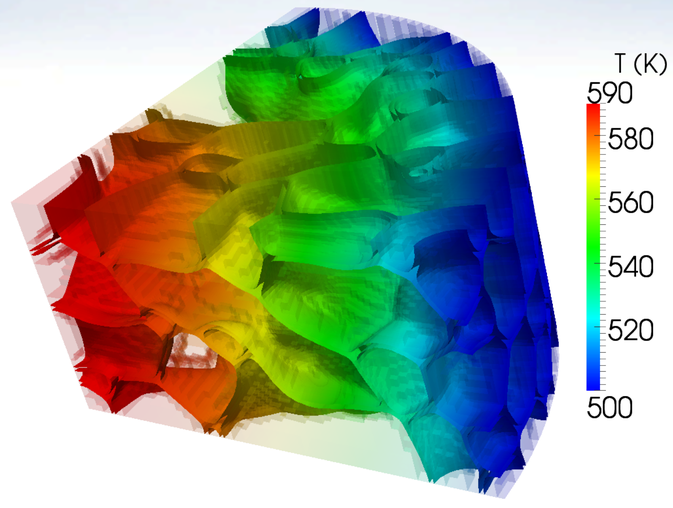
Rapid Phase Field Model Development using the Open Source MOOSE Framework

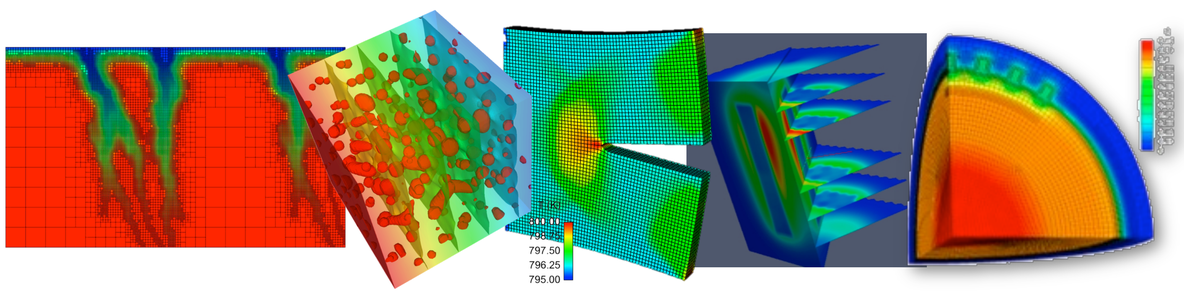


The Power of Mesoscale Modeling…

Multiphysics mesoscale simulation provides a powerful tool for designing materials to provide specific properties. These simulations predict the coevolution of microstructure and properties due to applied load, temperature, and other effects. However, they require an advanced multiphysics modeling capability that can fully take advantage of large high performance computing clusters.

MOOSE – Multiphysics Object Oriented Simulation Environment

- MOOSE is a finite-element, multiphysics framework that **simplifies the development** of advanced numerical applications.
- It provides a high-level interface to **sophisticated nonlinear solvers** and **massively parallel computational capability**.



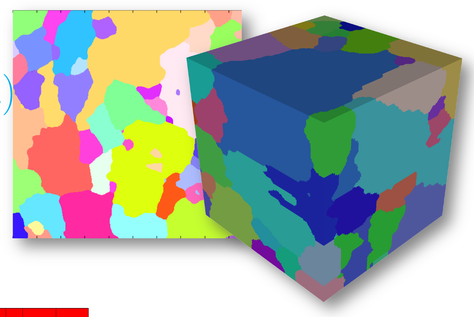
- MOOSE has been used to model thermomechanics, neutronics, geomechanics, reactive transport, microstructure modeling, computational fluid dynamics, and more every day!
- The developers follow a robust quality assurance approach where tests are run after every commit to ensure your results don't change.
- It is open source and freely available at **mooseframework.org**
- MOOSE is in use at universities, laboratories, and industry across the world.

MOOSE -Phase Field

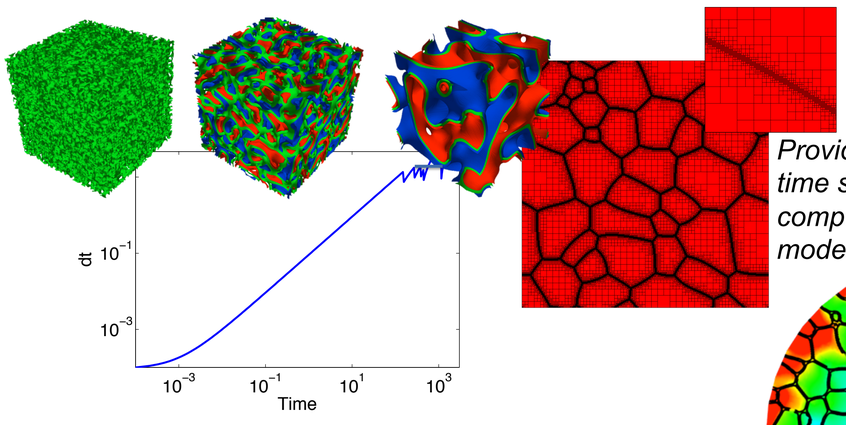
- You can rapidly develop an FEM-based application that predicts microstructure evolution in a large range of materials with the MOOSE phase Field module.
- It also provides a fully functional grain growth model that can efficiently model large polycrystals in 2D and 3D.

