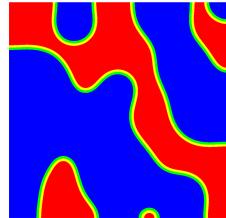


PRISMS Center Annual Workshop

August 3-6, 2021



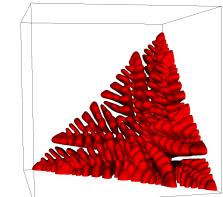
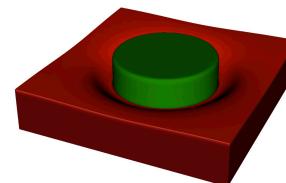
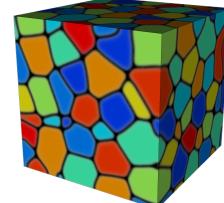
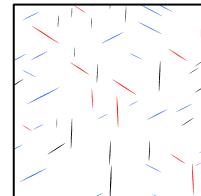
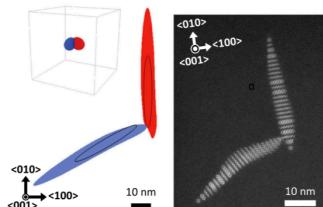
PRISMS-PF

An Open-Source Phase Field Modeling Framework

PRISMS-PF Training Session I

David Montiel

Department of Materials Science and Engineering, University of Michigan



Overview

- Introductions to the Phase Field Method (~30 mins)
- Introduction to PRISMS-PF (~30 mins)
- Q&A Period (~10 mins)
- Interactive demo session (50 mins)
- A set of **exercises** and some **useful links** will be sent to **all participants** on the second half of the session.
- If there is any time left, you can start working on the problem set.
- We will spend the entire session on **Wednesday** answering questions about the exercises (and PRISMS-PF usage in general)

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Announcements

- To simultaneously follow the steps of the interactive part on your computer you must have installed...
 - PRISMS-PF
 - VisIt (or ParaView) for results visualization
- **This session will be recorded.** I will make sure you have access to it ASAP so you can follow the demo part on your own.
- Please make sure you are **muted** and your **video is disabled**
- Post your questions on the chat and I will try to answer them all during the question period
- During the interactive session, **Bonnie Whitney** and **Kubra Karayagiz** will be answering the questions you post on the chat. We will create two breakout rooms in case you a question requires more time to answer.



Funding and Computational Resources



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Bryan Kinzer



Nicole Schuman



Susan Gentry



Pushkar Pandit



Thomas Flint



Xianyue Liu



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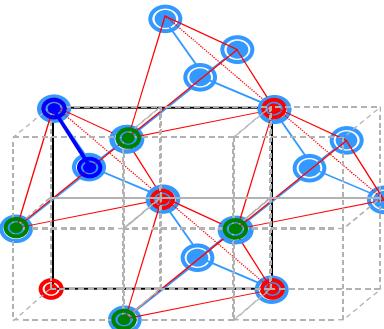
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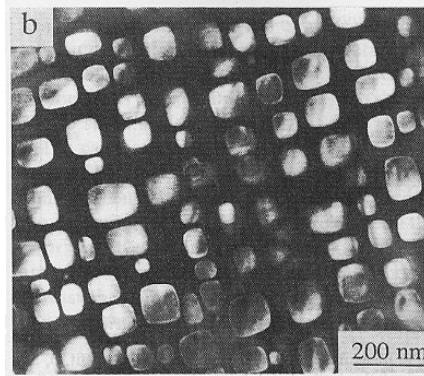
The Phase-Field Method



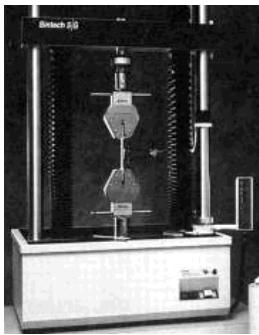
Motivation - The Paradigm of Materials Science



Processing



Structure



Properties

Fahrmann, et al., Acta Met. 45,1007 (1995)
Ni₃Al precipitates in a Ni-Al matrix



Performance

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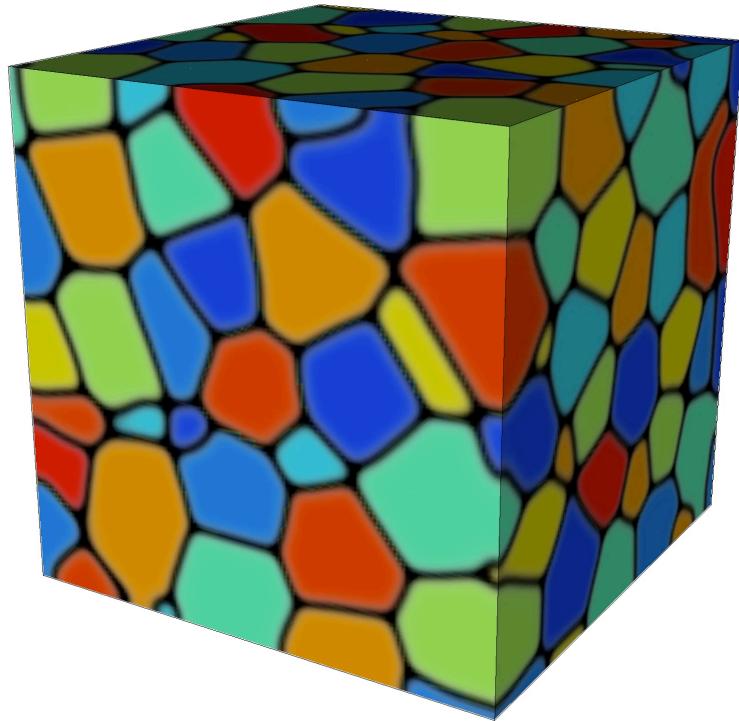
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Phase-Field Modeling

- In essence, phase field modeling is a method to simulate microstructure evolution, and in particular the evolution of interfaces and compositions of different constituents in a material.
- These simulations help us to understand the underlying mechanisms that give rise to different microstructures
- Being able to predict microstructure evolution is a powerful tool in the design processes that will give us a set of desired properties and performance



Phase Field Applications - Grain Growth



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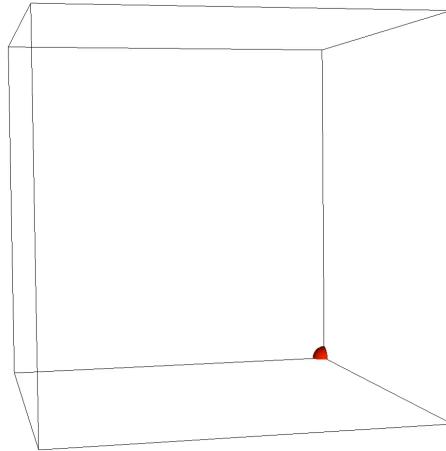
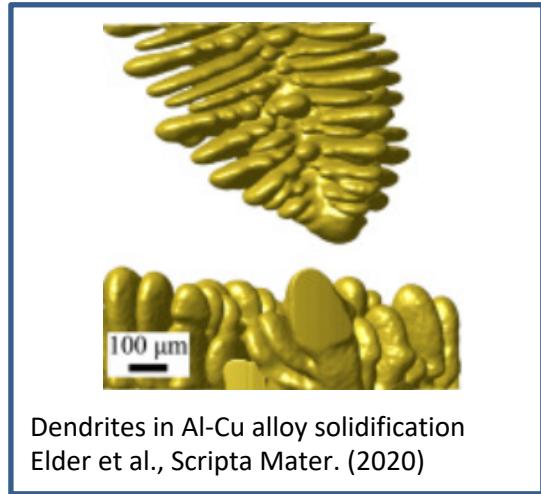


