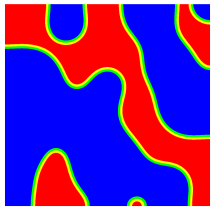
Annual PRISMS Center Workshop



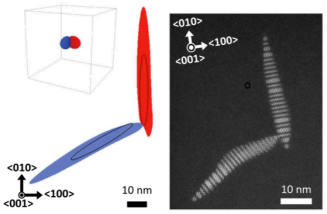
PRISMS-PF

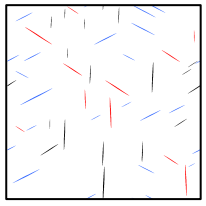
An Open-Source Phase Field Modeling Framework

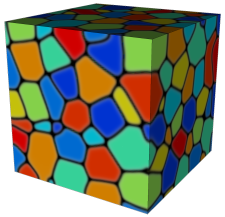
Training Session 2

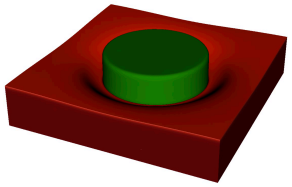
David Montiel

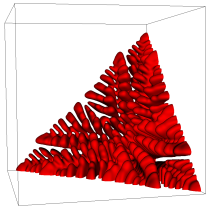
August 16, 2022











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PRISMS

Overview

Session 1

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

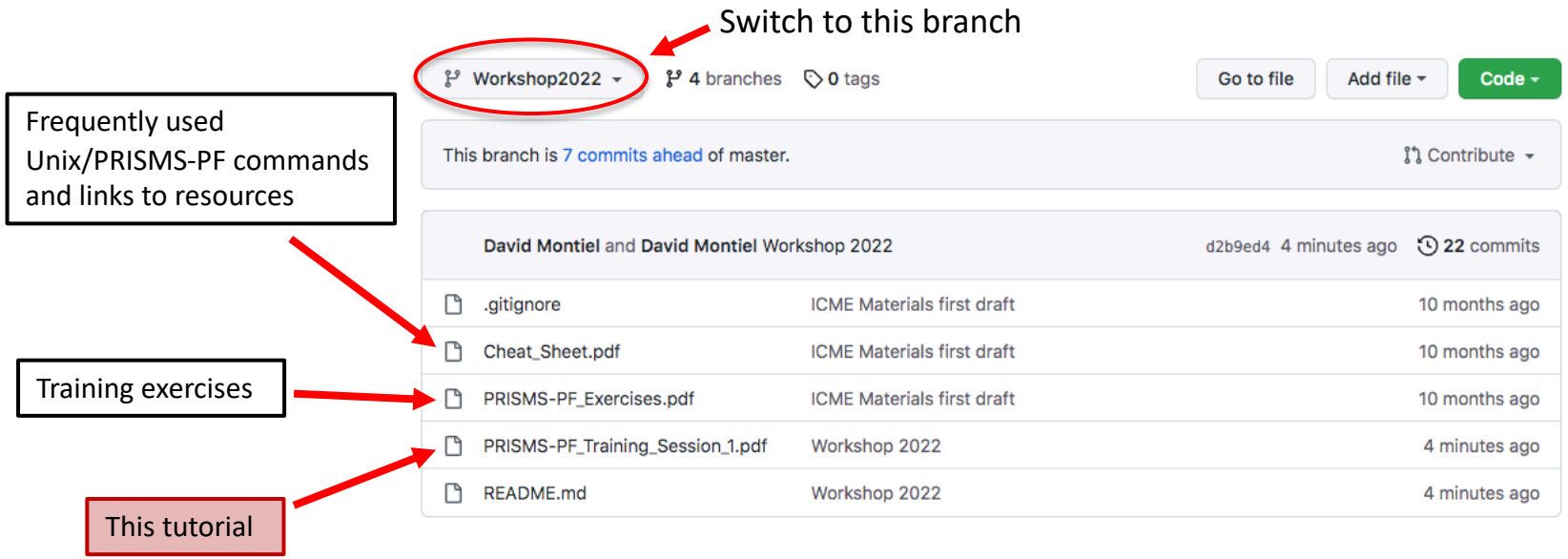
Session 2

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

PRISMS-PF Training

Training Materials / VM setup

https://github.com/prisms-center/PRISMS-PF_Training_Materials



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

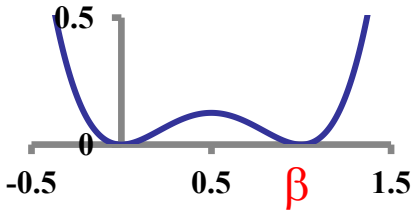
Example: Adding an undercooling term to the Allen-Cahn application

