Annual PRISMS Center Workshop

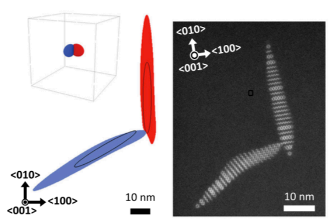
PRISMS-PF

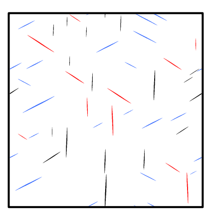
An Open-Source Phase Field Modeling Framework

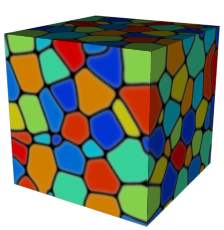
Training Session 2

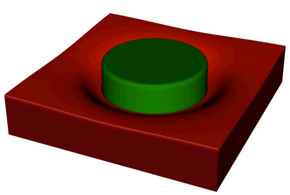
David Montiel

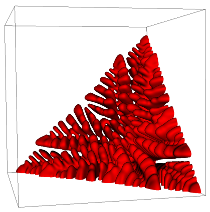
August 17, 2022











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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

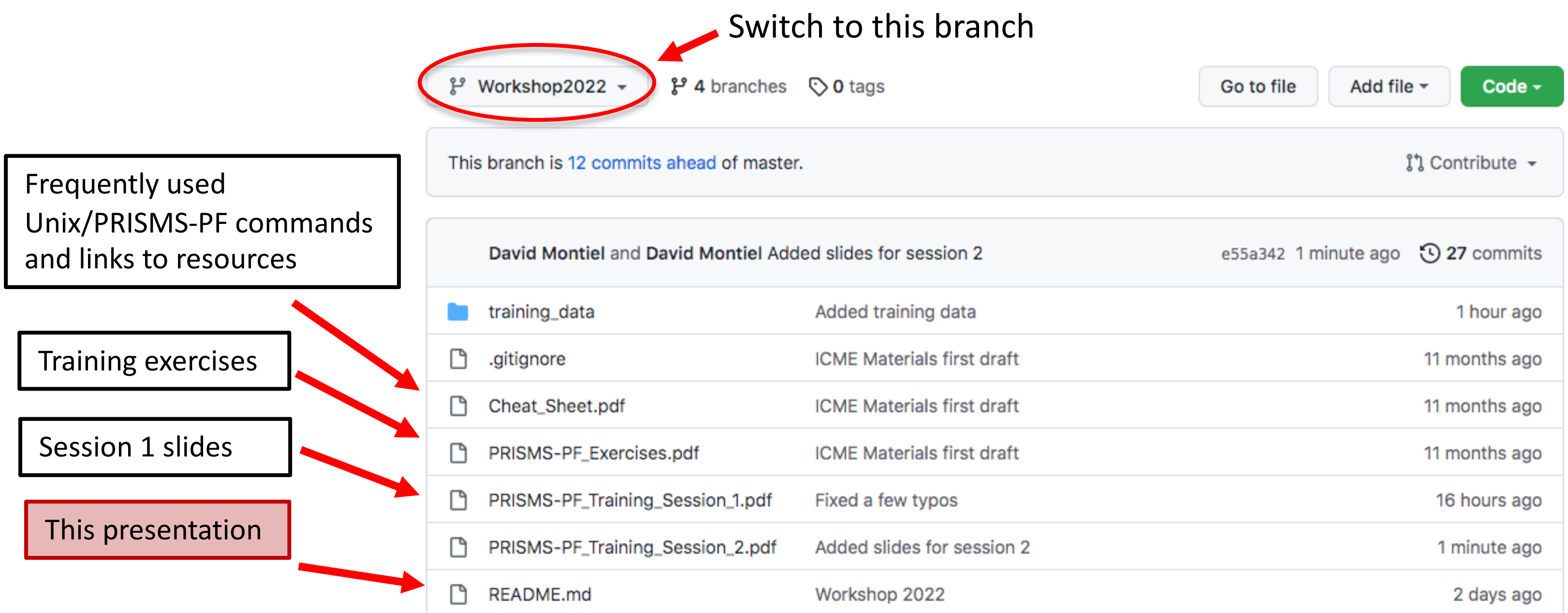
Session 2

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

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

Questions?