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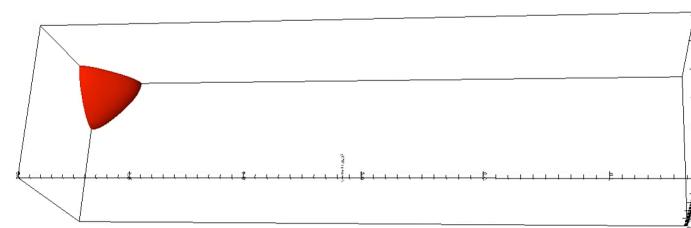
Phase Field Applications – Alloy solidification

Experiment



Equiaxed

Zhenjie Yao et al.
In preparation (2021)



Directional



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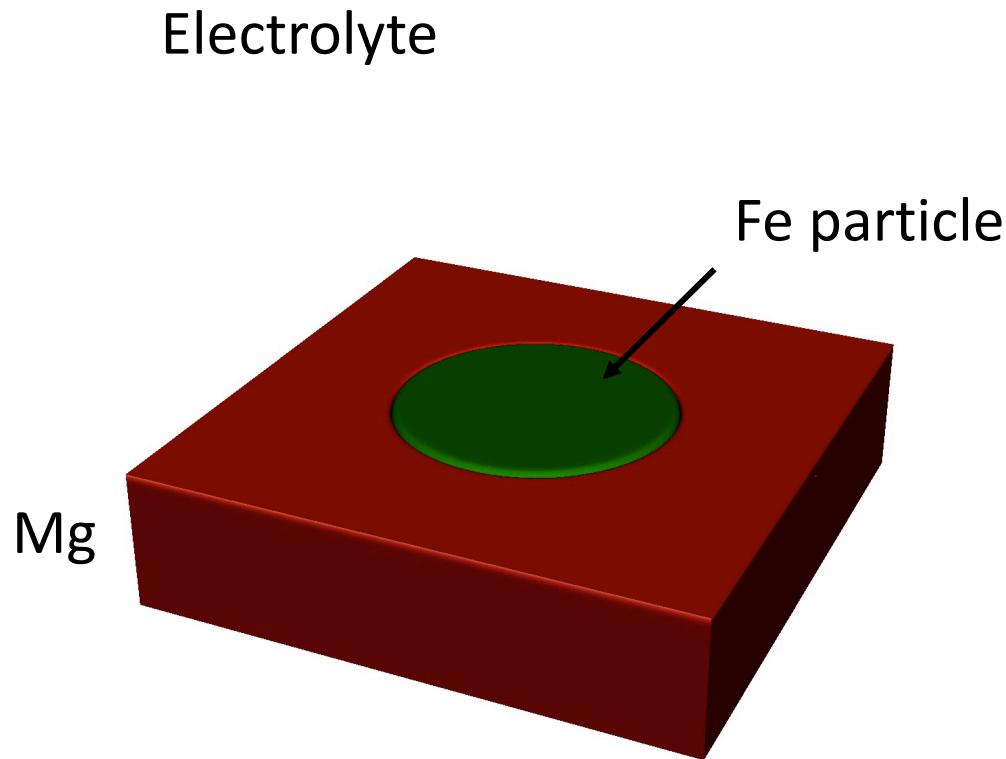
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Phase Field Applications - Corrosion



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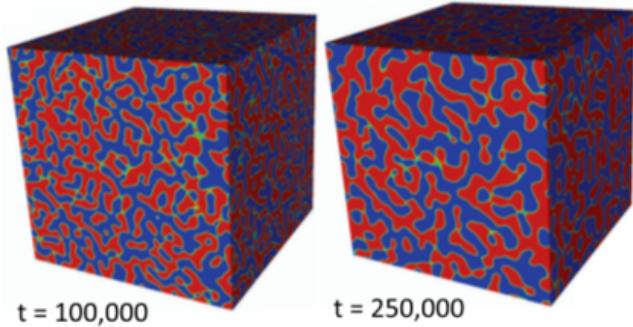


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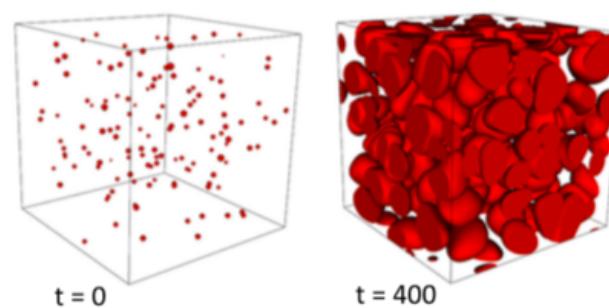
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PRISMS-PF Applications

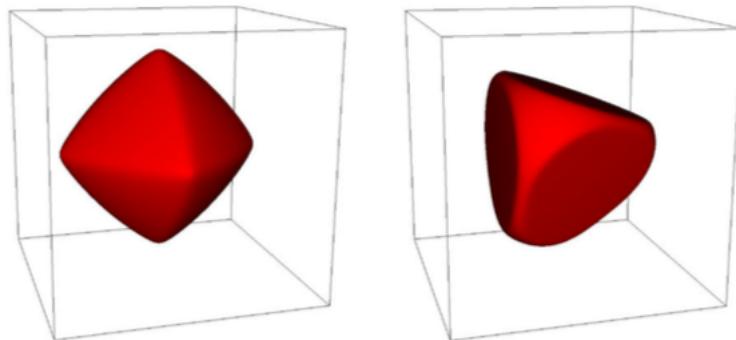
Spinodal decomposition and coarsening



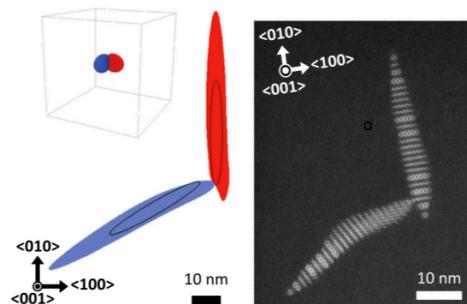
Nucleation and growth of particles



Evolution of particles with strong interfacial anisotropy



Interaction between Mg-Nd alloy precipitates



DeWitt, S. et al., Acta Mater. 136, 378–389 (2017)

