondition*, *InitialConditionVec*, *NonUniformDirichletBC*, and *NonUniformDirichletBCVec*. The first two functions in the file are used to set the initial conditions for scalar and vector variables, respectively, while the third and fourth functions set non-uniform Dirichlet boundary conditions for scalar and vector variables, respectively. For all of these functions, most users should only need to modify the sections between the lines.

6.2.1 InitialCondition and InitialConditionVec

Here's a look at the *InitialCondition* function for the coupled Allen-Cahn/Cahn-Hilliard example application:

```
template <int dim>
double InitialCondition<dim>::value (const Point<dim> &p, const unsigned int component) const
{
          double scalar_IC = 0;
          // ---------------------------------------------------------------------------
```

```
        // ENTER THE INITIAL CONDITIONS HERE FOR SCALAR FIELDS
        // ---------------------------------------------------------------------------
        // Enter the function describing conditions for the fields at point "p".
        // Use "if" statements to set the initial condition for each variable
        // according to its variable index.

        // The initial condition is two circles/spheres defined
        // by a hyperbolic tangent function. The center of each circle/sphere is
        // given by "center" and its radius is given by "rad".

        double center[2][3] = {{1.0/3.0,1.0/3.0,1.0/3.0},{3.0/4.0,3.0/4.0,3.0/4.0}};
        double rad[12] = {userInputs.domain_size[0]/5.0, userInputs.domain_size[0]/12.0};
        double dist;
        scalar_IC = 0;

        if (index == 0){
                scalar_IC = 0.009;
        }

        for (unsigned int i=0; i<2; i++){
                dist = 0.0;
                for (unsigned int dir = 0; dir < dim; dir++){
                        dist += (p[dir]-center[i][dir]*userInputs.domain_size[dir])
                                        *(p[dir]-center[i][dir]*userInputs.domain_size[dir]);
                }
                dist = std::sqrt(dist);

                // Initial condition for the concentration field
                if (index == 0){
                        scalar_IC += 0.5*(0.125)*(1.0-std::tanh((dist-rad[i])/(1.0)));
                }
                else {
                        scalar_IC += 0.5*(1.0-std::tanh((dist-rad[i])/(1.0)));
                }
        }

        // ---------------------------------------------------------------------------
        return scalar_IC;
}
```

In this function, the variable *scalarIC* should be set to the desired intitial condition. The (x,y,z) coordinates can be accessed by the *p* variable, with indices zero through 2. For example, if you wanted to initialize a field to $5xy$, you would enter:

```
scalarIC = 5.0 * p[0] * p[1];
```

The initial conditions given above are a bit more complicated. They set the initial conditions for two circular (spherical in 3D) particles. The initial condition for different variables is set using conditional statements and the *index* variable. The *index* variable refers to the variable index from the top of the "equations.h". This example uses conditional statements to set the initial conditions differently for the concentration (*index*==0) and the structural order parameter (*index*==0). The initial conditions for both fields are calculated using hyperbolic tangent functions that make use of the distance between the centers of the particles and the point *p*.

The model constants defined in 'parameters.in' can be used in the intial condition or boundary condition functions. However, the syntax is the same as in 'customPDE.h', not as in the residual functions. That is, they have to be extracted from the *userInputs* object. An example of this is in the dendriticSolidification application, where *deltaV* is set using one of the model constants.

Similarly, the initial conditions for vector fields are set in *InitialConditionsVec*. Here is the (somewhat trivial) *InitialConditionVec* function for the precipitateEvolution example application:

```
template <int dim>
void InitialConditionVec<dim>::vector_value (
        const dealii::Point<dim> &p,
        dealii::Vector<double> &vector_IC) const
```

```
{
            // ---------------------------------------------------------------------------
            // ENTER THE INITIAL CONDITIONS HERE FOR VECTOR FIELDS
            // ---------------------------------------------------------------------------
            // Enter the function describing conditions for the fields at point "p".
            // Use "if" statements to set the initial condition for each variable
            // according to its variable index.

            if (index==4){
                   vector_IC(0) = 0.0;
                   vector_IC(1) = 0.0;
            if (dim == 3){
                   vector_IC(2) = 0.0;
            }
            }
            // ---------------------------------------------------------------------------
}
```

The initial condition for each component is set using the *vector_IC* variable, where parentheses are used to select the x, y, or z component.