$$\left(\frac{\partial c_i}{\partial t},\phi_m\right)+\left(\kappa_i\nabla^2 c_i,\nabla\cdot(M_i\nabla\phi_m)\right)+\left(M_i\nabla\frac{\partial f_{loc}}{\partial c_i},\nabla\phi_m\right)+\left(M_i\nabla\frac{\partial E_d}{\partial c_i},\nabla\phi_m\right)$$

*Only the **derivatives of the free energy functionals** are coded to implement new phase field models.*

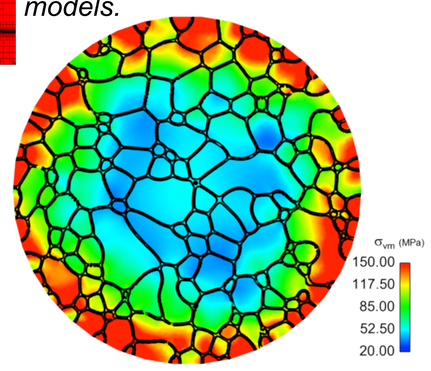


Initial microstructures can be generated or reconstructed from experimental data.



Provides easy access to mesh and time step adaptivity to minimize the computational expense of your models.

Can easily couple to multiple physics, such as finite deformation mechanics or heat conduction.

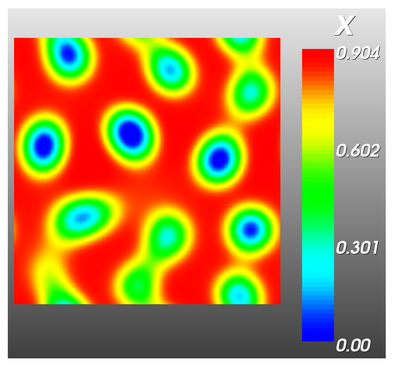


Rapid Phase Field model development

- **Automatic differentiation** assists model development
  - Free energies are specified in the input file
  - All necessary derivatives are generated automatically
  - Symbolic differentiation
- **No coding required**!
- Documentation on **http://mooseframework.org/wiki/PhysicsModules/PhaseField/DevelopingModels/ParsedFunctionKernels/**

A 30 Minute result

Iron concentration field in a spinodally decomposed FeCr alloy with a global chromium concentration of 30%. Chromium rich α'-precipitates (blue) embedded in an Iron rich α-phase (red) have formed. The phase concentrations are in good agreement with a common tangent construction on the analytical free energy surface.
Free energy taken in verbatim from *Schwen, D., E. Martinez, and A. Caro, J. Nuclear Mater. 439 (2013): 180–84.*



Kim-Kim-Suzuki model

S. G. Kim, W. T. Kim, T. Suzuki. "Phase-Field Model for Binary Alloys." Physical Review E 60 (1999): 7186.

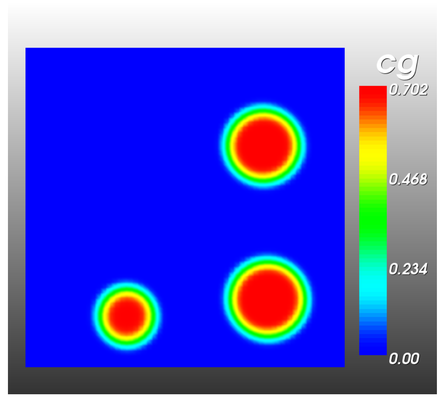
Thermodynamically consistent multi phase field model, where the free energies are specified for the individual phases.

$$c=h(\phi)c_S+[1-h(\phi)]c_L$$

$$f^S_{c_S}[c_S(x,t)]=f^L_{c_L}[c_L(x,t)]$$

$$f(c,\phi)=h(\phi)f^S(c_S)+[1-h(\phi)]f^L(c_L)+wg(\phi)$$

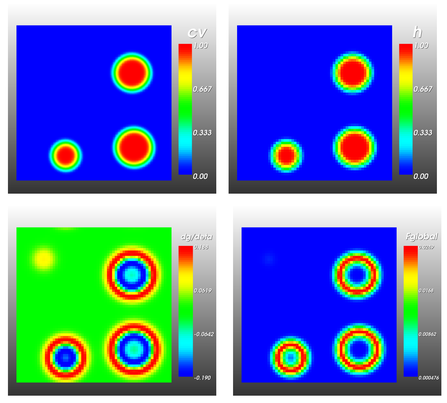
- Automatic differentiation support
- Currently in the restricted MARMOT code, move to the public MOOSE-PF is planned



Automatic differentiation

Free energies are supplied in the input files, and parsed using the Function Parser library and differentiated using a plugin developed in our group.

- Functions are compiled into byte code
- All necessary derivatives are generated at the start of the run from the byte code
- Computation overhead compared to hardcoded derivatives is about 20-30%
- Development time is shortened
- considerably (human error sources are eliminated)



KKS PF simulation of fission gas (c_g) and vacancies (c_v) in UO2 fuel.
Also shown are the switching function *h*, the order parameter derivative of the KKS double well function $dg/d\Phi$, and the bulk free energy density f_{global}. All derivatives are autogenerated.

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