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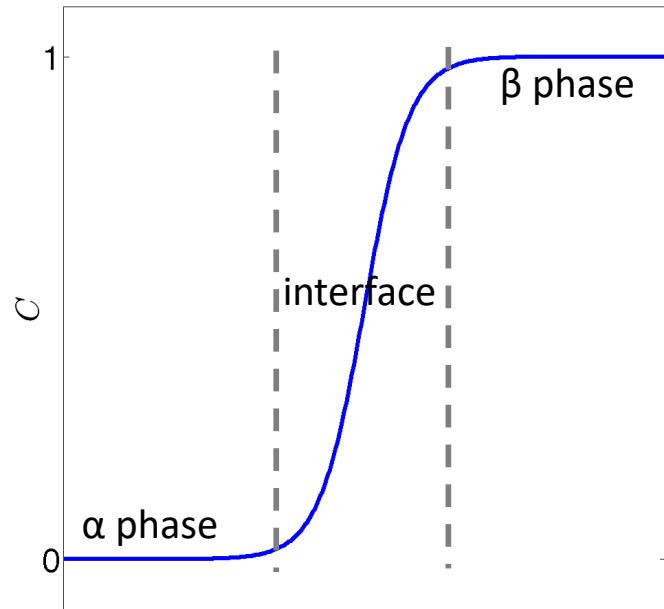
The Idea Behind the Phase-Field Model

- To model microstructure evolution, we need a method to describe and track interfaces
- If we treat interfaces as sharp 2D surfaces, the interfacial location must be tracked by markers. This is called the sharp interface model
- Challenging free boundary problem - mathematically and computationally intensive.



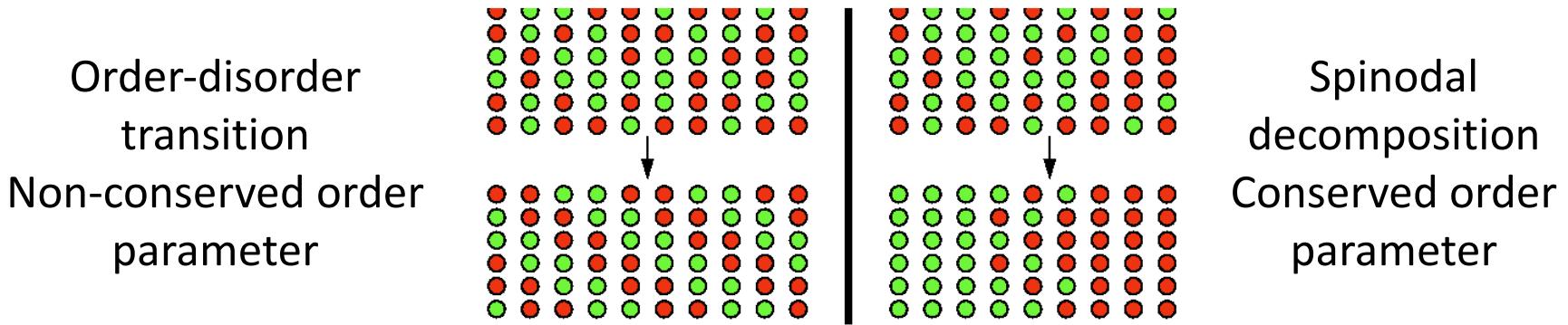
The Idea Behind the Phase-Field Model

- The phase-field model considers interfaces to be regions that have a finite volume where bulk quantities (order parameters) change gradually.
- Bulk quantities such as concentration are governed by partial differential equations (PDEs).
- Interfaces are identified as the regions where bulk quantities take their interfacial values
- The same PDEs can be applied everywhere (including the interface regions) thereby eliminating the need to explicitly track the interface



Order Parameter

- The evolution of interfaces is characterized using order parameters
- An order parameter is a continuous field that characterizes each phase
- Each order parameter has a governing equation (PDE) associated with it.
- Order parameters can be classified as conserved or non conserved



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What Determines Microstructure Evolution?

Thermodynamics and Kinetics (Dynamics)

- The equilibrium state is the state for which the free energy is a minimum
- For bulk phases, this state can be determined using phase diagrams and is characterized by a uniform chemical potential.
- Systems featuring complex microstructures observed in materials are not in thermodynamic equilibrium
- However, their evolution is still driven by the minimization of the free energy
- The driving force for phase transformation is proportional to the gradient of the chemical potential, but there is kinetic factor that determines how fast this transformation occurs.



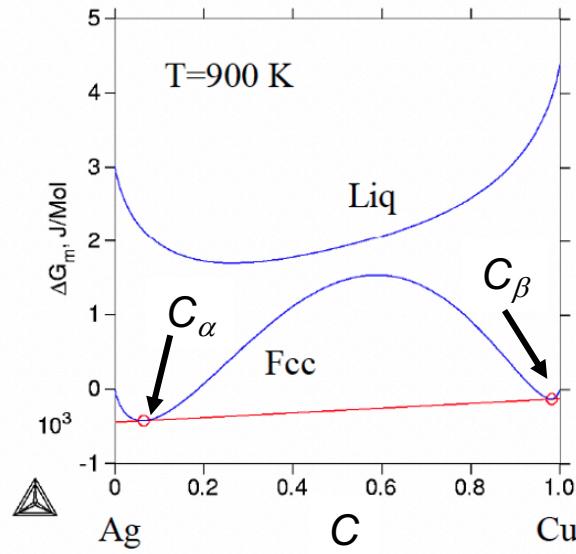
Dynamics

- Order parameter, ϕ

$$\phi = \frac{C - C_\alpha}{C_\beta - C_\alpha}$$

- Let $F\{\phi(\mathbf{r})\}$ be the free energy of the system which includes bulk and interfacial contributions

- Chemical potential: $\mu = \frac{\delta F}{\delta \phi}$



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Cahn-Hilliard Dynamics

Flux: $J = -M \nabla \mu$

Mass conservation: $\frac{\partial \phi}{\partial t} = -\nabla \cdot J$

Chemical potential: $\mu = \frac{\delta F}{\delta \phi}$

Combine all:
$$\frac{\partial \phi}{\partial t} = \nabla \cdot (M \nabla \mu) = \nabla \cdot \left(M \nabla \frac{\delta F}{\delta \phi} \right)$$

The Cahn-Hilliard equation



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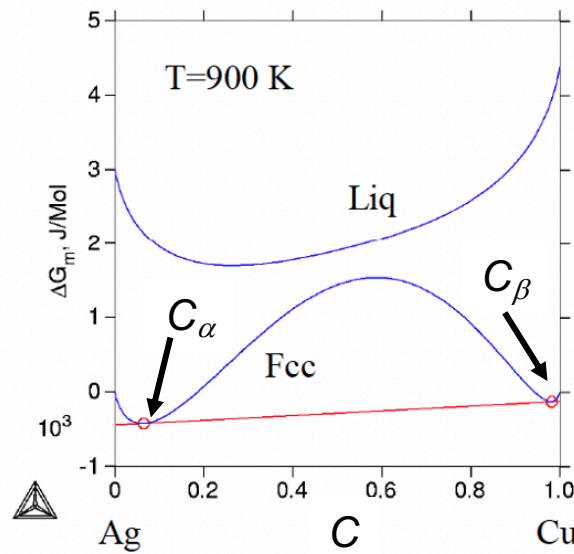


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Free Energy

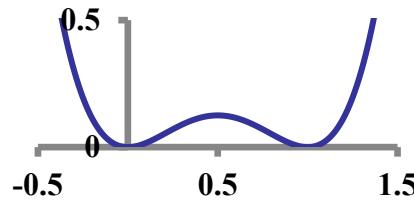
$$F = \int_{\Omega} \left[f(c) + \frac{1}{2} K |\nabla c|^2 \right] dV$$