6.2.2 NonUniformDirichletBC and NonUniformDirichletBCVec

These functions are needed when one or more boundaries are set to NON_UNIFORM_DIRICHLET. These functions are very similar to the initial condition functions above, the user sets an expression for *scalar_BC* or *vector_BC* at point *p*. Once again, the variable *index* is used to differentiate between variables based on their index from the top of the 'equations.h' file. For Dirichlet boundary conditions that vary in time, the current time can be accessed via the variable *time*.

Currently, the one of the only two applications that use a non-uniform Dirichlet boundary condition is CHiMaD_benchmark6a (the other is CHiMaD_benchmark6b). Here is the *NonUniformDirichletBC* function from CHiMaD_benchmark6a:

```
template <int dim>
double NonUniformDirichletBC<dim>::value (
         const dealii::Point<dim> &p,
         const unsigned int component) const
{
     double scalar_BC=0;
     // ---------------------------------------------------------------------------
     // ENTER THE NON-UNIFORM DIRICHLET BOUNDARY CONDITIONS HERE FOR SCALAR FIELDS
     // ---------------------------------------------------------------------------
     // Enter the function describing conditions for the fields at point "p".
     // Use "if" statements to set the boundary condition for each variable
     // according to its variable index. This function can be left blank if there
     // are no non-uniform Dirichlet boundary conditions.

     if (index == 2){
          if (direction == 1){
               double x=p[0];
               double y=p[1];
               scalar_BC=std::sin(y/7.0);
          }
     }
     // ---------------------------------------------------------------------------
     return scalar_BC;
}
```

6.3 postprocess.h

Unlike the files discussed so far in this section, the 'postprocess.h' file is optional. This file allows users to specify fields other than the primary model variable to output. It also includes an option to integrate over a field variable (e.g. to check conservation of a field). In the example problems, this file is often used to calculate the total free energy of the system, which should be monotonically decreasing for most phase field problems. It also is convienent for calculating somewhat complicated expressions such as chemical potentials, stresses, and strains.

Note: Two restrictions are currently in place for the postprocessor. First, postprocessing variables can only be scalars, not vectors. Second, the postprocessor won't work if the primary model variable with index zero is a vector. (This is because postprocessor uses the mesh of the zeroth primary variable to calculate and output the postprocessed field.) These restrictions will be lifted in future versions of PRISMS-PF.

6.3.1 loadPostProcessorVariableAttributes

Similar to the 'equations.h' file, 'postprocess.h' begins with a function called *loadPostProcessorVariableAttributes*, which sets the attributes of the postprocessing variables. Here is the *loadPostProcessorVariableAttributes* function from the coupledCahnHilliardAllenCahn application, where the postprocessed field is "f_tot", the total free energy:

```
void variableAttributeLoader::loadPostProcessorVariableAttributes(){

        // Variable 0
        set_variable_name                (0,"f_tot");
        set_variable_type                (0,SCALAR);

        set_need_value_residual_term     (0,true);
        set_need_gradient_residual_term  (0,false);

        set_output_integral              (0,true);

}
```

As in 'equations.h', a series of attributes for each variable are set using a series of C++ function calls. The following table lists the functions and a description of the attributes they set:

Function	*Options*	*Required*	*Default*	*Description*
set_variable_name	String	no	var	Sets the name of the variable.
set_variable_type	SCALAR, VECTOR	no	SCALAR	Sets whether the variable is a scalar or a vector (Currently only scalar fields are allowed).
set_need_need_value _residual_term	Boolean	no	false	Sets whether the expression for the postprocessed field has a value residual term.
set_need_need_gradient _residual_term	Boolean	no	false	Sets whether the expression for the postprocessed field has a gradient residual term.
set_output_integral	Boolean	no	false	Sets whether the integrated value of the postprocessed field is calculated. The integrated value is output to the file 'integratedFields.txt'.

