

Introduction to the phase field method and the MOOSE phase field module

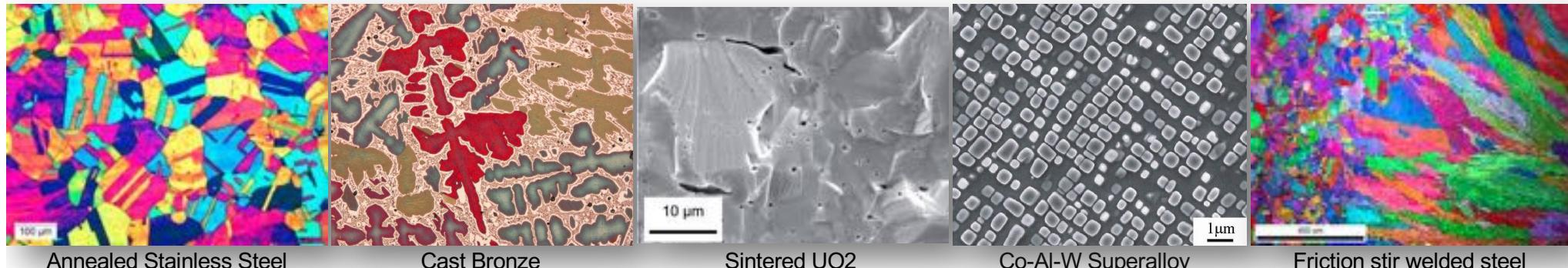
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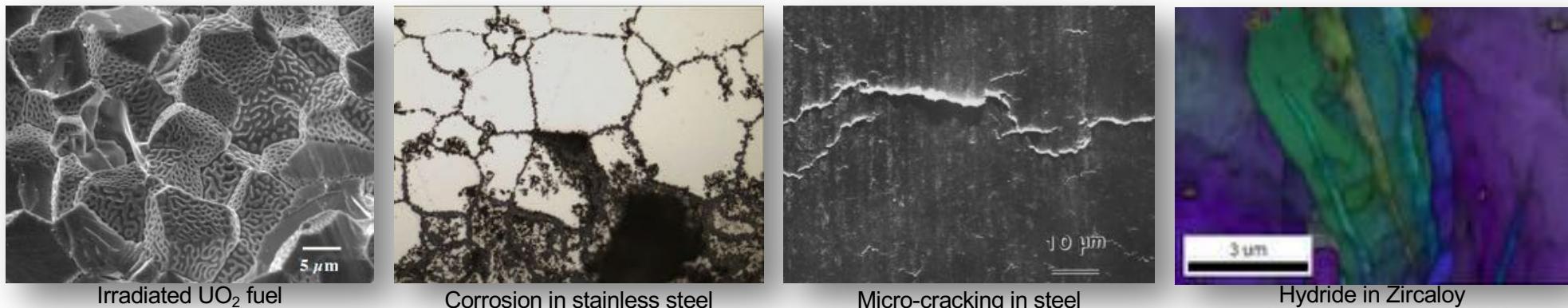
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The purpose of the phase field method is to model microstructure evolution

- The microstructure is established during fabrication

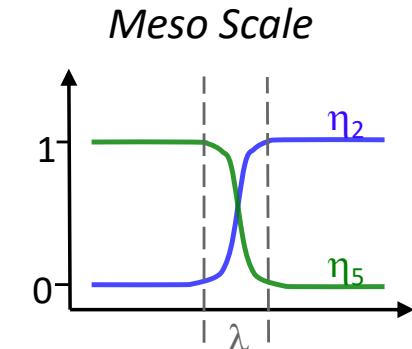
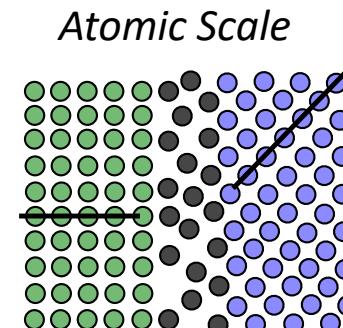
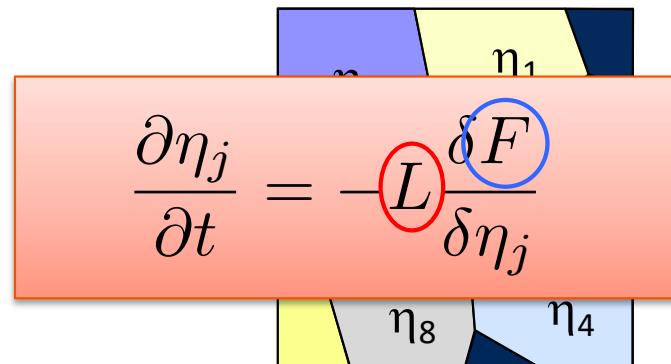


- It can continue to evolve during operation

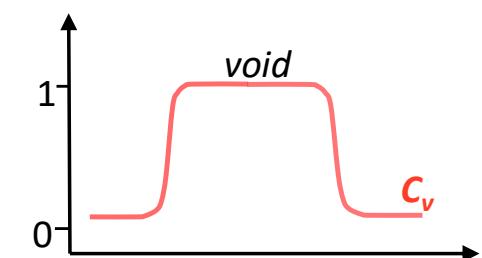
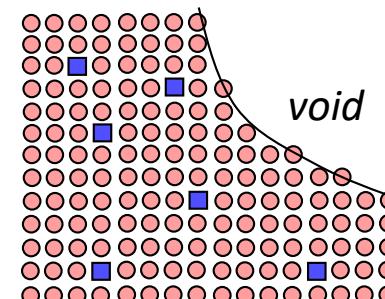
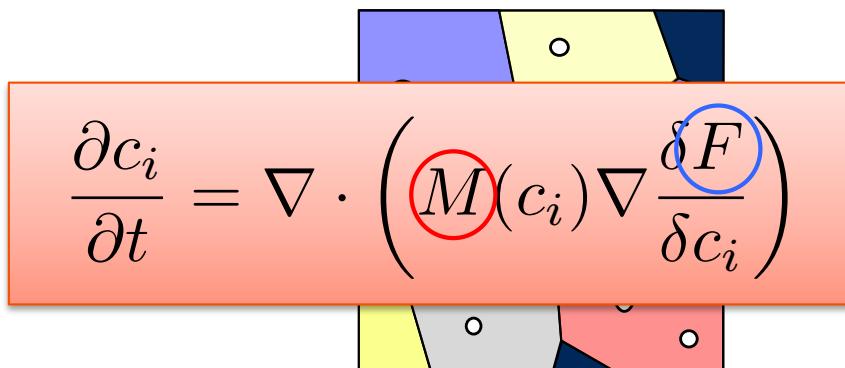


In the phase field method, the microstructure is described by continuous variables