Free Energy

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

$$f(c) = Wc^2(1-c)^2$$



“Double well” free energy with minima at $c=0$ and $c=1$



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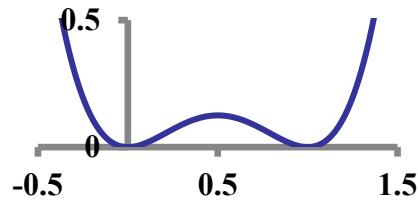
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Free Energy

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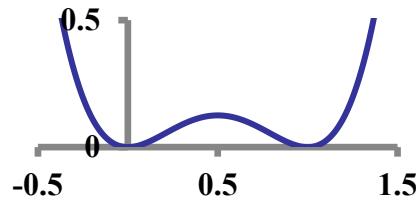
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Free Energy

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$$f(c) = Wc^2(1-c)^2$$



“Double well” free energy with minima at $c=0$ and $c=1$

Dynamics:

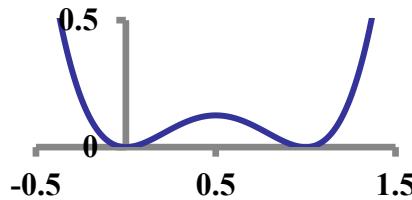
$$\frac{\partial c}{\partial t} = \nabla \cdot \left(M \nabla \frac{\delta F}{\delta c} \right)$$



Free Energy

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

$$f(c) = Wc^2(1-c)^2$$



“Double well” free energy with minima at $c=0$ and $c=1$

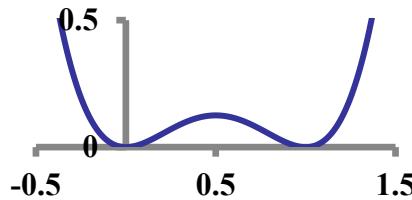
Dynamics: $\frac{\partial c}{\partial t} = \nabla \cdot \left(M \nabla \frac{\delta F}{\delta c} \right)$

$$\frac{\delta F}{\delta c} = 2Wc(c-1)(2c-1) - K\nabla^2 c$$

Free Energy

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

$$f(c) = Wc^2(1-c)^2$$



“Double well” free energy with minima at $c=0$ and $c=1$

Dynamics: $\frac{\partial c}{\partial t} = \nabla \cdot \left(M \nabla \frac{\delta F}{\delta c} \right)$

$$\frac{\delta F}{\delta c} = 2Wc(c-1)(2c-1) - K\nabla^2 c$$

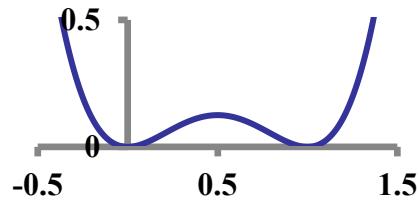
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Allen-Cahn Dynamics

Free energy functional

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

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



“Double well” free energy with minima at $\phi=0$ and $\phi=1$

Dynamics $\frac{\partial \phi}{\partial t} = -M \frac{\delta F}{\delta \phi} = -M \left[2W\phi(\phi-1)(2\phi-1) - K\nabla^2\phi \right]$

Remarks

- Most phase field formulations employ the governing equations we've covered today to describe the evolution of order parameters
- Depending on the system we want to study, we can incorporate different “physics” into the free energy (e.g., elasticity, interaction between different order parameters, interaction with an external electric or magnetic field, etc.)
- Many applications of the phase field model require multiple orders parameter that need to be solved simultaneously



Questions?

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The PRISMS-PF framework

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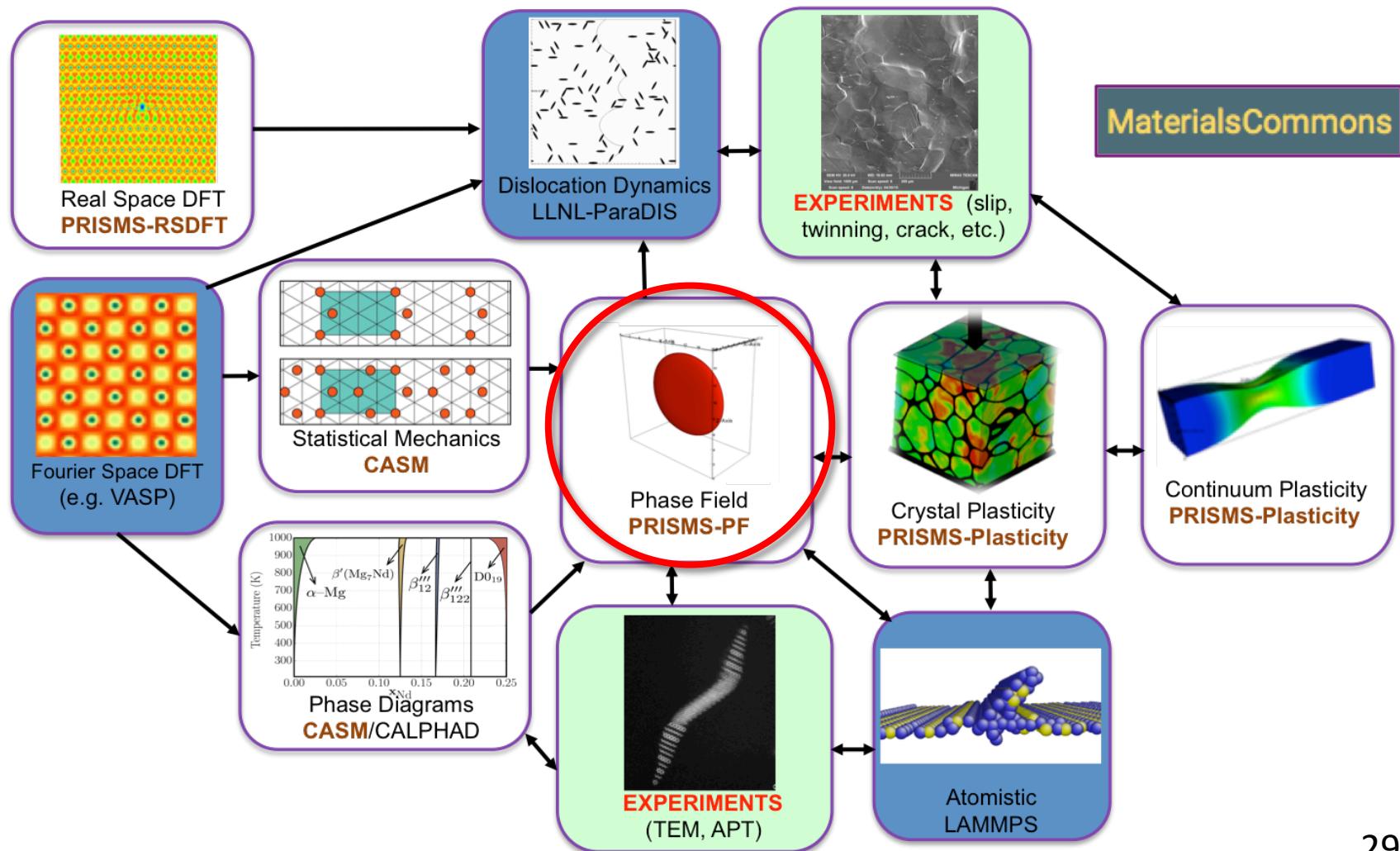
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PRISMS Center Integrated Framework



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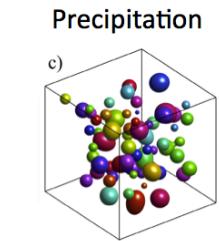
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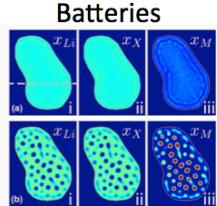
Motivation:

What's hard about writing a phase field code?