6.3.2 postProcessedFields

The second function in the 'postprocess.h' file is similar to the residual functions in 'equations.h'. The primary difference is that, while the primary model fields are read in from *variable_list*, the residuals are submitted to *pp_variable_list*. Otherwise, the structure is similar and expressions can be copied from one function to another.

Here is the *postProcessedFields* from the coupledCahnHilliardAllenCahn application:

```
template <int dim,int degree>
void customPDE<dim,degree>::postProcessedFields(const variableContainer<dim,degree,dealii::VectorizedArray
                                              variableContainer<dim,degree,dealii::VectorizedArray<double> > & pp_variab
                                                                                                    const deal

//c
scalarvalueType c = variable_list.get_scalar_value(0);

//n
scalarvalueType n = variable_list.get_scalar_value(1);
scalargradType nx = variable_list.get_scalar_gradient(1);

// Free energy for each phase
scalarvalueType faV = (-1.6704-4.776*c+5.1622*c*c-2.7375*c*c*c+1.3687*c*c*c*c);
scalarvalueType fbV = (5.0*c*c-5.9746*c-1.5924);

// Interpolation function
scalarvalueType hV = (10.0*n*n*n-15.0*n*n*n*n+6.0*n*n*n*n*n);

// The homogenous free energy
scalarvalueType f_chem = (constV(1.0)-hV)*faV + hV*fbV;

// The gradient free energy
scalarvalueType f_grad = constV(0.5*KnV)*nx*nx;

// The total free energy
scalarvalueType f_tot;
f_tot = f_chem + f_grad;

// Residuals for the equation to evolve the order parameter
pp_variable_list.set_scalar_value_residual_term(0, f_tot);


}
```

6.4 nucleation.h

The 'nucleation.h' file is also an optional file that is only needed when explcit nucleation is needed for the application. It contains the function *getNucleationProbability*, which calculates the probability of nucleation in a given volume element dV at a particular point in space p at time *this->currentTime*. Please refer to Note 3 in Sec. 5 for a description of the nucleation model in PRISMS-PF.

The values of the primary field variables can be accessed through the *variable_value* input, using the variable index from 'equations.h'. Only variables where *set_need_value_nucleation* was set to true the *loadVariableAttributes* function in 'equations.h' can be accessed.

Here is *getNucleationProbability* from the nucleationModel application:

```
template <int dim, int degree>
double customPDE<dim,degree>::getNucleationProbability(variableValueContainer variable_value, double dV, d
{
//Supersaturation factor
double ssf;
if (dim ==2) ssf=variable_value(0)-calmin;
if (dim ==3) ssf=(variable_value(0)-calmin)*(variable_value(0)-calmin);

// Calculate the nucleation rate
double J=k1*exp(-k2/(std::max(ssf,1.0e-6)))*exp(-tau/(this->currentTime));
double retProb=1.0-exp(-J*userInputs.dtValue*((double)userInputs.steps_between_nucleation_attempts)*dV);
return retProb;
}
```

6.5 customPDE.h

The final header file in each application folder is 'customPDE.h'. This file contains the declarations for all of the functions and variables specific to the application. In C++ terminology, it is the declaration for the customPDE class, which is a subclass of MatrixFreePDE. For most users, the relevant section is labeled as "Model constants specific to this subclass", which is where the model constants from 'parameters.in' are extracted from the *userInputs* object. There is a separate function to extract constants of each type. These are:

- get_model_constant_double
- get_model_constant_int
- get_model_constant_bool
- get_model_constant_rank_1_tensor
- get_model_constant_rank_2_tensor
- get_model_constant_elasticity_tensor

Each of these take the variable name from 'parameters.in' as an input and output the appropriate type.

