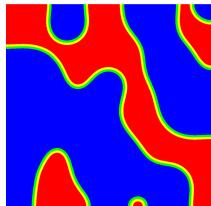


# Annual PRISMS Center Workshop



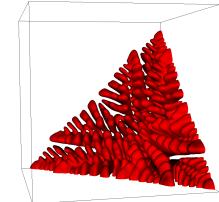
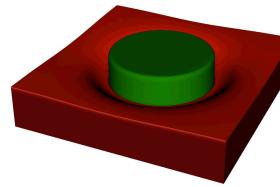
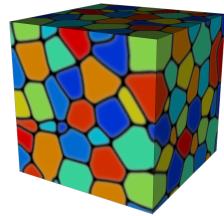
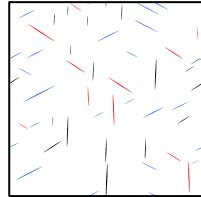
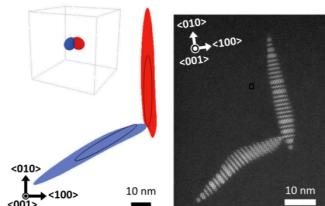
# PRISMS-PF

An Open-Source Phase Field Modeling Framework

## Training Session 2

David Montiel

*August 16, 2022*



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# Overview

## Session 1

- Introduction to the Phase Field Method
- Introduction to the Finite Element Method
- PRISMS-PF Overview
- Interactive Session
- Questions

## Session 2

- Questions about session 1 and exercises (10 min.)
- Results Visualization and Analysis
- Overview of Postprocessing scripts
- In class exercises/questions

2



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# PRISMS-PF Training

## Training Materials / VM setup

[https://github.com/prisms-center/PRISMS-PF\\_Training\\_Materials](https://github.com/prisms-center/PRISMS-PF_Training_Materials)

Frequently used Unix/PRISMS-PF commands and links to resources

Training exercises

This tutorial

Switch to this branch

Workshop2022

4 branches 0 tags

This branch is 7 commits ahead of master.

Contribute

David Montiel and David Montiel Workshop 2022 d2b9ed4 4 minutes ago 22 commits

.gitignore ICME Materials first draft 10 months ago

Cheat\_Sheet.pdf ICME Materials first draft 10 months ago

PRISMS-PF\_Exercises.pdf ICME Materials first draft 10 months ago

PRISMS-PF\_Training\_Session\_1.pdf Workshop 2022 4 minutes ago

README.md Workshop 2022 4 minutes ago

Step 1: Install Virtual Box

Step 2: Download the PRISMS Workshop Tutorials Virtual Box Image

Step 4: Launch VirtualBox and Import the VM Image

**Step 4: Start the VM Image**

user: **prismstools**

password: **prisms\_user**



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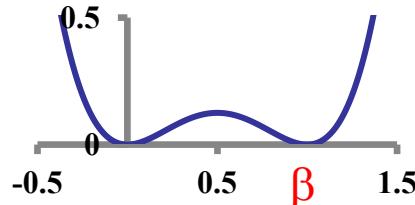
# Example: Adding an undercooling term to the Allen-Cahn application

## Free energy

$$F = \int_{\Omega} \left[ f(\phi) + \frac{1}{2} K |\nabla \phi|^2 \right] dV$$

- **Symmetric** double well: phases  $\alpha$  and  $\beta$  are equally stable

$$f(\phi) = \phi^2(1 - \phi)^2$$



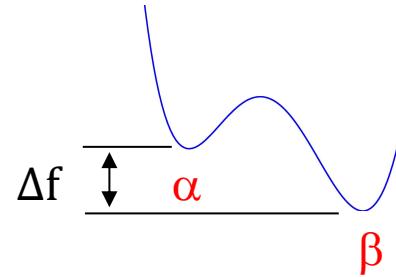
- System domains evolves in such way to minimize interface area until one of the phases disappears

- **Asymmetric** double well: one of the phases becomes more stable than the other

$$f(\phi) = \phi^2(1 - \phi)^2 - \Delta f p(\phi)$$

$\Delta f$  is a constant factor  
 $p(\phi)$  is an interpolation function

$$p(\phi) = \phi^3(10 - 15\phi + 6\phi^2)$$



- Phase  $\beta$  has lower energy than phase  $\alpha$



# Dynamics

## New governing equation

$$\frac{\partial \phi}{\partial t} = -M \frac{\delta F}{\delta \phi}$$

$$\frac{\delta F}{\delta \phi} = \frac{\partial f}{\partial \phi} - K \nabla^2 \phi$$

- We need to include a new term into  $\partial f / \partial \phi$

$$\frac{\partial f}{\partial \phi} = 2W\phi(\phi - 1)(2\phi - 1) - \text{30}\Delta f\phi^2(\phi - 1)^2$$



# Implementation (I)

1) Create a new application starting from the ***allenCahn*** application. Inside the ***applications*** folder type:

```
$ cp -r allenCahn allenCahn_undercooling
```

(you may choose any name you want for the new application)

2) Go to the **allenCahn\_undercooling** directory

3) We will modify the **parameters.prm** to include the constant value for  $\Delta f$ . We will choose  $\Delta f=0.025$

Add the following line to the end of **parameters.prm**:

```
set Model constant delf = 0.025, DOUBLE
```

4) Add a member variable with the same name to the class **customPDE**.