- Non-conserved order parameters describe the atomic order

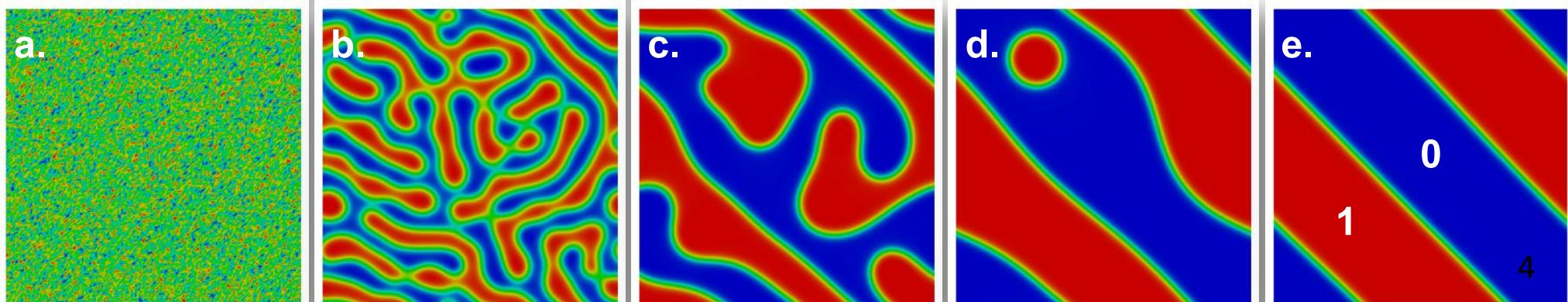
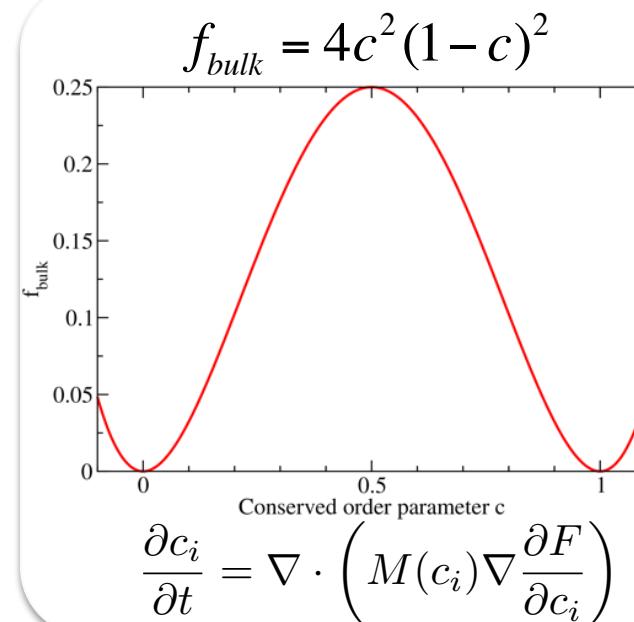
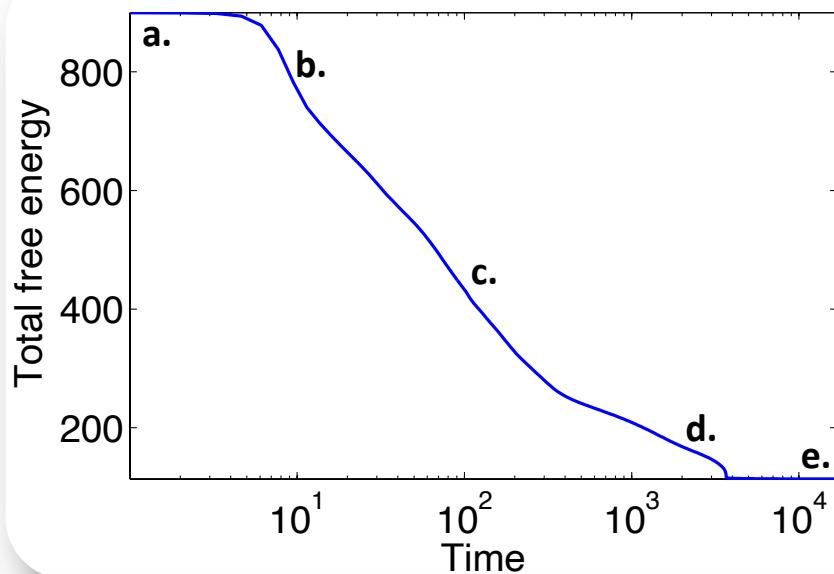


- Conserved concentrations describe atom concentrations

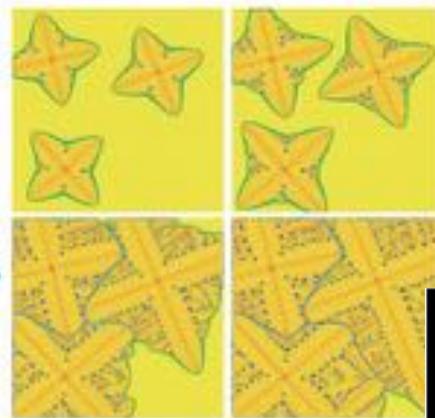


- The variables evolve to minimize a functional defining the free energy

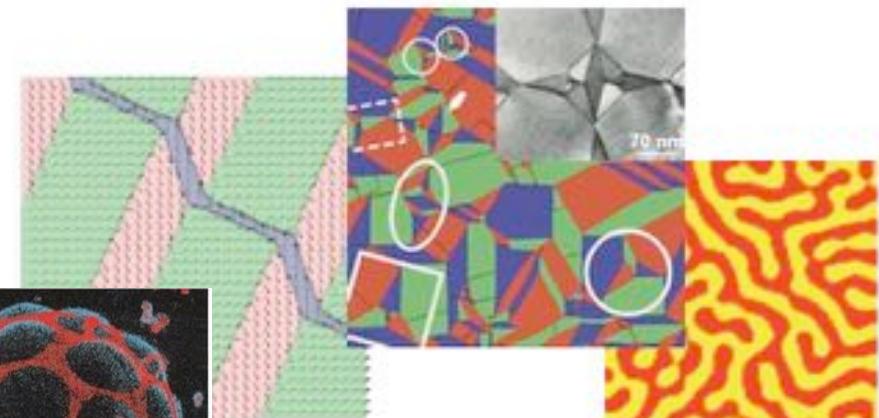
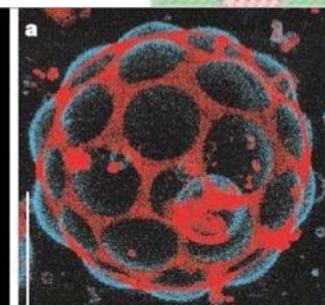
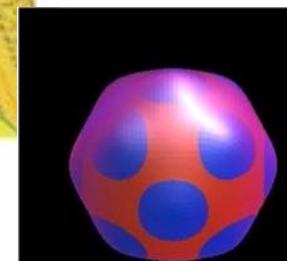
Spinodal Decomposition Example: the microstructure evolves from its initial state to lower the free energy



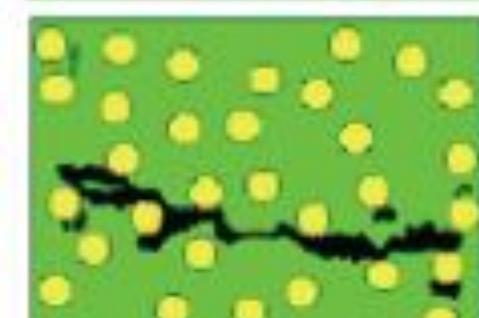
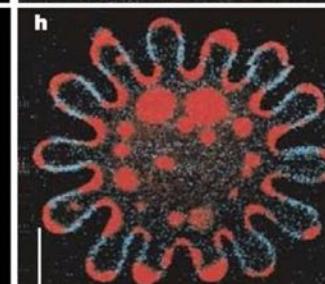
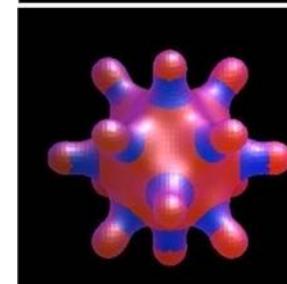
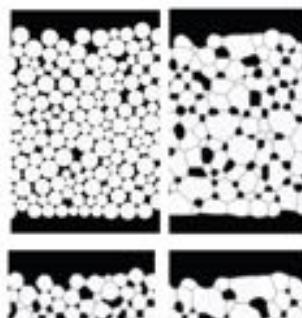
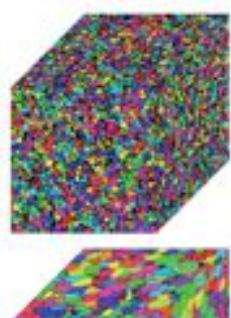
Phase Field Has Been Used in Many Areas



solidification (dendrite growth)