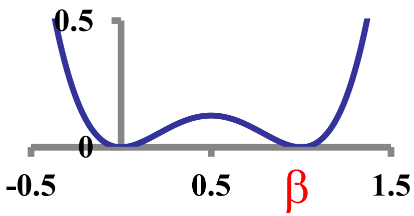
Example: Adding an undercooling term to the Allen-Cahn application

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

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



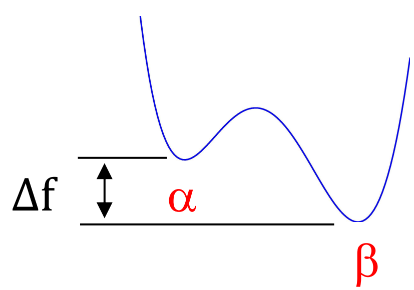
- System domains evolves in such way to minimize interface area until one of the phases disappears

- ***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

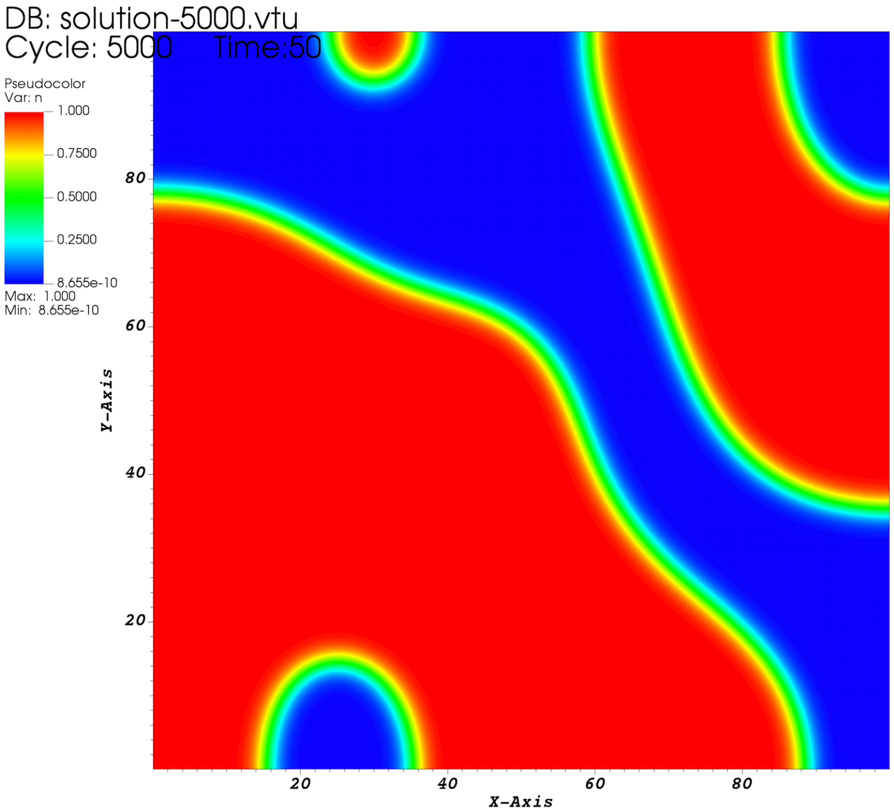
$$p(\phi) = \phi^3(10 - 15\phi + 6\phi^2)$$



