# MedeA PhaseField

Simulate years of microstructure evolution – in minutes

## At-a-Glance

The *MedeA*[1] *PhaseField* module employs the phase field method to predict grain growth, phase separation, other microstructural evolution phenomena, and stress response in metal alloys, organic materials, and ceramics at length and time scales inaccessible to atomistic simulation methods.

## Key Benefits

- *Models Realistically the microstructural evolution in diverse materials*
- *Accesses time and length scales of days and micrometers, unreachable with atomistic simulations*
- *Accepts material property input available from first principles and atomistic MedeA modules*
- *Flexible and scalable finite element-based simulations*

Phase field modeling is the method of choice for simulating material microstructures, enabling prediction of properties like mechanical strength, phase transitions, and environmental degradation behavior. By simulating the evolution of material phases under different conditions, *MedeA PhaseField* can predict behaviors like grain growth, phase separation, corrosion and hydriding behavior, stress evolution, and much more.

*MedeA PhaseField* is a versatile finite element based solver[2] for coupled phase field, mass transport, and linear elasticity equations. This coupling enables detailed simulations of microstructure evolution in metals, ceramics, and other materials in which mechanical properties are influenced by phase changes. *PhaseField* supports diverse boundary conditions, making it applicable to a wide range of real world scenarios.

The user defines an initial microstructure and phase properties such as free energies, bulk diffusion coefficients, and interfacial properties such as interface energies and grain boundary diffusivities. If unknown, many such properties can be calculated directly from first principles or atomistics using *MedeA*'s powerful tool suite.

Once a simulation is initialized, the finite element grid evolves adaptively, even to complex geometries, as the simulation progresses, enabling optimal trades between fidelity and speed.

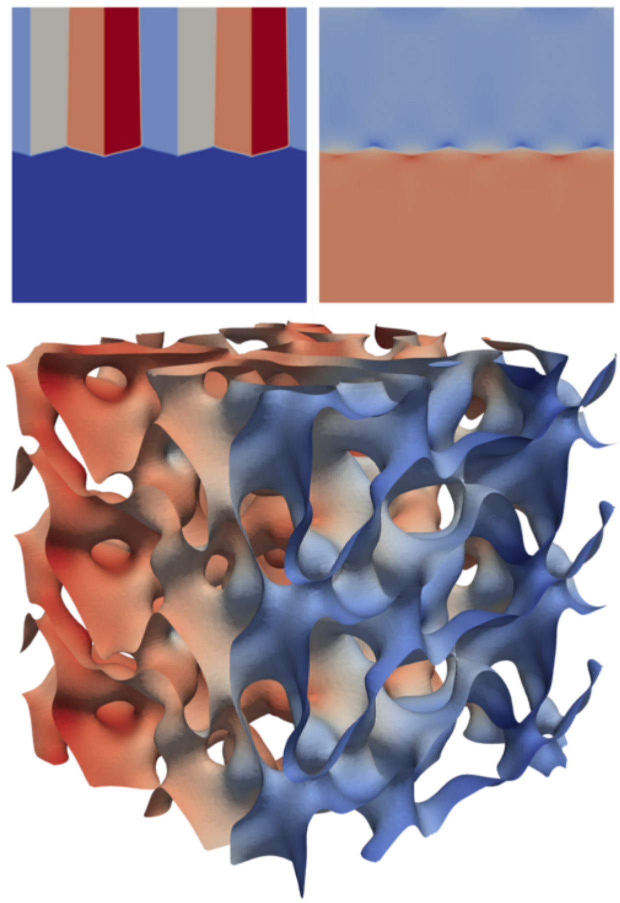

*Figure 1: Examples of microstructure evolution simulated with* MedeA PhaseField*. (Top) A 2D simulation of columnar oxide growing a metal substrate, with phases shown in the left panel and the stress response in the right panel. (Bottom) Interfaces in a Ag-Cu eutectic system modeled in 3D.*

*MedeA PhaseField* empowers users to simulate many, and varied phenomena of engineering im-

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

[2] Anderson et al., *MFEM: A modular finite element methods library. Computers & Mathematics with Applications* **81**, 42-74 (2021)

portance. For example, the figure shows snapshots of a 2D simulation of an oxidation process, and a 3D simulation of phase separation in an Ag-Cu binary eutectic alloy. In both cases, elastic effects are critical for predicting the formation of microstructural features. Elastic anisotropy, phase transformation kinetics, and the coupling between phase and mechanical fields are key features that can be adjusted to match experimental data or theoretical models.

Advanced users can modify the finite element mesh, refine the phase field equations, or introduce custom boundary conditions to further enhance the realism and accuracy of simulations. Integration of the phase field and elasticity equations enables self-consistent calculations of stress and strain, making *PhaseField* suitable for studying deformation-induced phase transformations and the interaction between microstructure and mechanical properties.

*PhaseField* simulation results are exportable to post-processing tools for further analysis, including visualization and data extraction for validation against experimental findings.

## Key Features

- Finite element-based simulation of microstructure evolution
- Coupled phase field, mass transport, and linear elasticity equations
- Access to first-principles and atomistic material property values inside *MedeA*
- Adaptive mesh refinement and adaptive timestepping for optimal convergence
- Easily exportable results for post-processing and visualization

## Required Modules

- *MedeA Environment*
- *MedeA PhaseField*

## Recommended Modules

- *MedeA VASP*
- *MedeA Diffusion*
- *MedeA UNCLE*
- *MedeA Interfaces*

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