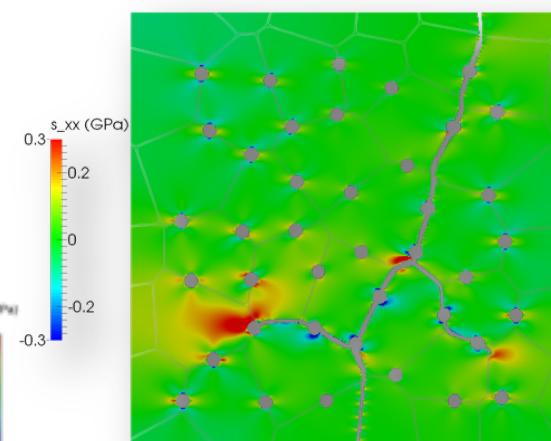
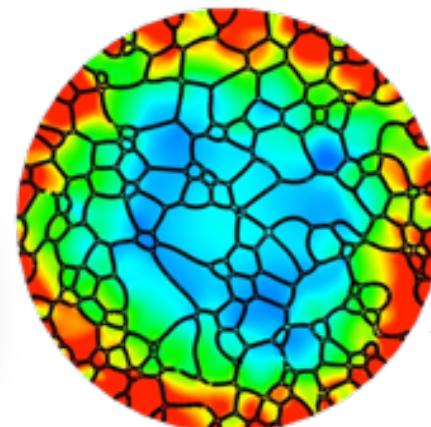
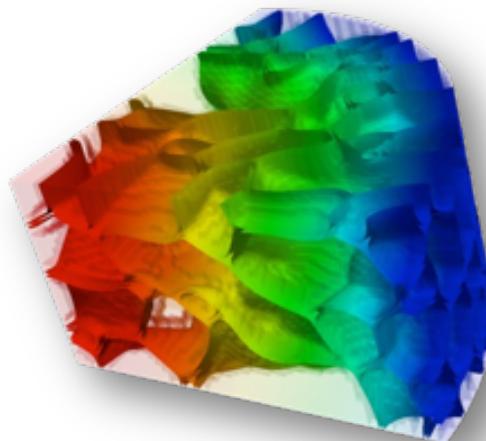
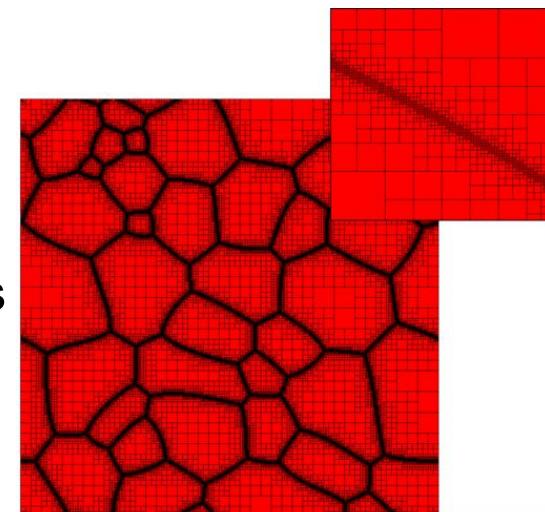
phase transformations



- The primary strengths of the phase field method are:
 - It is easy to have multiple physical phenomenon occurring at once, including mechanics
 - It is quantitative and can represent real materials

The phase field PDEs can be solved in various ways, but we use the finite element method

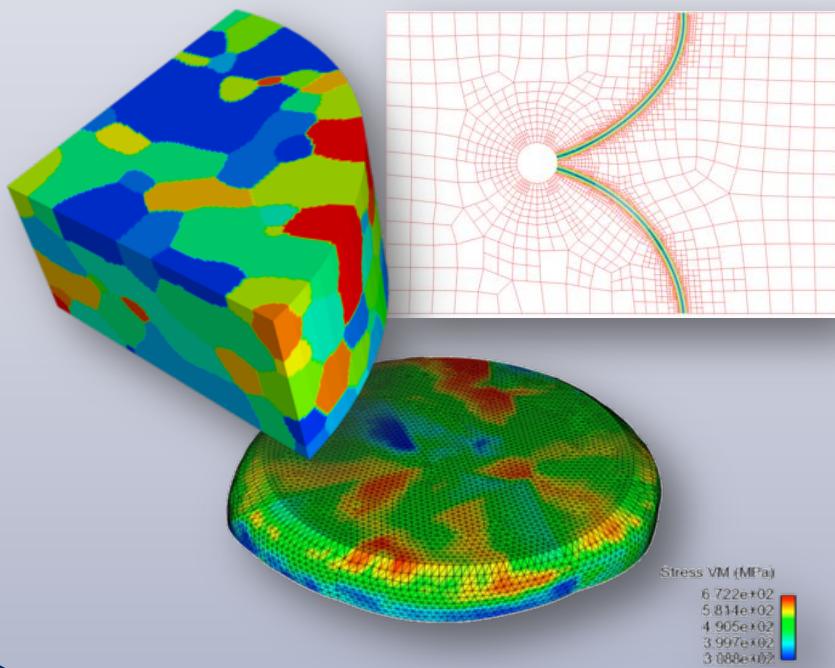
- Methods include finite difference, finite volume, FFT, and FEM.
- Benefits of FEM (MOOSE)
 - Can model any domain shape
 - Can employ a large range of different boundary conditions
 - Scales well up to large numbers of processors
 - Can easily couple to multiple physics



FEM with MOOSE has great flexibility in domain shape and boundary conditions

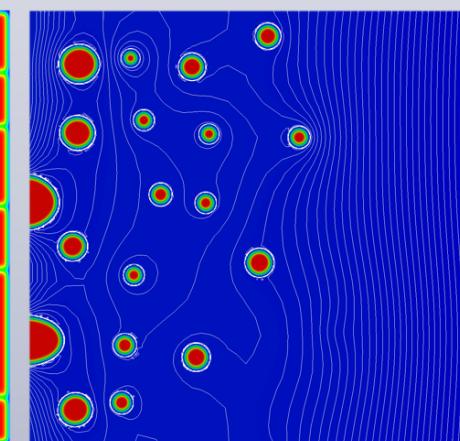
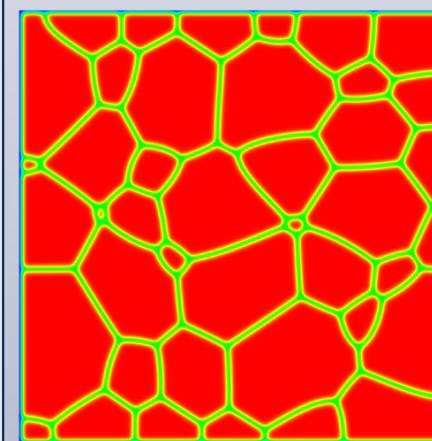
Flexible Domain Shapes

- With FEM, you can model any domain that you can mesh. Therefore, nearly any domain shape can be modeled.
- You can also mesh microstructural features, such as grains or pores



Flexible Boundary Conditions

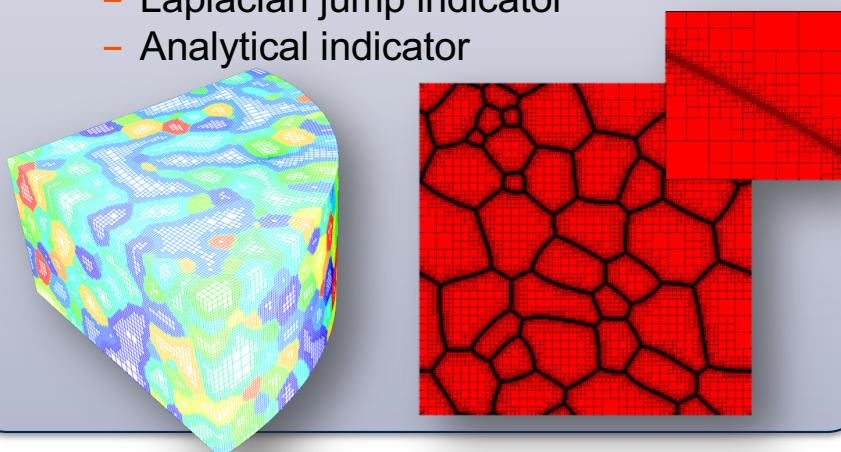
- A large range of different boundary conditions are available in MOOSE
 - Periodic BCs
 - Dirichlet BCs (specified values on boundary or defined by function)
 - Neumann BCs (integrated BC in residual, often used to define flux)
- Users can add new boundary conditions