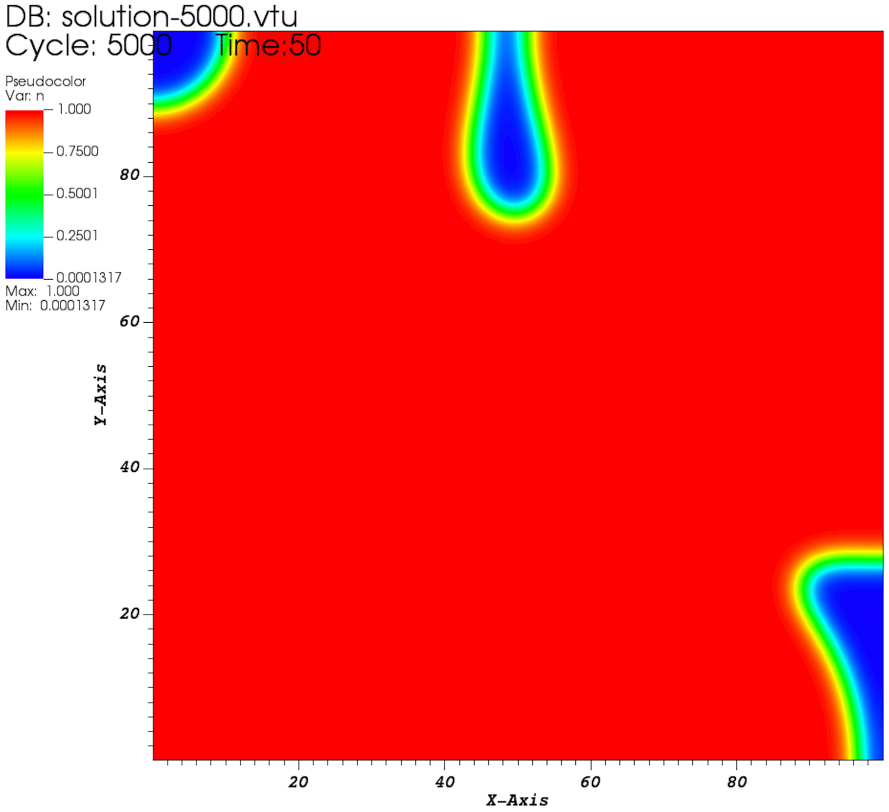
- Phase β has lower energy than phase α

Simulation Result

Original allenCahn application



Additional undercooling term

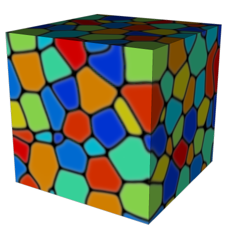


Motivation

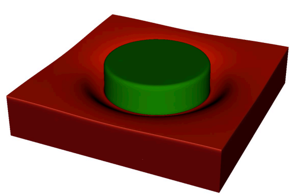
- Data visualization and analysis are key components needed to make sense of results in computational materials science

- Simulation outputs often consists in large datasets. This requires tools that can efficiently use computer resources, including **compute engines** that can run in **parallel** on a cluster.

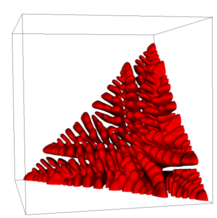
- **VisIt** and **ParaView** are two popular **open-source** visualization and graphical analysis tools



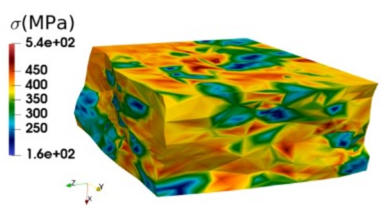
Polycrystal microstructure



Migro-galvanic corrosion on the surface of a Mg Alloy



Alloy solidification



Deformed polycrystal after compression (von Mises equivalent strain)

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VisIt

User Guide:

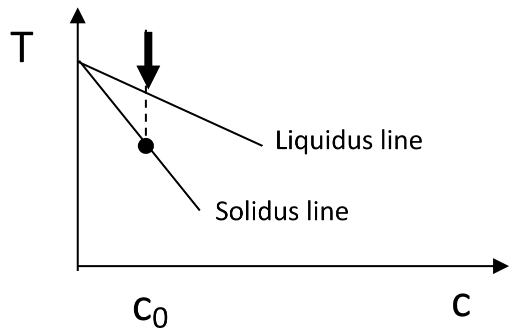
https://wci.llnl.gov/simulation/computer-codes/visit/manuals