When the code runs it will read the text from **parameters.prm** and assign the value of 0.025 to the new variable. On line 56 of **customPDE.h** add the line:

```
double delf = userInputs.get_model_constant_double("delf");
```

# Implementation (II)

5) We are going to add the new undercooling term to the governing equation for “n” (In the code, the order parameter  $\phi$  is named “n”)

Open the file **equations.cc** and add the new term to line 50, i.e., replace line 50 with:

```
scalarvalueType fnV = 4.0*n*(n-1.0)*(n-0.5) -  
constV(30.0*delf)*n*n*(n-1.0)*(n-1.0);
```

6) Finally, add the corresponding term to the free energy calculation in **postprocess.cc**. Open the file and add the new term in line the 60

```
scalarvalueType f_tilt = -constV(delf)*(n*n*n)*(10.0-  
15.0*n+6.0*n*n);
```

Also add the contribution of `f_tilt` to `f_tot` (close to line 71) :

```
f_tot = f_chem + f_tilt + f_grad;
```

7) Save all changes and close the files.

8) Delete the file **CMakeCache.txt** (the compilation will fail otherwise)

9) Compile and run the code and visualize the results using VisIt.

How do the results differ from those of the allenCahn application?

# Homework – Problem set

PRISMS-PF\_Exercises.pdf

## PRISMS-PF Training Exercises:

Here is a set of exercises to familiarize yourself with PRISMS-PF. Most users find that these problems take several hours to complete in a training environment where questions can be answered in real time. The problems are approximately in ascending order of difficulty. We recommend **copying and renaming the example app directories before making modifications** so that you still have the original versions to refer to. **Delete the file “CMakeCache.txt” in the newly created directory.** If the only required changes are to the parameters file (problems 1-2), then you can create a new parameters file with a different name in the original app directory.

### 1. Boundary Conditions I:

*Changing boundary conditions for the Allen-Cahn example problem*

- a. Change the BCs in the Allen-Cahn application to zero flux (the natural BC) on the top boundary, eta = 0 on the bottom boundary (a Dirichlet BC), and periodic on the two side boundaries (see diagram below)



# Resources

Website: <https://prisms-center.github.io/phaseField>

Repository: <https://github.com/prisms-center/phaseField>

PRISMS Center YouTube Channel: <https://www.youtube.com/channel/UCZXc3007JuBCGKDcneD>

Email: [prismsphasefield.dev@umich.edu](mailto:prismsphasefield.dev@umich.edu)

## PRISMS-PF

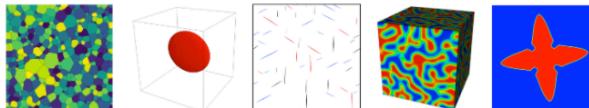
An open-source, general purpose framework for high-performance phase field modeling

GitHub Repository  
User Manual  
User Registration Link  
PRISMS-PF Forum  
YouTube Channel  
Community of Practice



### Overview

PRISMS-PF is a powerful, massively parallel finite element code for conducting phase field and other related simulations of microstructural evolution. The phase field method is commonly used for predicting the evolution of microstructures under a wide range of conditions and material systems. PRISMS-PF provides a simple interface for solving customizable systems of partial differential equations of the type commonly found in phase field models, and has 24 pre-built application modules, including for precipitate evolution, grain growth, dendritic solidification, and spinodal decomposition.

A screenshot of the GitHub repository page for "prisms-center/phaseField". The page shows the repository's structure, including branches (master, 14 branches), tags (14 tags), and recent commits. A sidebar on the right provides information about the repository, including its purpose ("An Open-Source Phase-Field Modeling Framework"), releases (14, with the latest being Version 2.1.2), packages (none published), and contributors (6).

File	Description	Date
applications	added vtk conversion scripts	3 days ago
include	Changed default extension to .prm to make the code compatible with ...	5 months ago
postprocess_scripts	Update README.md	3 months ago
src	added option for more frequent timing print out. v2.1.2 done.	2 years ago
tests	propagated all changes to the adaptivity input file changes	2 years ago
.gitattributes	added a .gitattributes file to prevent the html files from being coun...	4 years ago
.gitignore	can now output the grain ids for the grain growth apps. Free energy ou...	3 years ago
.travis.yml	fixed travis file to truncate the 'v' in the branch name for the gltf...	3 years ago
CMakelists.txt	added the reassignment code to the core MatrixFreePDE, but FloodFI...	3 years ago
LICENSE	added doxygen documentation files	6 years ago
README.md	Add citation information	11 months ago
authors	Added David Montiel to authors	4 years ago
logo_v2.png	more updates to the README	3 years ago
test_ci.sh	Merge branch 'master' into master	4 years ago
version	added option for more frequent timing print out. v2.1.2 done.	2 years ago
version_changes.md	added option for more frequent timing print out. v2.1.2 done.	2 years ago



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# Acknowledgments



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