Any model implemented with MOOSE has access to mesh and time step adaptivity

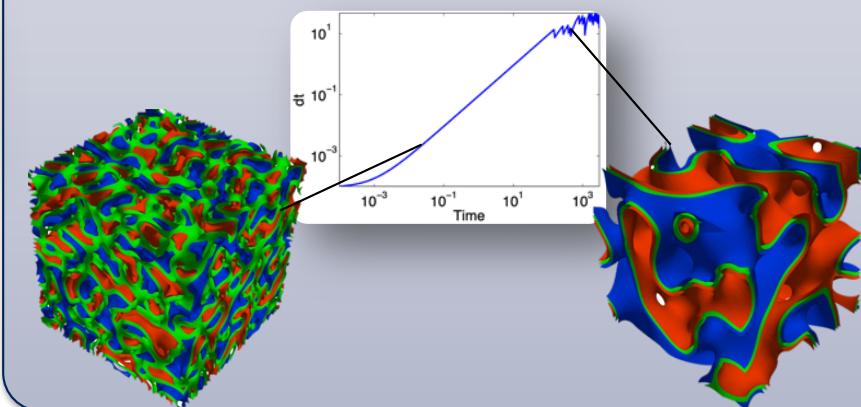
Mesh Adaptivity

- Requires no code development
- Refinement or coarsening is defined by a marker that be related to
 - An error estimator
 - Variable values
 - Stipulated by some other model
- Error indicators include the
 - Gradient jump indicator
 - Flux jump indicator
 - Laplacian jump indicator
 - Analytical indicator



Transient Time Step Adaptivity

- The time step in transient simulations can change with time
- Various time steppers exist to define dt :
 - Defined by a function
 - Adapts to maintain consistent solution behavior
 - Adapts to maintain consistent solution time
- Users can write new time steppers



Solving the phase field equations is a boundary value problem with PDEs

- The equations are:
 - Allen-Cahn $\frac{\partial \eta_j}{\partial t} = -L_j \frac{\delta F}{\eta_j}$
 - Cahn-Hilliard $\frac{\partial c_i}{\partial t} = -\nabla \cdot M_i \nabla \frac{\delta F}{c_i}$
 - The initial conditions define the initial state of the microstructure
 - The boundary conditions depend on the problem being solved
- To solve the PDE in time, we use implicit time integration
 - $c_i(t + dt) = c_i(t) + f(c_i(t + dt))$
 - We solve the nonlinear equation using Newton's method or similar methods

The phase field variables evolve as dictated by functional derivatives of a free energy function

- The symbol δ indicates the functional derivative

$$\frac{\partial \eta_j}{\partial t} = -L_j \frac{\delta F}{\eta_j} \quad \frac{\partial c_i}{\partial t} = -\nabla \cdot M_i \nabla \frac{\delta F}{c_i}$$

- The free energy functional includes the local energy (thermodynamic), deformation energy and gradient energy terms

$$F = \int_V \left(f_{loc}(c_i, \eta_j, \dots, T) + E_d(c_i, \eta_j) + \sum_i \frac{\kappa_i}{2} (\nabla c_i)^2 + \sum_j \frac{\kappa_j}{2} (\nabla \eta_j)^2 \right) dV$$

Here is more information regarding the functional derivative

- From Wikipedia, “functional derivative”:
The functional (or variational) derivative relates a change in a functional to a change in a function that the functional depends on.
 - Let $F = \int f(r, c, \nabla c) dV$, where F is the total free energy and f is the free energy density
 - $\frac{\delta F}{\delta c} = \frac{\partial f}{\partial c} - \nabla \cdot \frac{\partial f}{\partial \nabla c}$
- So, the derivatives of our free energy functional are

$$F = \int_V \left(f_{loc}(c_i, \eta_j, \dots, T) + E_d(c_i, \eta_j) + \sum_i \frac{\kappa_i}{2} (\nabla c_i)^2 + \sum_j \frac{\kappa_j}{2} (\nabla \eta_j)^2 \right) dV$$

$$\frac{\delta F}{\delta \eta_j} = \left(\frac{\partial f_{loc}}{\partial \eta_j} + \frac{\partial E_d}{\partial \eta_j} - \nabla \cdot \kappa_j \nabla \eta_j \right)$$

$$\frac{\delta F}{\delta c_i} = \left(\frac{\partial f_{loc}}{\partial c_i} + \frac{\partial E_d}{\partial c_i} - \nabla \cdot \kappa_i \nabla c_i \right)$$

The basic phase field equations have local, deformation, and gradient contributions

- Allen-Cahn: $\frac{\partial \eta_j}{\partial t} = -L_j \left(\frac{\partial f_{loc}}{\partial \eta_j} + \frac{\partial E_d}{\partial \eta_j} - \nabla \cdot \kappa_j \nabla \eta_j \right)$
- Cahn-Hilliard: $\frac{\partial c_i}{\partial t} = \nabla \cdot M_i \nabla \left(\frac{\partial f_{loc}}{\partial c_i} + \frac{\partial E_d}{\partial c_i} - \nabla \cdot \kappa_i \nabla c_i \right)$
- The form of the equations are fairly standard in most phase field models
- Phase field models differ due to their
 - Energy terms: f_{loc} , E_d ,
 - Interfacial parameters: κ_j , κ_i
 - Kinetic terms: L_j , M_i

The phase field module simplifies the development of new phase field models

- Kernels that implement the weak form of the phase field equations have been created in the phase field module:
https://mooseframework.org/modules/phase_field/index.html
- The correct kernels are automatically created when non-conserved and conserved variables are defined
- The required free energy functions and interfacial and kinetic parameters are defined by the user as materials
 - Energy terms: f_{loc} , E_d ,
 - Interfacial parameters: κ_j , κ_i
 - Kinetic terms: L_j , M_i

All MOOSE phase field simulations need four types of objects

Variables

c_i, η_j

Define non-conserved and conserved quantities to represent the microstructure

[Modules]

```
[./PhaseField]
[./Nonconserved]
...
[../]
[../]
[]
```

ICs (Initial Conditions)

Defines the initial microstructure, as defined by the initial variable values

[ICs]

```
...
[]
```

Free energy, material properties

L, M, K, f_{loc}

Are used in the kernels, but are material specific. Can be functions of other variables.

[Materials]

```
...
[]
```

Boundary Conditions

L, M, K, f_{loc}

Define the state of the material at the domain boundaries, e.g. $c_i = 0$ at $x = 0$. Could be periodic or involve gradients

[BCs]

```
...
[]
```

Non-conserved variables are created in the phase field module block

- $\frac{\partial \eta_j}{\partial t} = -L_j \left(\frac{\partial f_{loc}}{\partial \eta_j} + \frac{\partial E_d}{\partial \eta_j} - \nabla \cdot \kappa_j \nabla \eta_j \right)$
- This block creates a nonconserved variable called eta and all the corresponding kernels
 - f_{loc} + E_d is stored in a material property called F
 - κ_j is stored in a property called kappa_eta
 - L_j is stored in a property called L

```
[Modules]
./PhaseField
./Nonconserved
./eta
free_energy = F
kappa = kappa_eta
mobility = L
[..]
[..]
[..]
[]
```

Conserved variables are also created in the phase field module block

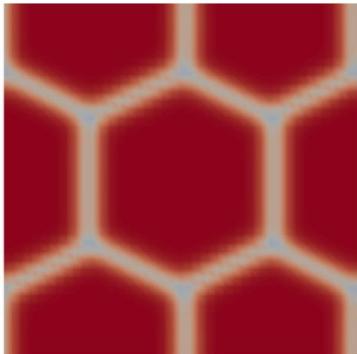
- $\frac{\partial c_i}{\partial t} = \nabla \cdot M_i \nabla \left(\frac{\partial f_{loc}}{\partial c_i} + \frac{\partial E_d}{\partial c_i} - \nabla \cdot \kappa_i \nabla c_i \right)$, however we often split it into two
- $\frac{\partial c_i}{\partial t} = \nabla \cdot M_i \nabla(\mu_i)$ and $\mu_i = \frac{\partial f_{loc}}{\partial c_i} + \frac{\partial E_d}{\partial c_i} - \nabla \cdot \kappa_i \nabla c_i$
- This block creates conserved variable `c` and the corresponding kernels, and it splits the equations, if desired
 - f_{loc} + E_d is stored in a material property called `F`
 - κ_i is stored in a property called `kappa_c`
 - M_i is stored in a property called `M`
 - `Solve_type` determines if the equation is split
 - `direct`: No split (3rd order elements)
 - `forward_split`: New variable `chem_pot_c` is created
 - `backward_split`: Same, but residuals reversed

```
[Modules]
[./PhaseField]
[./Conserved]
[./c]
free_energy = F
kappa = kappa_c
mobility = M
solve_type = forward_split
[..]
[..]
[..]
[]
```