- Opening databases (sample PRISMS-PF data)
- Basic plots: Pseudocolor, Contour, Spreadsheet, Lineout
- Operators: Slicing
- Querries (e.g., integration over volume of a variable)
- Expressions
- Commands window
- Scripts

Interactive Session

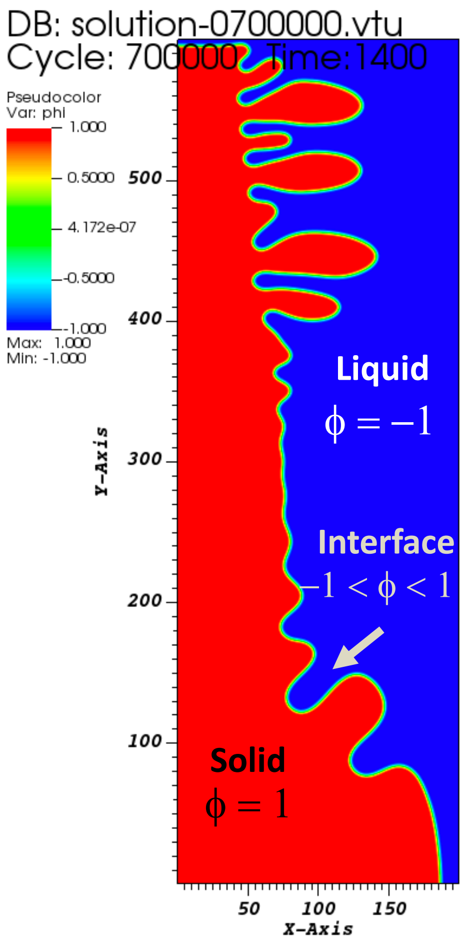
VisIt Example 1 – Alloy Solidification

Example: Dendritic solidification of an alloy under constant cooling rate (temperature is spatially inform)

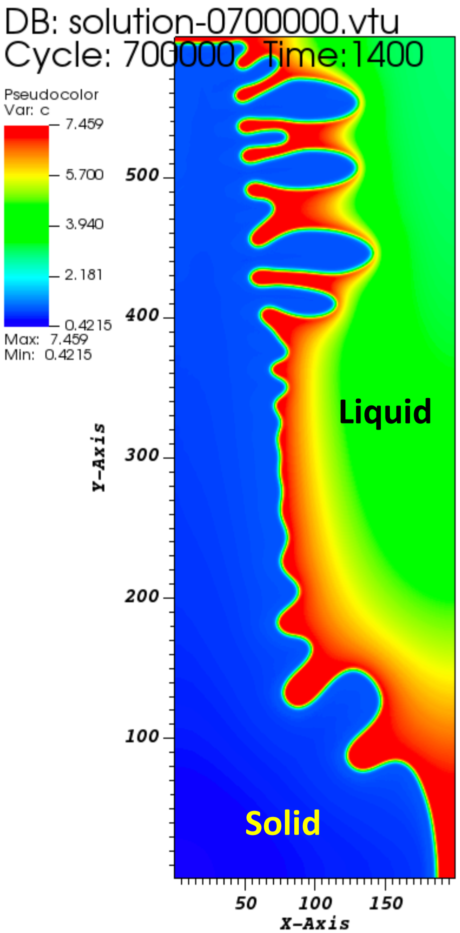


- Rejected solute by the solid creates a morphological instability, leading to dendrites

Order parameter, phi



Solute concentration, c



Exercise - 1

1) Create a Pseudocolor plot for the solute concentration variable (”c”)
2) Set the Time slider to the last frame of the simulation (1,000,000).
3) Select the Lineout mode icon on top of the plot window
4) Draw an approximately horizontal line across the entire system in the x-direction and at y~300
5) A new window will appear showing a simple ”Y vs. X”plot
6) On the left panel switch make sure the active window is that of the 1D plot and that in the list of plots the “Curve-Lineout(c)” plot is selected.
7) On the top menu of the left panel, go to Operator Attributes (Opp Atts) -> Analysis -> Lineout
8) Edit the endpoints of the lineout to the following [x y z] limits