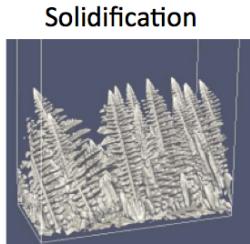
1. Wide diversity of models and coupled physics makes code reuse difficult



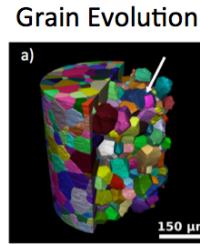
Poulsen, Voorhees, Acta Materialia (2016)



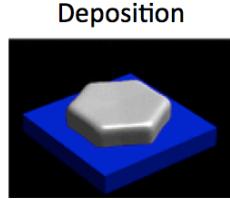
Yu, et al. J. Phase Equil. Diff. (2016)



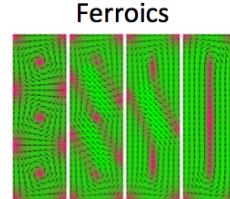
Shimokawabe, et al., SC '11 (2011)



McKenna, et al. Acta Materialia (2014)



DeWitt, et al. J. Electrochem. Soc. (2016)



Chen, Zheng, Wang, Appl. Phys. Lett. (2012)

No “typical” governing equations

Large variety of formulations and terms



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Motivation:

What's hard about writing a phase field code?

2. Simulating large, physically representative systems is computationally intensive



nersc.gov

Simulations often take days on
10s-100s of cores

Simulations are often done in 2D
for tractability

Physical fidelity requires strong
numerical performance



Four Principles Guiding PRISMS-PF Development

1. Its computational performance, including parallel scalability, should meet or exceed that of typical phase field codes
2. It should accommodate a wide variety of phase field models and applications
3. The interface for creating or modifying governing equations should be simple, quick, and separate from the numerical implementation.
4. It should be open source with a permissive license so it is available to everyone and advances can be shared by the community

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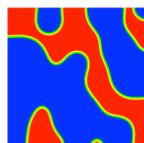
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PRISMS-PF

An Open-Source Phase-Field Modeling Framework

Advanced capabilities

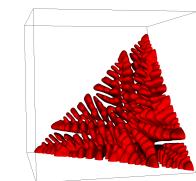
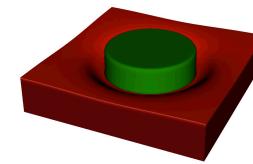
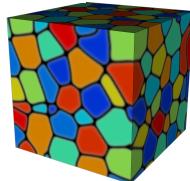
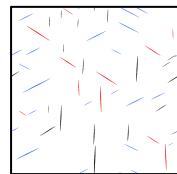
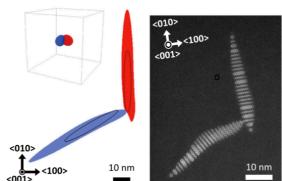
- Matrix-free finite element approach
- Solution of an arbitrary number of coupled PDEs
 - Higher-order elements
 - Multi-level parallelism
 - Adaptive meshing
 - Explicit nucleus placement
 - Grain-remapping
 - Newton/Picard nonlinear solver

Implicit time integration capability <- Coming soon!

Functionalities / Ease of Use

- Simple interface
- Detailed online user guide
- 27 pre-built applications
- Simple Docker-based installation
- nanoHUB tool w/ GUI for educational use
- Integrated with Materials Commons
- Postprocessing scripts for results analysis
- YouTube video tutorials

DeWitt et al., npj Comput. Mater. 6, 29 (2020)



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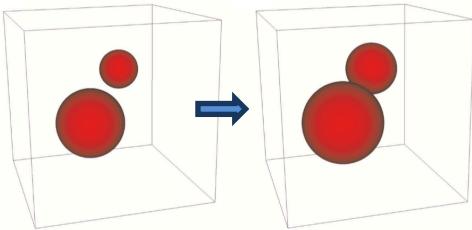
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Performance of PRISMS-PF

Comparison to finite difference code

- Two growing particles in 3D



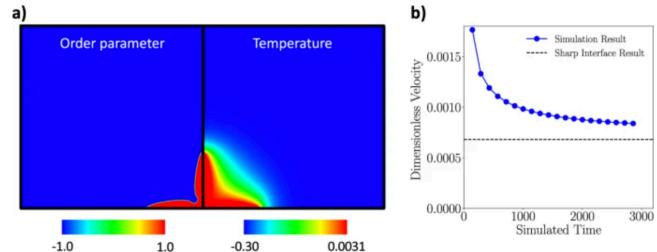
| Element/Mesh Type | Speedup vs. FD* |
|-------------------|-----------------|
| Linear/Regular | 0.028 |
| Quadratic/Regular | 0.90 |
| Cubic/Regular | 1.9 |
| Cubic/Adaptive | 12.0 |

Comparison is at the same error with respect to a highly-resolved simulation in time in space

[DeWitt et al., npj Comput. Mater. 6, 29 (2020)]

Comparison to other Open Source Codes

- Solidification benchmark problem
(<https://pages.nist.gov/pfhub/benchmarks/benchmark3.ipynb/>)



- PRISMS-PF performance was compared to MOOSE, AMPE and FiPy
- The PRISMS-PF calculations required **three orders of magnitude fewer** normalized core hours than **AMPE** and **FiPy**, while having similar or lower error.
- The fastest calculations using PRISMS-PF and **MOOSE** have **similar computational cost** and tip velocity error.