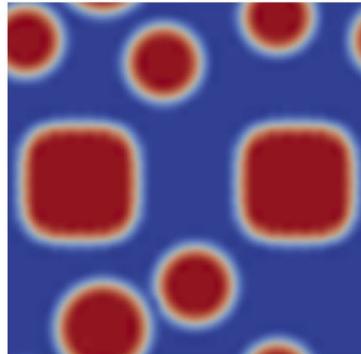
The initial stage of the microstructure is defined by the variable ICs

- There are many different ICs available in MOOSE to define your initial microstructure

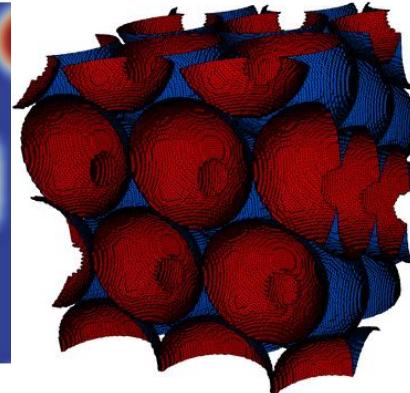
PolycrystalHexGrainIC



BimodalSuperellipsoidsIC



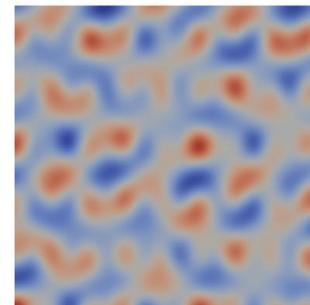
ClosePackIC



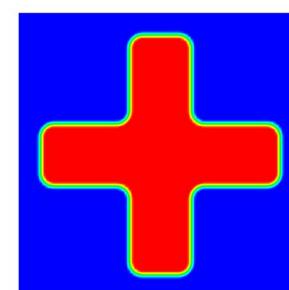
RndBoundingBoxIC



FunctionIC



CrossIC



[ICs]

[./eta_IC]

type = SmoothCircleIC

variable = eta

x1 = 200

y1 = 200

radius = 20

int_width = 7

invalue = 1

outvalue = 0.0065

[..]

[]

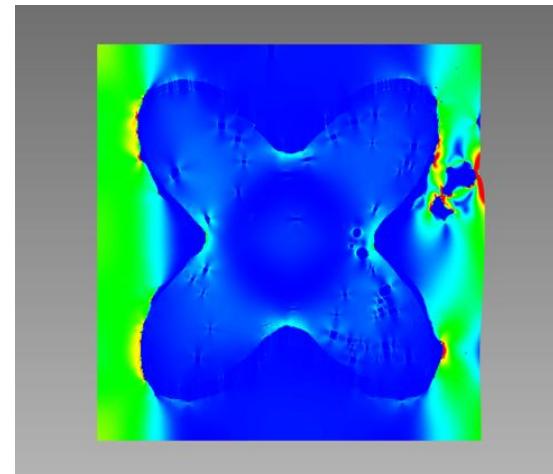
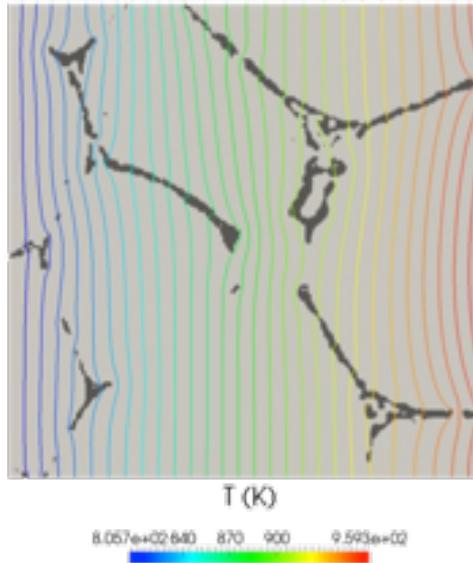
The ImageFunction can be used to create any IC you like from an image

```
[Functions]
[./image_func]
type = ImageFunction
file = Example.png
[..]
[]
```

```
[Mesh]
type = ImageFunction
file = Example.png
dim = 2
[]
```

```
[ICs]
[./var_ic]
type = FunctionIC
function = image_func
variable = var
[..]
[]
```

- Values can be read in directly from the color intensity or you can use a cut-off threshold



We need many derivatives of material properties for residuals and Jacobians

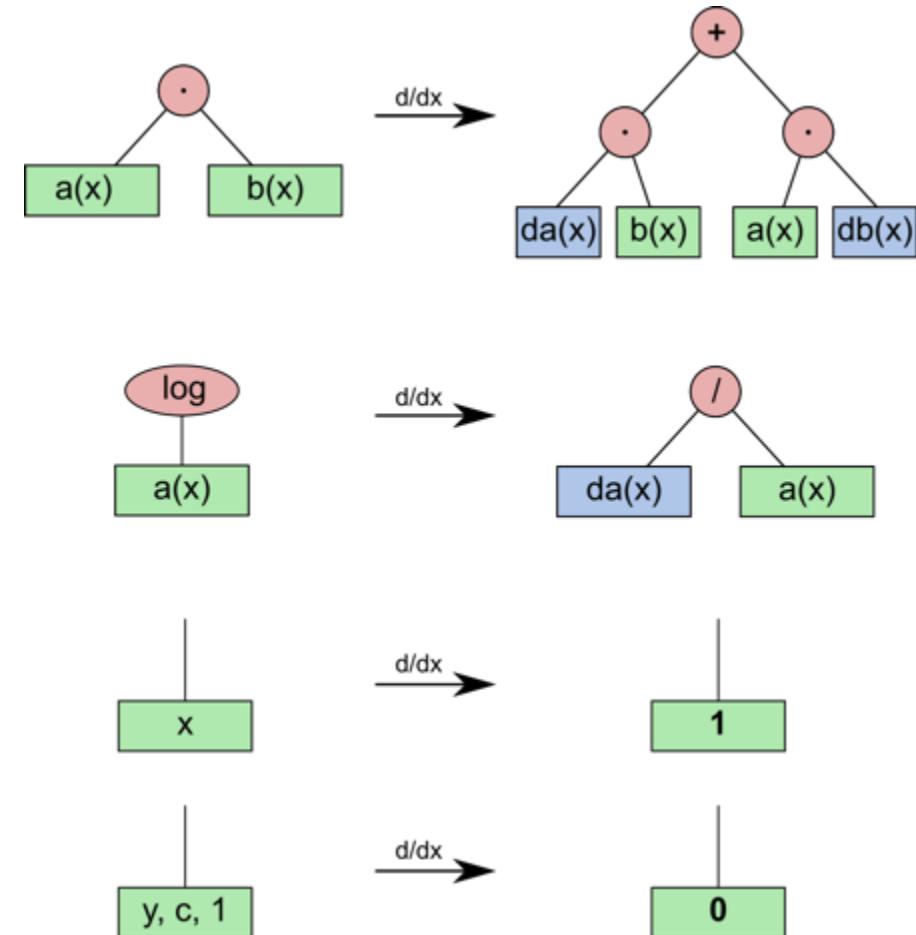
- Allen-Cahn: $\frac{\partial \eta_j}{\partial t} = -L_j \left(\frac{\partial f_{loc}}{\partial \eta_j} + \frac{\partial E_d}{\partial \eta_j} - \nabla \cdot \kappa_j \nabla \eta_j \right)$
 - $\frac{\partial f_{loc}}{\partial \eta_j}, \frac{\partial^2 f_{loc}}{\partial \eta_j^2}, \frac{\partial E_d}{\partial \eta_j}, \frac{\partial^2 E_d}{\partial \eta_j^2}, \frac{\partial L_j}{\partial \eta_j}, \dots$
- Cahn-Hilliard: $\frac{\partial c_i}{\partial t} = \nabla \cdot M_i \nabla \left(\frac{\partial f_{loc}}{\partial c_i} + \frac{\partial E_d}{\partial c_i} - \nabla \cdot \kappa_i \nabla c_i \right)$
 - $\nabla \frac{\partial f_{loc}}{\partial c_i} = \frac{\partial^2 f_{loc}}{\partial c_i^2} \nabla c_i, \frac{\partial^3 f_{loc}}{\partial c_i^3}, \nabla \frac{\partial E_d}{\partial c_i} = \frac{\partial^2 E_d}{\partial c_i^2} \nabla c_i, \frac{\partial^3 E_d}{\partial c_i^3}, \frac{\partial M_i}{\partial c_i}, \dots$
- Split Cahn-Hilliard: $\frac{\partial c_i}{\partial t} = \nabla \cdot M_i \nabla(\mu_i)$ and $\mu_i = \frac{\partial f_{loc}}{\partial c_i} + \frac{\partial E_d}{\partial c_i} - \nabla \cdot \kappa_i \nabla c_i$
 - $\frac{\partial f_{loc}}{\partial c_i}, \frac{\partial^2 f_{loc}}{\partial c_i^2}, \frac{\partial E_d}{\partial c_i}, \frac{\partial^2 E_d}{\partial c_i^2}, \frac{\partial M_i}{\partial c_i}, \dots$