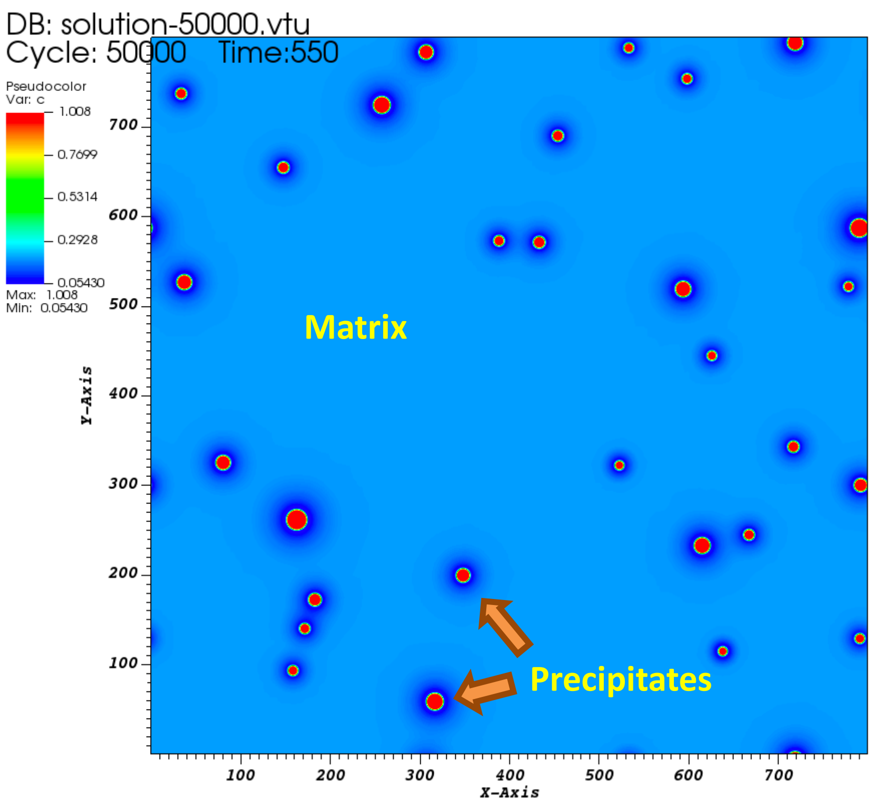
Point 1	0 300 0
Point 2	200 300 0

9) Click on “Apply” and then “Dismiss” (to close the window)
10) Drag the time slider (or use and the buttons to go back and forth in time. What do you observe? Comment on the chat.

VisIt Example 2 – Homogeneous Nucleation of Precipitates

Example: nucleation and growth of precipitate particles in an alloy

- Alloying element originally is in solid solution.
- Temperature decreases to a value where the alloying element is no longer soluble (coexistence region) leading to nucleation and growth
- As precipitates growth the solute around them is depleted



Postprocessing Scripts

- PRISMS-PF contains a suite of postprocessing scripts in Python that calculate the commonly useful properties of the system. These scripts use the VisIt CLI. These scripts are included in the folder phaseField/postprocess_scripts/
  (see: https://github.com/prisms-center/phaseField/tree/master/postprocess_scripts)

  - **plot_and_save.py**: Creates pseudocolor (in 2D) or contour (in 3D) plots for each frame and saves the images

  - **interface_area.py**: Calculates the total interfacial area (in 3D) or length (in 2D) between two phases

  - **phase_fraction.py**: Calculates the phase fraction as the ratio of the volume (area) of the phase defined by n=1 over the volume (area) of the whole system.

  - **domain_stats.py**: Counts the number of independent domains of the phase characterized by n=1. Also obtains the average area (volume) for each domain and the standard deviation around the area.

Postprocessing Scripts

1) Copy all the scripts from phaseField/postprocess_scripts into the directory where the series of .vtu files are located,

```
$ cp ../../postprocess_scripts/*.py .
```

2) Run each script, one by one as

```
$ visit –cli -s <script.py>
```

3) Inspect the new output files generated by the scripts

Exercise - 2

The alloy solidification database shown in earlier is for a 2D simulation of solidification of Al-Cu alloy under a constant (and spatially uniform) cooling rate.