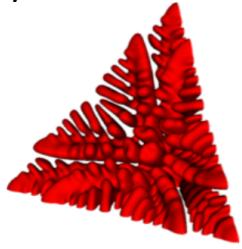
New and Upcoming Features - Built-in Apps

Recent

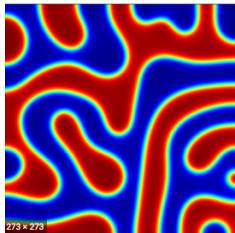
Corrosion



Alloy Solidification

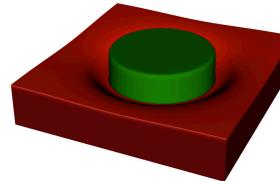


Spinodal Decomposition

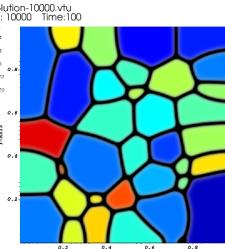


Coming soon

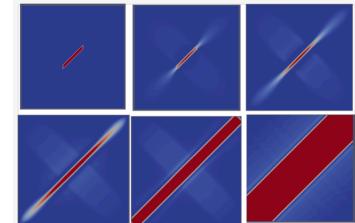
Microgalvanic Corrosion



Grain Growth (with Stored Energy)



Martensitic Transformation*



* Pushkar Pandit (IIT Hyderabad, India) and Bonnie Whitney (WPI)



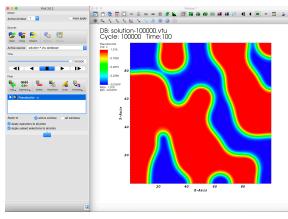
New and Upcoming Features - YouTube Video Tutorials



PRISMS Center
219 subscribers

Installing, running, and visualizing results

PRISMS-PF



Installation of prerequisites

p4est

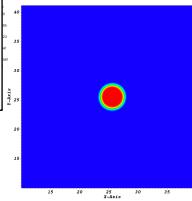
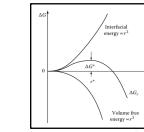


deal.II

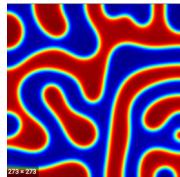
VISIT

ParaView

Nucleation and Growth



Spinodal Decomposition



Coming soon:

Advanced Application



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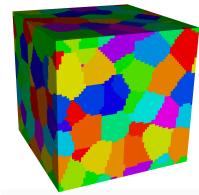
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PRISMS

New and Upcoming Features - Integration Tools

Integration with DREAM.3D

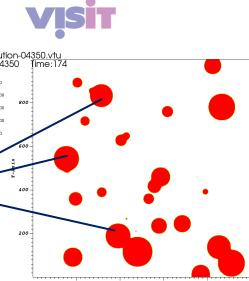
DREAM.3D



PRISMS-PF
An Open-Source Phase-Field Modeling Framework

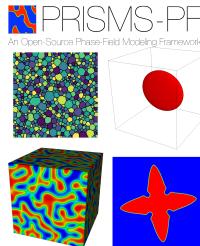
Recently upgraded script to import microstructure from DREAM.3D (using the VisIt CLI)

visIt



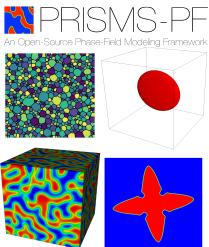
Postprocessing scripts

New scripts for results analysis of PRISMS-PF simulations:

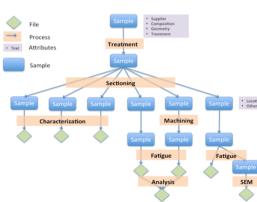


- Phase fraction
 - Interface area
 - Domain count
- ... more to come

Materials Commons CLI



Materials Commons 2.0



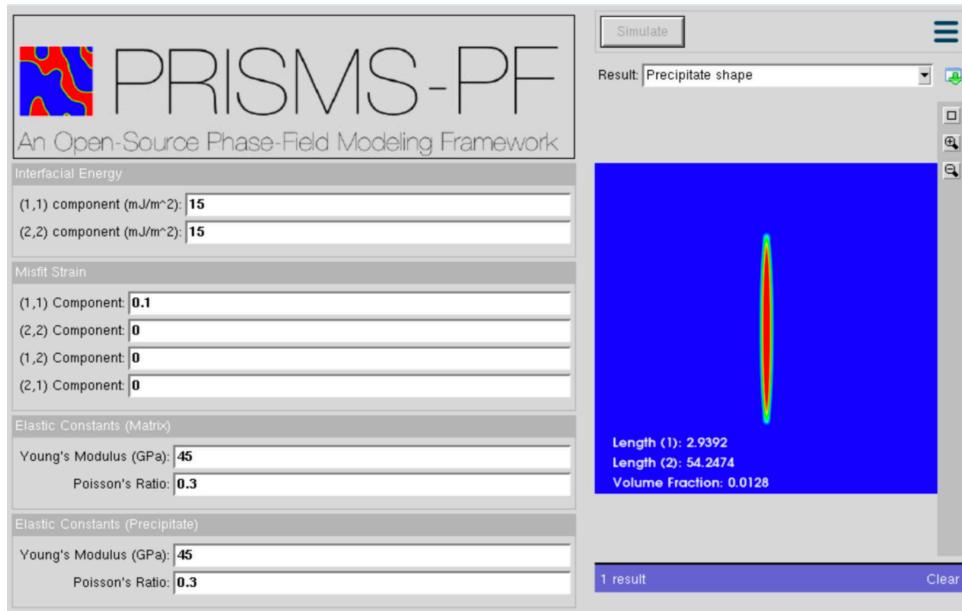
The newly-developed CLI for Materials Commons will facilitate creating scripts to automate the creation of projects, upload data, create and publish datasets, and edit communities of practice



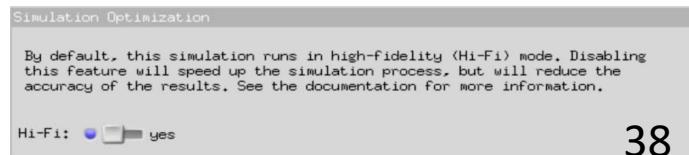
PRISMS-PF nanoHUB Module

<https://nanohub.org/resources/prismspfmisfit>

PRISMS-PF: Equilibrium Shape for a Misfitting Precipitate*



- 2D equilibrium shape of a precipitate taking into account the effects of interfacial and strain energy
- Targeted for classroom use
- Recently optimized to include a low-fidelity option which produces a faster, preliminary calculation



*S. DeWitt (UM), N. Shuman (UC Davis), and S. Gentry (UC Davis)



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PRISMS

Ongoing and Future Development

Applications (ongoing development)

- Static recrystallization (coupled with PRISMS-Plasticity)
- Additive manufacturing - Tom Flint (University of Manchester, UK), Bryan Kinzer (UM), Bonnie Whitney (WPI)
- Fluid dynamics - Xianyue Liu (SUSTech, China)

Performance improvement

- Implementation of GPU acceleration capability
- Adaptive time-stepping
- Nonzero Neumann boundary conditions

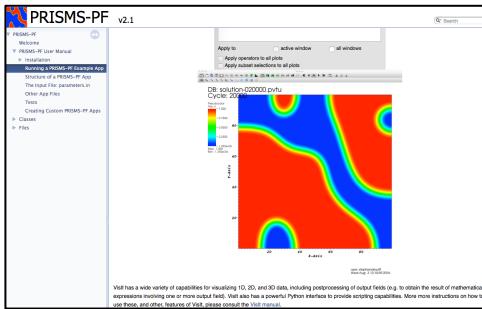
Integration and ease-of-use

- Integration with Thermo-Calc for direct access databases that contain thermodynamic and kinetic information
- Integration with CASM for loading free energy surfaces
- Adding integration with Materials Commons to existing NanoHUB tool
- Expand postprocessing suite



Community support

Online user manual



The screenshot shows a page from the PRISMS-PF v2.1 online user manual. It includes a heading 'PRISMS-PF v2.1', a table of contents, and a detailed explanation of the Allen-Cahn and Cahn-Hilliard equations. The equations are shown with mathematical notation involving integrals and variables like ΔM , f_0 , f_1 , $H^{(1)}$, $H^{(2)}$, and V . Below the equations is a code snippet in C++ illustrating how to implement these functions.