DerivativeParsedMaterial ***in MOOSE defines a material property and its derivatives***

- Each MOOSE Material class can provide **multiple Material Properties**
- DerivativeParsedMaterial provides a well defined set of Material Properties
 - A function value, stored in the material property `f_name`
 - All necessary derivatives with respect to the variables `f_name` depends on
- The derivatives are regular Material Properties with an enforced naming convention
 - Example F , dF/dc , d^2F/dc^2 , $dF/deta$, $d^2F/dcdeta \dots$
 - You don't need to know the property names besides `f_name`, unless you want to look at them in the output!
- The material property `f_name` could be used as a free energy, mobility, or whatever else you need

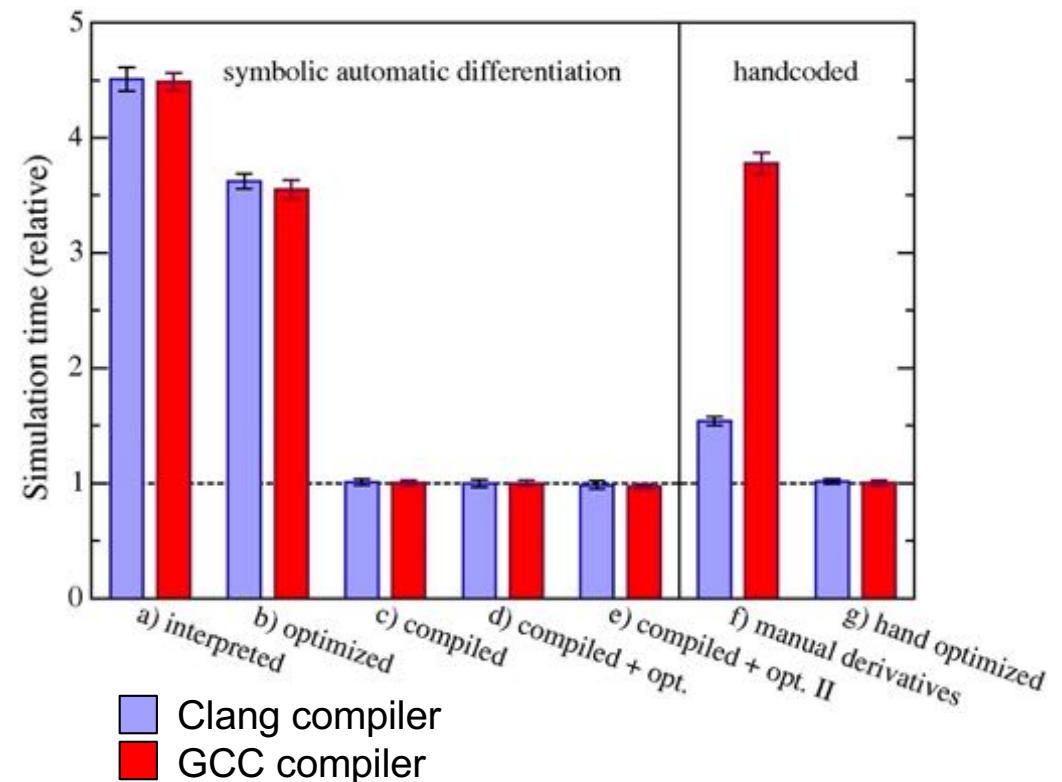
You define your functions directly in the input file and the derivatives are taken automatically

- Based on FunctionParser library
<http://warp.povusers.org/FunctionParser/>
 to allow **runtime** specification of mathematical expressions
 - Mathematical expressions become tree data structures connected by operators
 - Differentiation rules are applied recursively starting at the root of the tree
- Automatic differentiation:
 - Eliminates sources of human error
 - Conserves developer time



The interpreted functions are just as fast as compiled functions

- Just In Time (JIT) compilation speeds up the FParser functions
- ~80ms compile time per function. Results cached.
- There is no reason not to use the interpreted functions with automatic differentiation



The functions are defined in the input file using natural and straight forward syntax

- The automatic differentiation was developed specifically for phase field
- You can use:
 - Coupled non-linear and auxiliary variables
`args = 'cv ci'`
 - Material properties
`material_property_names = 'w cv_eq'`
 - Constants
`constant_names = 'T kB EfV cmveq cbveq'
constant_expressions = '1800 8.6173324e-5 3.0 exp(-EfV/(kB*T)) 1'`
 - The entire feature set of FunctionParser in MOOSE, including
 - Conditionals `if(a>b,B,C)`
 - Inline variables `y:=x^2; sin(2*y)`

Material property dependencies can be included, including derivatives

`material_property_names =`

- | | |
|-----------------------------------|--|
| <code>F</code> | A material property called F with no declared variable dependencies (i.e. vanishing derivatives) |
| <code>F(c,phi)</code> | A material property called F with declared dependence on c and phi |
| <code>d3x:=D[x(a,b),a,a,b]</code> | The third derivative $\partial^3 x / \partial a^2 \partial b$ of the a , b-dependent material property x, which will be referred to as d3x in the function expression |
| <code>dF:=D[F,c]</code> | Derivative of F w.r.t. c. Although the c-dependence of F is not explicitly declared using the round-bracket-notation, it is implicitly assumed as a derivative w.r.t. c is requested |

Example 1: Polynomial free energy function

- $f_{loc} = A(c - c_A^{eq})^2(c - c_B^{eq})^2$

```
[Materials]
[./f_loc]
  type = DerivativeParsedMaterial
  f_name = f_loc
  args = c
  function = 'A*(c - ca)^2*(c - cb)^2'
  constant_names = 'A ca cb'
  constant_expressions = '5 0.3 0.7'
[./]
```

Example 2: Ideal solution model free energy function

- $f_{loc} = E_f c + k_b T(c \ln c + (1 - c) \ln(1 - c))$
- The `plog(val,tol)` function takes the natural log, unless `val < tol` and then switches to a Taylor approximation

```
[Materials]
[./f_loc]
  type = DerivativeParsedMaterial
  f_name = f_loc
  args = 'c T'
  function = 'Ef*c + kb*T*(c*plog(c, tol) + (1 - c)*plog(1 - c, tol))'
  constant_names = 'Ef kb tol'
  constant_expressions = '1.2 8.6173303e-5 1.0e-6'
[..]
[]
```

Example 3: Free energy functional composed of a combination of other free energies

- $f_{loc} = f_A(c)(1 - h(\eta)) + f_B(c)h(\eta) + W g(\eta)$
- $f_A(c)$, $f_B(c)$, $h(\eta)$ and $g(\eta)$ would be created separately with additional DerivativeParsedMaterial blocks

```
[Materials]
[./f_loc]
  type = DerivativeParsedMaterial
  f_name = f_loc
  args = 'c eta'
  function = 'fA*(1 - h) + fB*h + W*g'
  material_property_names = 'fA(c) fB(c) h(eta) g(eta)'
  constant_variables = 'W'
  constant_expressions = '1.0'
[..]
[]
```

Example 4: Mobility that is a function of the second derivative of the free energy density

