PRISMS-PF:
The PRISMS Phase Field Code

Trainers:

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Beck Andrews

David Montiel

Training Objective

Learn enough of PRISMS-PF to allow you to go home and start using it in your work

Plan for the Training

- Schedule:
  - Brief introductory comments
  - Guided walkthrough
    - Tour of the file system
    - Running example applications
    - Visualization
    - Tutorial on writing equations in the weak form
    - Walkthrough of the application files
  - Individual exercises using PRISMS-PF to modify existing applications and create new applications

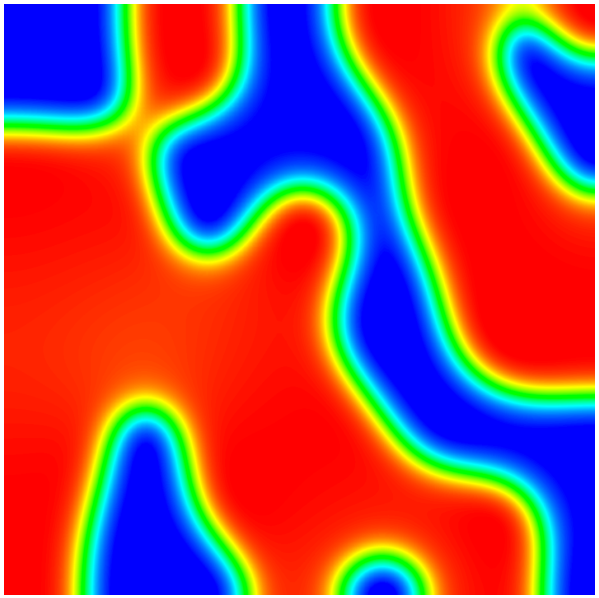
Now

This morning

This afternoon and Wednesday

One Slide on Phase Field Modeling

- Phase field modeling is a diffuse interface approach to modeling microstructure evolution
- Examines phase separation in systems with two or more minima in their free energy
- Two main equations:
  - Cahn-Hilliard: conserved dynamics (e.g. concentration)
  - Allen-Cahn: nonconserved dynamics (e.g. grain orientation)
- Applications include: solidification, precipitation, grain growth, phase separation in batteries, deposition, ferroics



Spinodal Decomposition (Cahn-Hilliard Equation)

PRISMS-PF:

An Open Source, Finite Element, General Purpose Phase-Field Platform

(github.com/prisms-center/phaseField)

User-Friendly:

Simple interface to solve an arbitrary number of PDEs

Detailed user guide

18 applications (and counting) to get you started

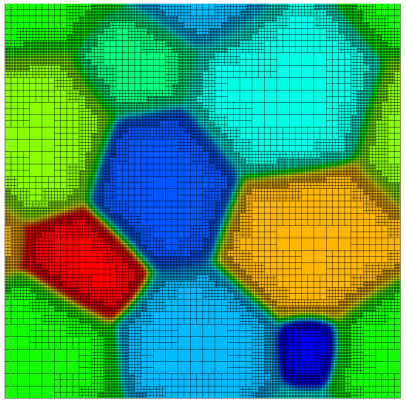
High-Performance:

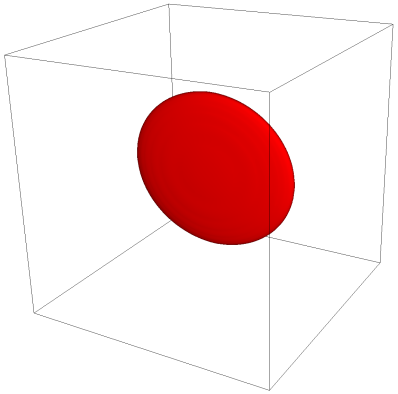
Ideal scaling for >1,000 processors

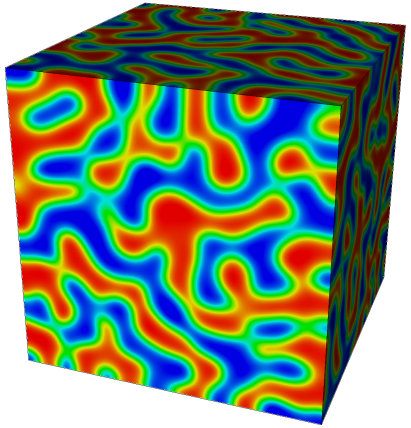
Matrix-free method permits >10^9 DOF

Adaptive meshing

Competitive performance with finite difference (even without adaptive meshing)