Write a Python code that uses the VisIt library (you can modify one of the existing scripts) to do the following:

i) Obtain the average concentration (C_s) on the solid side of the solid-liquid interface for all time frames (cycles) of the alloy solidification database.
ii) For the same data, obtain the solid fraction, f_s ,for all time frames.
iii) Plot C_s vs. f_s
iv) Compare the result to that of Scheil's equation (https://en.wikipedia.org/wiki/Scheil_equation/), which is an approximate relation to describe the solute redistribution during solidification of an alloy. It is given by

$$C_s = kC_0(1 - f_s)^{k-1}.$$

i) Show the simulation and the Scheil curves in the same plot (use values between 0 and 0.75 for the Scheil curve). Use the values k = 0.14 and C_0 = 3.
ii) What do you you observe? If there is a discrepancy between the plots, what can be the source(s) behind this discrepancy? Which of the assumptions listed in the in the "Scheil Equation" Wikipedia page do not hold for the simulation? Can you think if any other reasons for the discrepancy?

Q&A Session (All PRISMS Tools)

Date: **Friday, August 19**

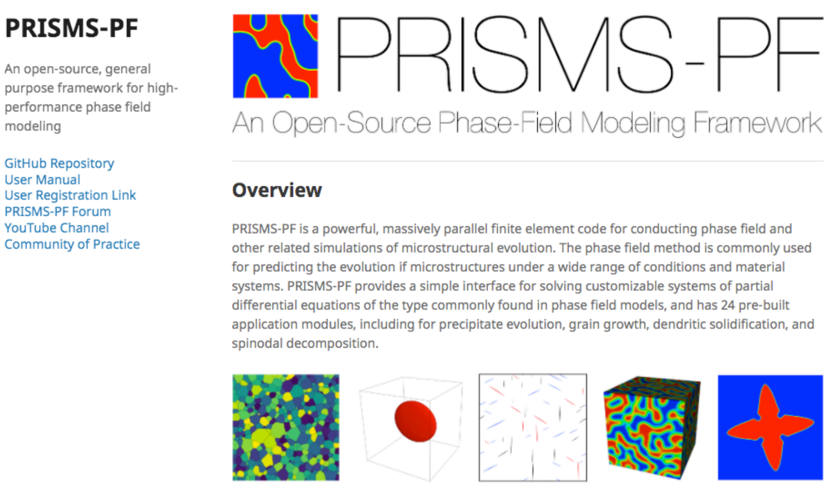
Time: **1pm-1pm EDT**

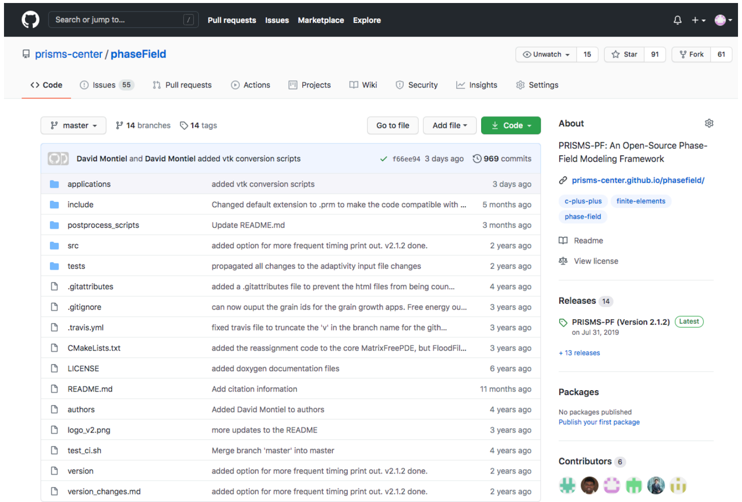
Meeting ID: **997 9138 8873**

Link: https://umich.zoom.us/j/99791388873

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





Acknowledgments

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