Allen-Cahn equation:

$$\int_{\Omega} \omega \nabla f_0^{\alpha \beta} \cdot \nabla f = \int_{\Omega} \left[\sqrt{1 + \Delta M} \left(f_0^{\alpha} - f_1^{\alpha} \right) M \right] + V \omega \left(- \sqrt{1 + \Delta M} \omega \nabla f \right) \cdot \nabla f$$

Cahn-Hilliard equation:

$$\int_{\Omega} \omega \nabla f^{(1)} \cdot \nabla f^{(2)} = \int_{\Omega} \left[\sqrt{1 + \Delta M} \left(f_0^{(1)} - f_1^{(1)} \right) M \right] + V \omega \left(- \sqrt{1 + \Delta M} \omega \nabla f^{(1)} \right) \cdot \nabla f^{(2)}$$

Online message board
(> 100 registered users)

☆ PRISMS-PF Users 99 members 1-30 of 144 < >

Welcome to the PRISMS-PF user forum! This is the place to ask any questions that you have regarding PRISMS-PF ranging from whether it is right for your work, installation, creating new applications, details about the internal workings of the code, or future directions. We work to make sure that postings are responded to within a few business hours. For additional help with PRISMS-PF, we also hold office hours on Skype on the first Tuesday of every month. See the "Skype Office Hours" thread for more details.

- Bryan Kinzer, dmontiel 8 Help with Loading Initial Conditions in Dream3D Example/Trying to add Particulates – Thanks... Feb 26 ☆
- dmontiel Updated vtk conversion scripts within the grainGrowth_dream3d application – Hello everyone, ... Feb 25 ☆
- Bryan Kinzer, dmontiel 3 CMAKE_PREFIX_PATH Not Found Question – Hey David, After clearing out the files when I ran ... Feb 19 ☆
- Bryan Kinzer, ... dmontiel 5 PRISMS-PF is running super slow on Computing Cluster – Hello, Bryan One source of poor per... Feb 17 ☆

Phase-Field Community of Practice (NEW)

Community: Phase-Field Simulations of Microstructure Evolution Edit Community

Overview Datasets Files Links

Name Phase-Field Simulations of Microstructure Evolution

Description A community of practice for sharing phase-field simulation results of microstructure evolution.

DONE

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PRiSMS

Three Types of PRISMS-PF Users

1. Using pre-built applications

- Modifying simulation parameters, boundary conditions, initial conditions.
- No C++ or deal.II knowledge required

2. Creating new applications

- Implementing governing equations and defining model parameters
- Basic C++ knowledge required
- No deal.II knowledge required

3. Developing new features and functionalities

- Editing the core library
- Knowledge of C++ and deal.II required



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
 - Using an app requires no C++ experience (parsed text input file)
 - Developing an app requires minimal C++ experience and no FEM experience
- Tests
 - Suite of unit and regression tests
 - Continuous integration testing with Travis CI

Structure of an application

Code files (all applications):

- `main.cc` – Parses user input data, builds the fields, loads initial conditions, calls the solver method.
- `parameters.in` – Text file with input data: system dimensions, mesh specification, time step, boundary conditions, output format and frequency, and user-defined simulation parameters.
- `equations.cc` – Declare the expressions (weak form) for the time dependent and time-independent equations
- `ICs_and_BCs.cc` – Set the initial conditions and non-uniform Dirichlet boundary conditions (if applicable).
- `customPDE.h` – Declare user-defined simulation parameters defined in `parameters.in`. Declare application-specific methods, or override methods from the core library.

Structure of an application

Code files (optional):

- `postprocess.cc` – Defines fields needed for analysis of the results, but not necessarily for the simulation, e.g., the free energy density.
- `nucleation.cc` – Defines the method to calculate the probability of nucleation (only needed when nucleation is enabled).



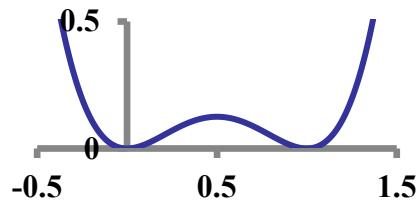
APPLICATION DEMO

1. allenCahn

Free energy
functional

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

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



“Double well” free
energy with minima
at $\phi=0$ and $\phi=1$

Dynamics $\frac{\partial \phi}{\partial t} = -M \frac{\delta F}{\delta \phi} = -M \left[2W\phi(\phi-1)(2\phi-1) - K\nabla^2\phi \right]$

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APPLICATION DEMO

Derivation of weak form of equations (Allen-Cahn model)

Free energy
functional

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

Governing equation

$$\frac{\partial \phi}{\partial t} = -M \frac{\delta F}{\delta \phi} = -M \left[\frac{\partial f}{\partial \phi} - K \nabla^2 \phi \right]$$

Time discretization
(forward Euler method)

$$\phi^{n+1} = \phi^n - M \Delta t \left[\frac{\partial f^n}{\partial \phi} - K \nabla^2 \phi^n \right]$$



APPLICATION DEMO

Derivation of weak form of equations (Allen-Cahn model)

- To obtain the weak formulation of the governing equation(s) we multiply both sides an arbitrary variation, ω , and integrate over the volume Ω :

$$\int_{\Omega} \omega \phi^{n+1} dV = \int_{\Omega} \left[\omega \phi^n - \omega \Delta t M \left(\frac{\partial f^n}{\partial \phi} - K \nabla^2 \phi^n \right) \right] dV$$

Rearranging terms, we have

$$\int_{\Omega} \omega \phi^{n+1} dV = \int_{\Omega} \omega \left[\phi^n - \Delta t M \frac{\partial f^n}{\partial \phi} \right] dV + \int_{\Omega} \left[\nabla \omega (-\Delta t M K) \cdot \nabla \phi^n \right] dV$$

r_{ϕ} $r_{\nabla \phi}$



Interactive Session

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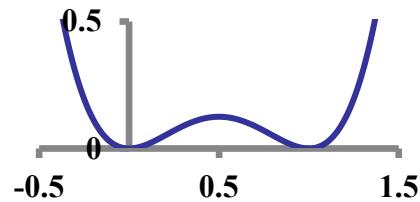
APPLICATION DEMO

2. Cahn-Hilliard

Free energy functional

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

$$f(c) = Wc^2(1-c)^2$$



“Double well” free energy with minima at $c=0$ and $c=1$

Dynamics

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(M \nabla \frac{\delta F}{\delta c} \right)$$