Here is 'customPDE.h' from the preciptiateEvolution application, where all of the different types of constants are used:

```
#include "../../include/matrixFreePDE.h"

template <int dim, int degree>
class customPDE: public MatrixFreePDE<dim,degree>
{
public:
	customPDE(userInputParameters<dim> _userInputs):
		MatrixFreePDE<dim,degree>(_userInputs) , userInputs(_userInputs) {};

private:
	#include "../../include/typeDefs.h"

	const userInputParameters<dim> userInputs;

	// Pure virtual method in MatrixFreePDE
	void residualRHS(
		variableContainer<dim,degree,dealii::VectorizedArray<double> > & variable_list ,
		dealii::Point<dim, dealii::VectorizedArray<double> > q_point_loc) const;

	// Pure virtual method in MatrixFreePDE
	void residualLHS(
		variableContainer<dim,degree,dealii::VectorizedArray<double> > & variable_list ,
		dealii::Point<dim, dealii::VectorizedArray<double> > q_point_loc) const;

	// Virtual method in MatrixFreePDE that we override if we need postprocessing
	#ifdef POSTPROCESS_FILE_EXISTS
	void postProcessedFields(
		const variableContainer<dim,degree,dealii::VectorizedArray<double> > & variable_list ,
		variableContainer<dim,degree,dealii::VectorizedArray<double> > & pp_variable_list ,
		const dealii::Point<dim, dealii::VectorizedArray<double> > q_point_loc) const;
	#endif

	// Virtual method in MatrixFreePDE that we override if we need nucleation
	#ifdef NUCLEATION_FILE_EXISTS
	double getNucleationProbability(variableValueContainer variable_value , double dV) const;
```

```
        #endif

        // ===================================================================
        // Methods specific to this subclass
        // ===================================================================


        // ===================================================================
        // Model constants specific to this subclass
        // ===================================================================

        double McV = userInputs.get_model_constant_double("McV");
        double Mn1V = userInputs.get_model_constant_double("Mn1V");
        double Mn2V = userInputs.get_model_constant_double("Mn2V");
        double Mn3V = userInputs.get_model_constant_double("Mn3V");
        dealii::Tensor<2,dim> Kn1 = userInputs.get_model_constant_rank_2_tensor("Kn1");
        dealii::Tensor<2,dim> Kn2 = userInputs.get_model_constant_rank_2_tensor("Kn2");
        dealii::Tensor<2,dim> Kn3 = userInputs.get_model_constant_rank_2_tensor("Kn3");
        bool n_dependent_stiffness = userInputs.get_model_constant_bool("n_dependent_stiffness");
        dealii::Tensor<2,dim> sfts_linear1 = userInputs.get_model_constant_rank_2_tensor("sfts_linear1");
        dealii::Tensor<2,dim> sfts_const1 = userInputs.get_model_constant_rank_2_tensor("sfts_const1");
        dealii::Tensor<2,dim> sfts_linear2 = userInputs.get_model_constant_rank_2_tensor("sfts_linear2");
        dealii::Tensor<2,dim> sfts_const2 = userInputs.get_model_constant_rank_2_tensor("sfts_const2");
        dealii::Tensor<2,dim> sfts_linear3 = userInputs.get_model_constant_rank_2_tensor("sfts_linear3");
        dealii::Tensor<2,dim> sfts_const3 = userInputs.get_model_constant_rank_2_tensor("sfts_const3");
        double A4 = userInputs.get_model_constant_double("A4");
        double A3 = userInputs.get_model_constant_double("A3");
        double A2 = userInputs.get_model_constant_double("A2");
        double A1 = userInputs.get_model_constant_double("A1");
        double A0 = userInputs.get_model_constant_double("A0");
        double B2 = userInputs.get_model_constant_double("B2");
        double B1 = userInputs.get_model_constant_double("B1");
        double B0 = userInputs.get_model_constant_double("B0");

        const static unsigned int CIJ_tensor_size =2*dim-1+dim/3;
        dealii::Tensor<2,CIJ_tensor_size> CIJ_Mg =
                userInputs.get_model_constant_elasticity_tensor("CIJ_Mg");
        dealii::Tensor<2,CIJ_tensor_size> CIJ_Beta =
                userInputs.get_model_constant_elasticity_tensor("CIJ_Beta");



        // ===================================================================
};
```