- $M = D / \frac{\partial^2 f_{loc}}{\partial c^2}$
- f_{loc} would be created by another derivative parsed material and D would be a standard material property

```
[Materials]
[./f_loc]
    type = DerivativeParsedMaterial
    f_name = f_loc
    args = 'c'
    function = 'D/D2f_loc'
    material_property_names = 'D D2f_loc:=D(f_loc, c, c)'
[..]
[]
```

MOOSE has a number of possible Boundary conditions that can be applied

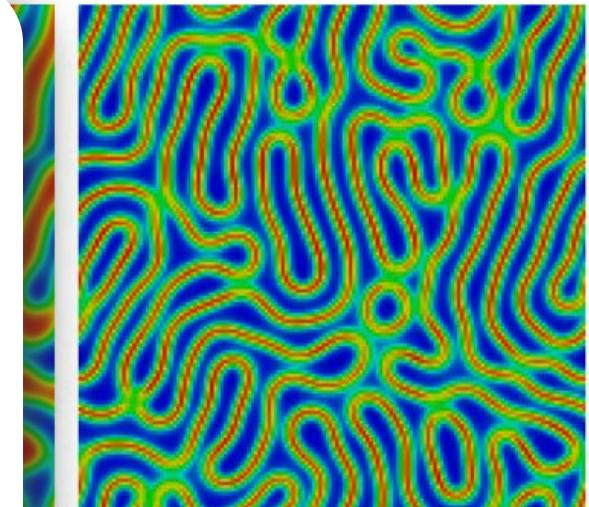
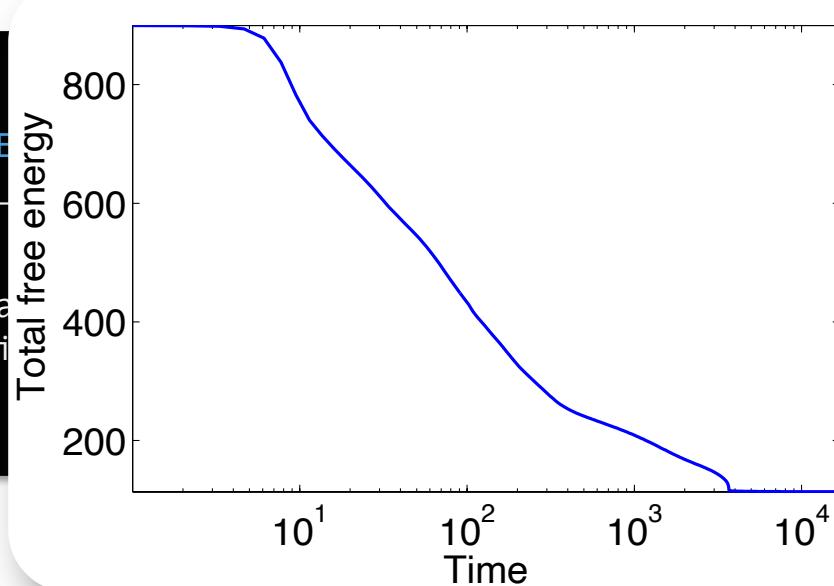
- Some of the existing boundary conditions are:
 - PresetBC – Assigns the value of a variable on a boundary
 - NeumannBC – Assigns the derivative of a variable
 - PeriodicBC – Makes a boundary periodic
- Users can also write their own BCs

```
[BCs]
[./Periodic]
[./all]
    auto_direction = 'x y'
[../]
[../]
[]
```

The TotalFreeEnergy auxkernel adds the gradient energy density to the other terms

- $f_{total} = f_{loc}(c_i, \eta_j, \dots, T) + E_d(c_i, \eta_j) + \sum_i \frac{\kappa_i}{2} (\nabla c_i)^2 + \sum_j \frac{\kappa_j}{2} (\nabla \eta_j)^2$
- The total free energy F in the system is computed using the ElementVariableIntegralPostprocessor
- **It is always a good idea to check to make sure that the total free energy is going down in your simulation**

```
[AuxKernels]
[./local_energy]
  type = TotalFreeE
  variable = local_
  f_name = fbulk
  interfacial_vars
  kappa_names = 'ka
  execute_on = 'ini
  [..]
[]
```



Free energy density

The evolving microstructure can be quantified using postprocessors

- FeatureFloodCount – A postprocessor that counts the number of distinct regions in a given variable, defined by a threshold value.
- FeatureVolumeVectorPostprocessor – A vector postprocessor that compiles accurate volumes from the FeatureFloodCount
- FeatureVolumeFraction – A postprocessor that computes the volume fraction defined by the FeatureFloodCount variable

```
[./feature_counter]
type = FeatureFloodCount
variable = c
threshold = 0.5
compute_var_to_feature_map = true
[../]
```

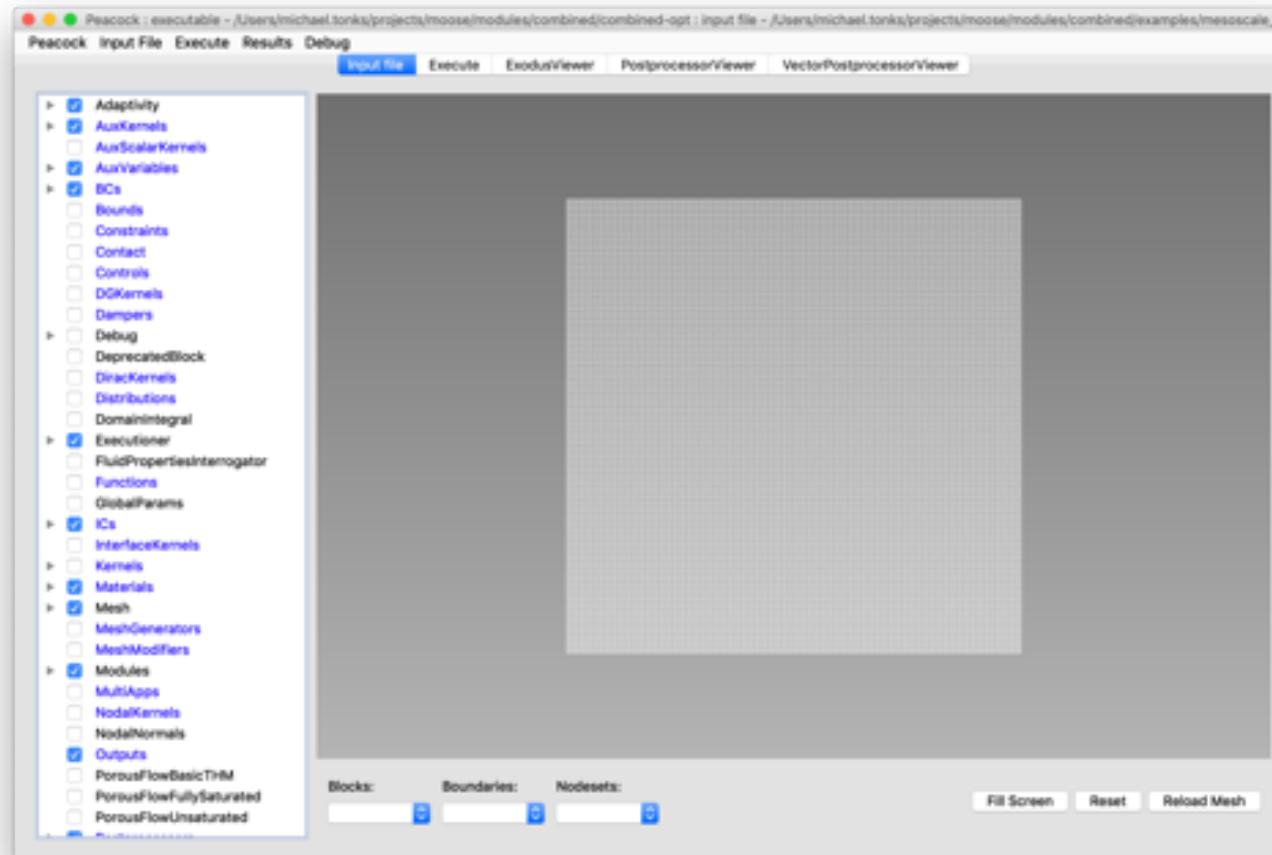
```
[VectorPostprocessors]
[./feature_volumes]
type = FeatureVolumeVectorPostprocessor
flood_counter = feature_counter
[../]
[]
```

```
[./Volume_Fraction]
type = FeatureVolumeFraction
mesh_volume = Volume
feature_volumes = feature_volumes
[../]
```