Free energy

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

- ***Symmetric*** double well: phases α and β are equally stable

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



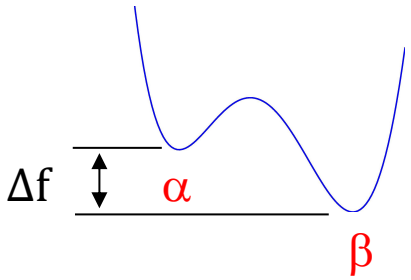
- System domains evolves in such way to minimize interface area until one of the phases disappears

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

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

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

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



- Phase β has lower energy than phase α

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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 $\partial f / \partial \phi$

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

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 Δf. We will choose Δf=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 ϕ 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

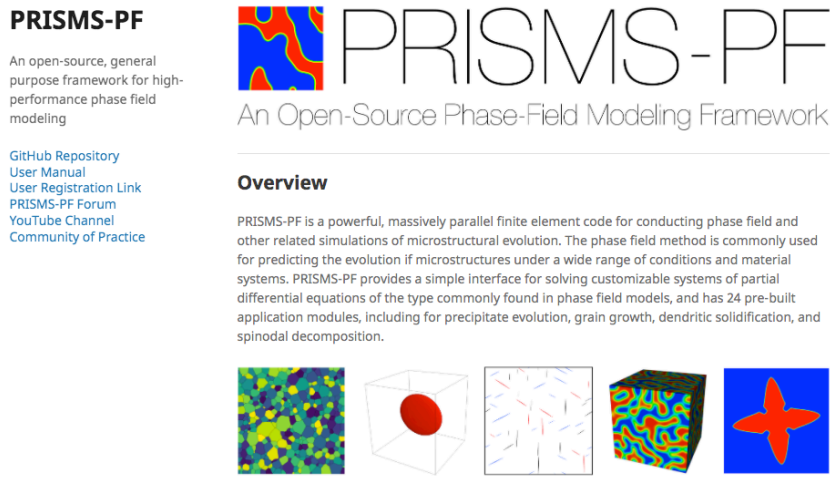
PRISMS-PF Training Exercises:

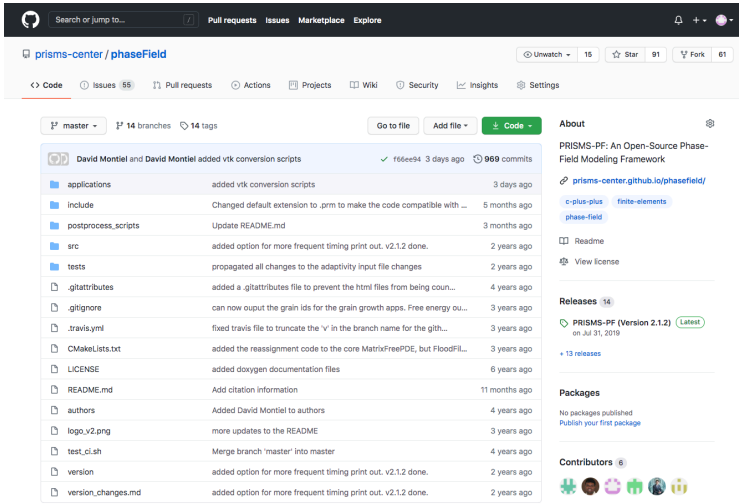
Here is a set of exercises to familiarize yourself with PRISMS-PF. Most users find that these problems take several hours to complete in a training environment where questions can be answered in real time. The problems are approximately in ascending order of difficulty. We recommend **copying and renaming 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_umA
Email: prismsphasefield.dev@umich.edu





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