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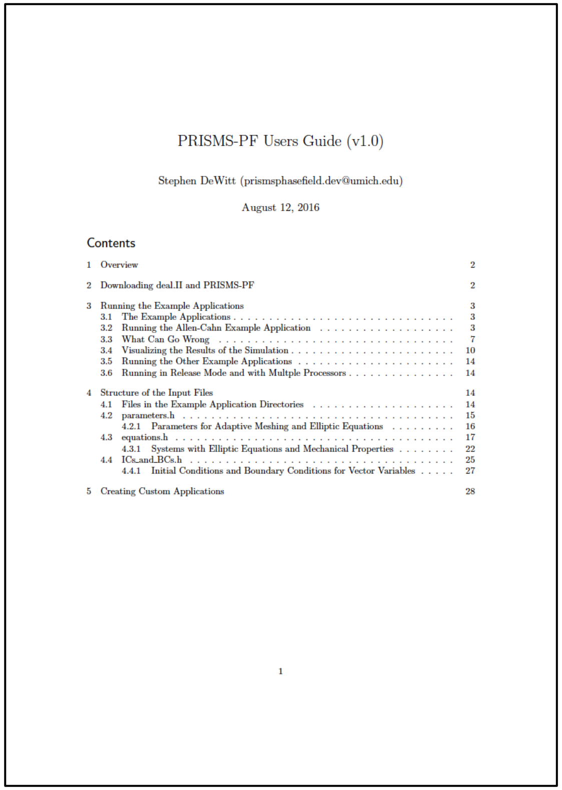
PRISMS

Structure of PRISMS-PF

- Core library
  - Generates mesh, does the finite element calculation, outputs files, etc.
- Apps
  - Each app is a directory that contains an input file and some application files
    - Governing equations, boundary conditions, initial conditions, numerical and model parameters, postprocessing expressions
  - Copy and paste an app directory to create a new app
- Tests
  - Suite of unit and regression tests

User’s Guide

- Instructions for downloading and installing PRISMS-PF and pre-requisites
- Instructions for running the pre-built applications and visualizing the results
- A description of the application files and how to create custom applications



PRISMS-PF Users Guide (v1.0)

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

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 8.2.1. 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:

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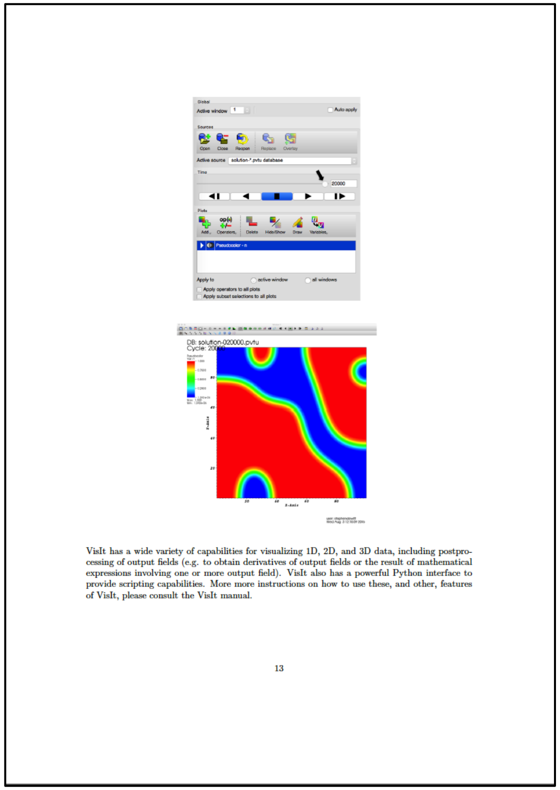

VisIt has a wide variety of capabilities for visualizing 1D, 2D, and 3D data, including postprocessing of output fields (e.g. to obtain derivatives of output fields or the result of mathematical expressions involving one or more output field). VisIt also has a powerful Python interface to provide scripting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