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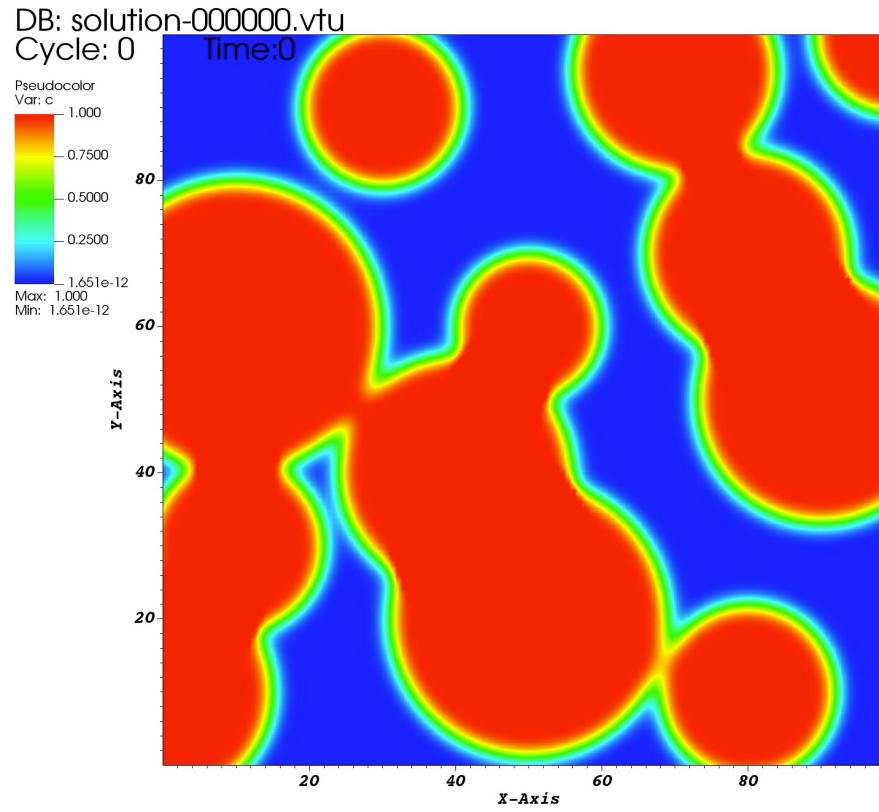


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APPLICATION DEMO

2. Cahn-Hilliard



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APPLICATION DEMO

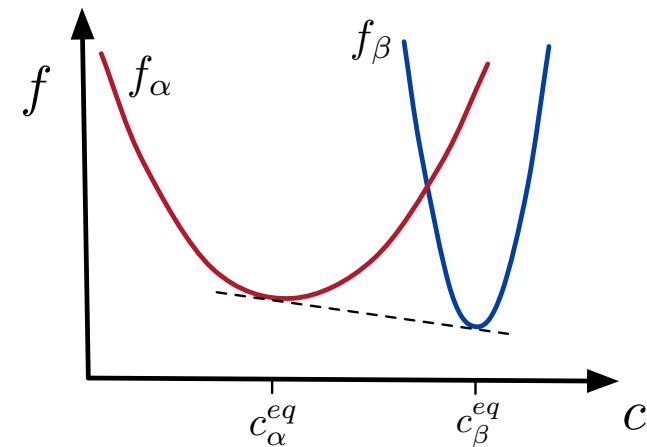
3. Coupled Cahn-Hilliard/Allen-Cahn

Free energy functional
$$F = \int_{\Omega} \left[f_{\alpha}(c)[1 - H(\phi)] + f_{\beta}(c)H(\phi) + \frac{1}{2}K |\nabla \phi|^2 \right] dV$$

f_{α}, f_{β} - Free energy curves for phases α and β

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

(Interpolation function)



Dynamics

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(M \nabla \frac{\delta F}{\delta c} \right)$$

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

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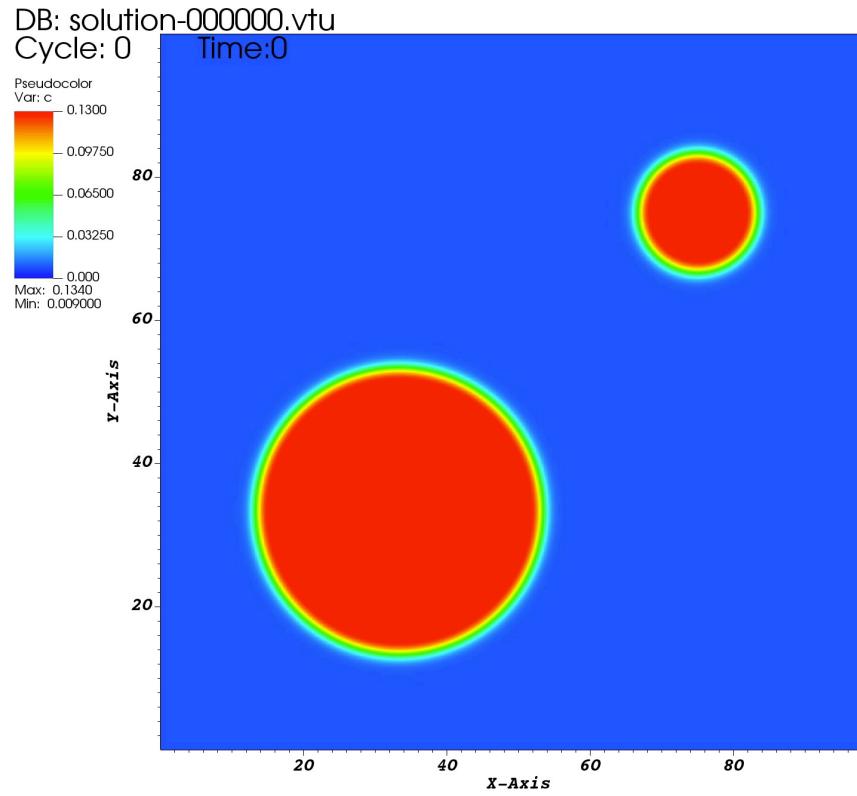


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APPLICATION DEMO

3. Coupled Cahn-Hilliard/Allen-Cahn



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Thank you!

Interested in PRISMS-PF?

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

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

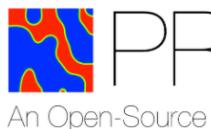
PRISMS Center YouTube Channel: https://www.youtube.com/channel/UCZXc3007JuBCGKDcneD_umA

Email: prismsphasefield.dev@umich.edu

PRISMS-PF

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

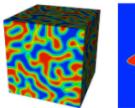
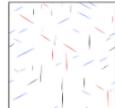
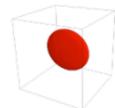
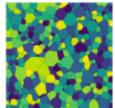
GitHub Repository
User Manual
User Registration Link
PRISMS-PF Forum
YouTube Channel
Community of Practice



An Open-Source

Overview

PRISMS-PF is a powerful, massively parallel simulation framework for predicting the evolution of microstructures. PRISMS-PF provides a simple interface to solve a wide range of differential equations of the type commonly found in materials science application modules, including for spinodal decomposition.



PRISMS-PS Training Sessions

- Monday 10-12 EST (8/9/2021)
- Wednesday 10-12 EST (8/11/2021)

The screenshot shows the GitHub repository page for PRISMS-PF. Key details include:

- Commits:** 969
- Watchers:** 15
- Stars:** 91
- Forks:** 61
- Languages:** C-plus-plus, Finite-elements, phase-field
- Readme:** View license
- Releases:** 14 (Latest: PRISMS-PF (Version 2.1.2) on Jul 31, 2019)
- Packages:** No packages published. Publish your first package
- Contributors:** 6



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