This file can also be used to declare new member functions for the application. One example of this is the *seedNucleus* function in the nucleationModel application.

Furthermore, for advanced users, the customPDE class can be used to override MatrixFreePDE functions from the core PRISMS-PF library. One example of this is in the CHiMaD_benchmark6b application, where the *makeTriangulation* function is overridden to create a non-square mesh.

6.6 main.cc

The final file in the application directory is the C++ 'main.cc' file. This file controls the overall flow of the code and is unlikely to be modified by most users. For all of the example applications, 'main.cc' is identical. One situation where a user may want to modify 'main.cc' is if they wanted to run several simulations with different parameter sets for one execution of the code.

7 Tests

The ‘tests’ folder in the root directory contains some tests to ensure that PRISMS-PF is working properly. A battery of automated tests can be found in the ‘automated_tests’ directory. These can be run by running the python script ‘run_automatic_tests.py’. This will run a series of unit and regression tests, printing a summary of the results to the screen and writing to the file ‘test_results.txt’. This python file can also be used as an example of automating PRISMS-PF simulations.

The ‘unit_tests’ directory contains a driver for a series of unit tests. To run them enter:

```
$ cmake .
$ make debug
$ mpirun -n 1 main
```

A summary of the tests will print to the screen.

8 Creating Custom Applications

You can create your own PRISMS-PF applications by making simple modifications to the input files described in the previous section. To create a new application, simply create a new folder in the applications directory and copy the files from a related example application. Currently, the new application folder must be in the applications directory, otherwise it will not be able to find the required files in the core PRISMS-PF library. **If the file “CMakeCache.txt” exists, delete it** (this file contains paths to the original application, and if left would cause the compiler to compile the code from the original application). Then, make your desired modifications (changing the initial or boundary conditions, changing the residual equations, etc.) and compile and run your application the same way you would one of the example applications.

Once your have your own applications running, we’d love to help you share them with the community. Please contact us at prismsphasefield.dev@umich.edu if you need help using GitHub to generate a pull request so that we can add your work to the public repository.

9 Appendix I: The userInputs Object

In all of the application files, the user has access to an object called “userInputs”. This object contains all of the input parameters from parameters.in and the variable attributes from the top of equations.h and postprocess.h. The following table lists the member variable names to access these parameters (excluding a few that are only useful in the core code). Using standard C++ syntax, all of these can be accessed using the following syntax: userInputs.exampleVariable, where “exampleVariable” is the member variable name.

userInputs Member Variables

Variable Name	*Type*	*parameters.in Text*	*Description*
domain_size	std::vector<double>	Domain size X, Domain size Y, Domain size Z	A vector containing the dimensions of the domain.
subdivisions	std::vector<unsigned int>	Subdivisions X, Subdivisions Y, Subdivisions Z	A vector containing the number of subdivisions of the domain.
refine_factor	unsigned int	Refine factor	Directly from parameters.in.
degree	unsigned int	Element degree	Directly from parameters.in.
h_adaptivity	bool	Mesh adaptivity	Directly from parameters.in.
max_refinement_level	unsigned int	Max refinement level	Directly from parameters.in.
min_refinement_level	unsigned int	Min refinement level	Directly from parameters.in.
refine_criterion_fields	std::vector<unsigned int>	Refinement criteria fields	Converts variable names to their variable index.
refine_window_max	std::vector<double>	Refinement window max	Directly from parameters.in.
refine_window_min	std::vector<double>	Refinement window min	Directly from parameters.in.
skip_remeshing_steps	unsigned int	Steps between remeshing operations	Directly from parameters.in.
dtValue	double	Time step	Directly from parameters.in.
finalTime	double	Simulation end time, Number of time steps	End time for the simulation, set based whichever will happen first, the specified time or number of time steps.
totalIncrements	double	Simulation end time, Number of time steps	Number of time steps for the simulation, set based whichever will happen first, the specified time or number of time steps.
output_file_type	std::string	Output file type	Directly from parameters.in.
output_file_name	std::string	Output file name	Directly from parameters.in.
outputTimeStepList	std::vector<unsigned int>	List of time steps to output	Holds the list of time steps to output for all output conditions, not just LIST.
skip_print_steps	unsigned int	Skip print steps	Directly from parameters.in.