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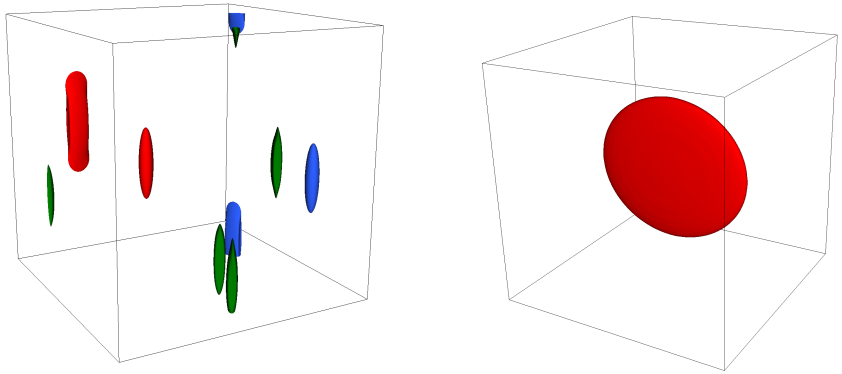
Three Types of PRISMS-PF Users

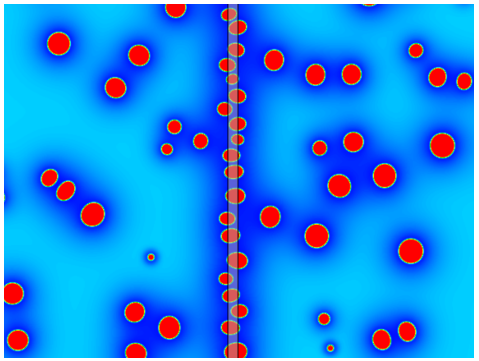
1. Uses PRISMS-PF applications
   - No C++ knowledge needed
   - No deal.II knowledge needed
2. Creates PRISMS-PF applications
   - Minimal C++ knowledge needed
   - No deal.II knowledge needed
3. Extends PRISMS-PF itself
   - C++ knowledge needed
   - deal.II knowledge needed

Phase Field Modeling with PRISMS-PF at UM

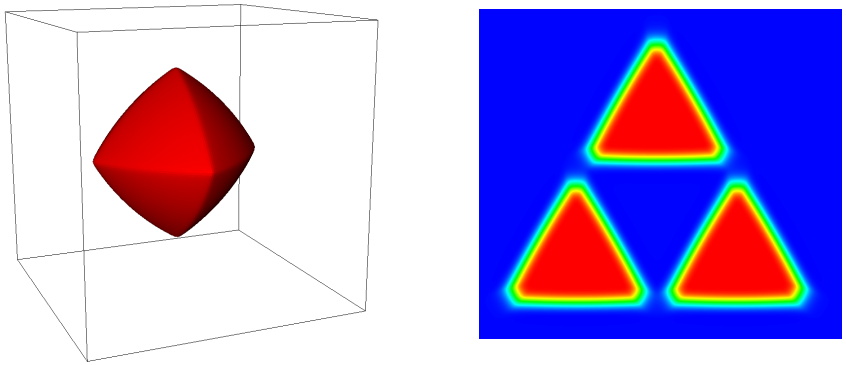
Mg-RE Precipitates



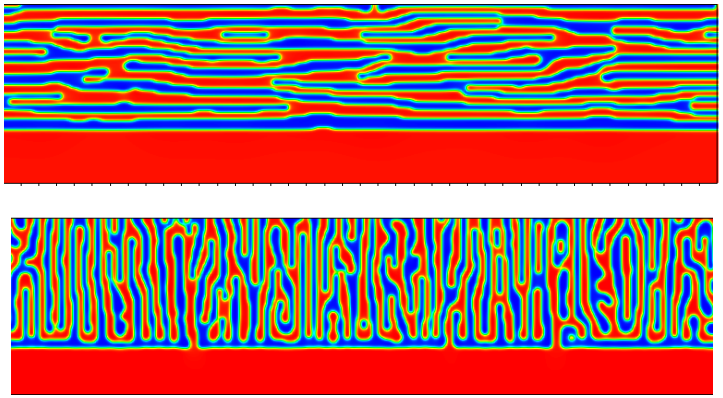
Precipitation near Grain Boundaries



Strong Interfacial Energy Anisotropy



Spinodal Decomposition in Strained Thin Films (Non-PRISMS)



Downloading PRISMS-PF

https://github.com/prisms-center/phaseField

Setting Environment Variables

Type this on the command line:

source /afs/umich.edu/user/s/t/stvdwtt/Public/prismspf_script.sh

```
dukenukem% source /afs/umich.edu/user/s/t/stvdwtt/Public/prismspf_script.sh
```