userInputs Member Variables			
Variable Name	*Type*	*parameters.in Text*	*Description*
solverType	std::string	Linear solver	Directly from parameters.in.
abs_tol	bool	Use absolute convergence tolerance	Directly from parameters.in.
solver_tolerance	double	Solver tolerance value	Directly from parameters.in.
max_solver_iterations	unsigned int	Maximum allowed solver iterations	Directly from parameters.in.
load_ICs	std::vector<bool>	Load intial conditions	Directly from parameters.in.
load_parallel_file	std::vector<bool>	Load parallel file	Directly from parameters.in.
load_file_name	std::vector<std::string>	File names	Directly from parameters.in.
load_field_name	std::vector<std::string>	Variable names in the files	Directly from parameters.in.
BC_list	std::vector< varBCs<dim>>	Boundary conditions for variable [variable name]	Vector of one object per component of each variable that stores the BCs.
nucleus_semiaxes	std::vector<double>	Nucleus semiaxes (x,y,z)	Directly from parameters.in.
order_parameter _freeze_semiaxes	std::vector<double>	Freeze zone semiaxes (x,y,z)	Directly from parameters.in.
no_nucleation _border_thickness	double	Nucleation-free border thickness	Directly from parameters.in.
nucleus_hold _time	double	Freeze time following nucleation	Directly from parameters.in.
min_distance_between _nuclei	double	Minimum allowed distance between nuclei	Directly from parameters.in.
nucleation_order _parameter_cutoff	double	Order parameter cutoff value	Directly from parameters.in.
steps_between _nucleation_attempts	double	Time steps between nucleation attempts	Directly from parameters.in.

userInputs Member Variables			
Variable Name	*Type*	*parameters.in Text*	*Description*
number_of_variables	unsigned int		Counts the number of variables in loadVariableAttributes in equations.h.
var_name	std::vector<std::string>		Vector of the variable names from loadVariableAttributes in equations.h.
var_type	std::vector<fieldType>		Vector of the variable types from loadVariableAttributes in equations.h.
var_eq_type	std::vector<PDEType>		Vector of the variable equation types from loadVariableAttributes in equations.h.
nucleation_occurs	bool		Set true if any variables are set to nucleate in loadVariableAttributes in equations.h.
nucleating _variable_indices	std::vector<unsigned int>		Vector of the variable indices for variables that are set to nucleate in loadVariableAttributes in equations.h.
nucleation _need_value	std::vector<unsigned int>		Vector of the variable indices for variables that are set to be needed in the nucleation calculation in loadVariableAttributes in equations.h.
pp_number_of_variables	unsigned int		Counts the number of variables in loadPostProcessorVariableAttributes in postprocess.h.
num_integrated_fields	unsigned int		Counts the number of variables marked to be integrated in loadPostProcessorVariableAttributes in postprocess.h.
pp_var_name	std::vector<std::string>		Vector of the variable names from loadPostProcessorVariableAttributes in postprocess.h.
pp_var_type	std::vector<fieldType>		Vector of the variable types from loadPostProcessorVariableAttributes in postprocess.h.