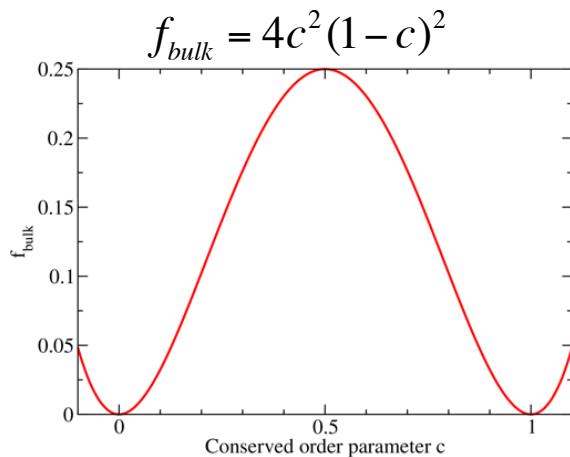
```
[./Volume]
type = VolumePostprocessor
execute_on = 'INITIAL'
[../]
```

MOOSE comes with a graphic user interface called PEACOCK

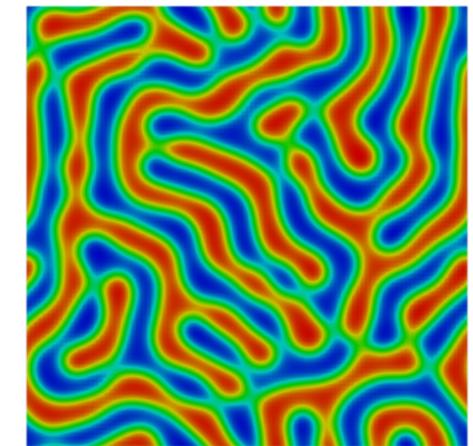
- PEACOCK simplifies the creation of input files, execution of MOOSE, and visualization of results



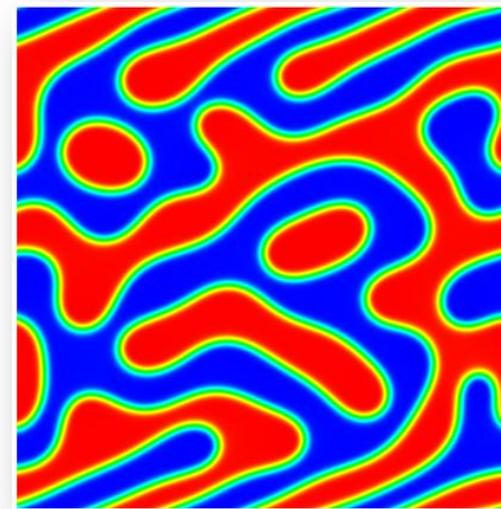
To summarize, the phase field method is a useful tool and MOOSE makes it easy



```
[Materials]
[./f_loc]
type = DerivativeParsedMaterial
f_name = f_loc
args = c
function = '4.0*c^2*(c - 1)^2'
[./]
```

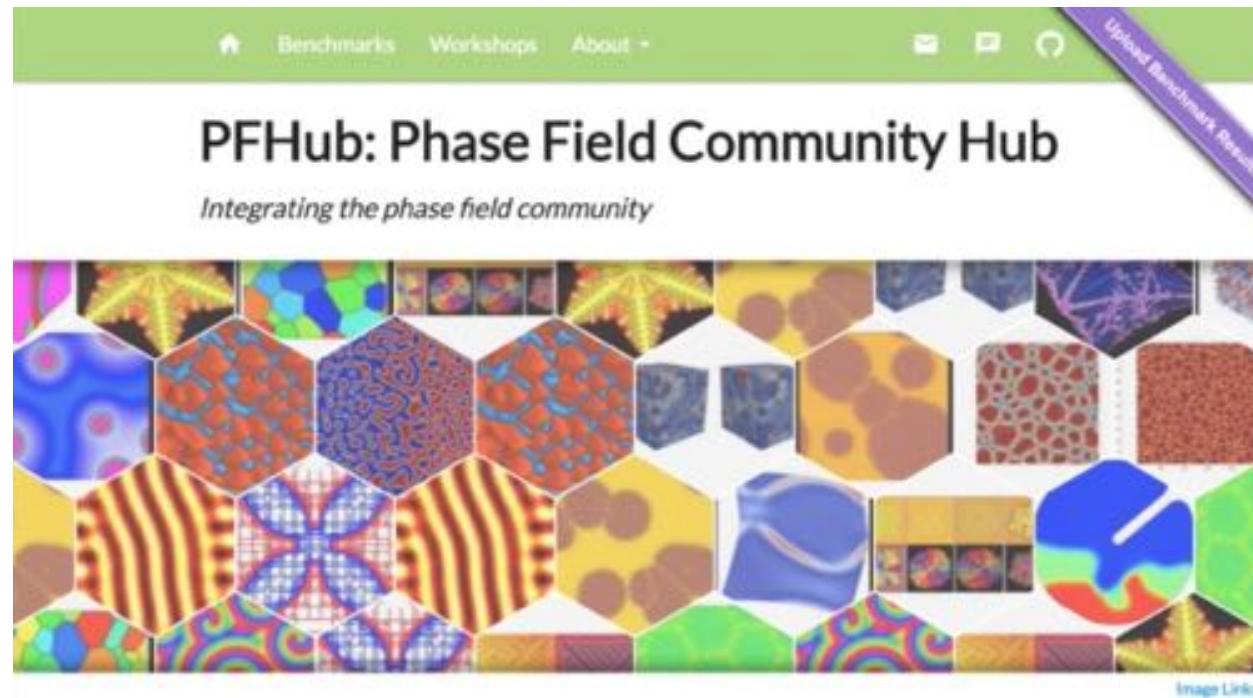


First example problem



CHiMaD/NIST Spinodal Decomposition Benchmark Problem

- <https://pages.nist.gov/pfhub/benchmarks/benchmark1.ipynb/>



Welcome to the PFHub! If you're a beginner, you'll soon find resources and a crash course on the technique. If you're an expert, you'll find tools to verify and showcase the quality of your simulations. If you're anywhere in-between, you'll find a community built around a shared interest in phase-field and a commitment to opening up our research for the benefit of all.

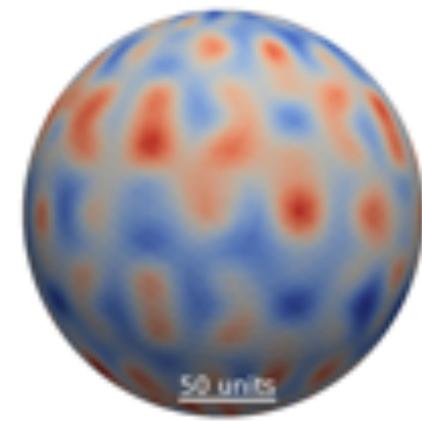
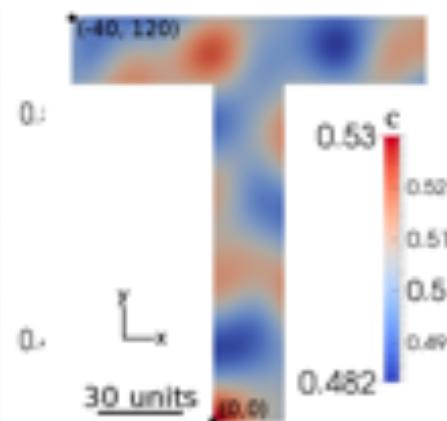
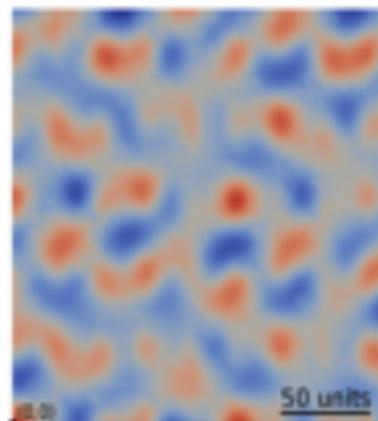
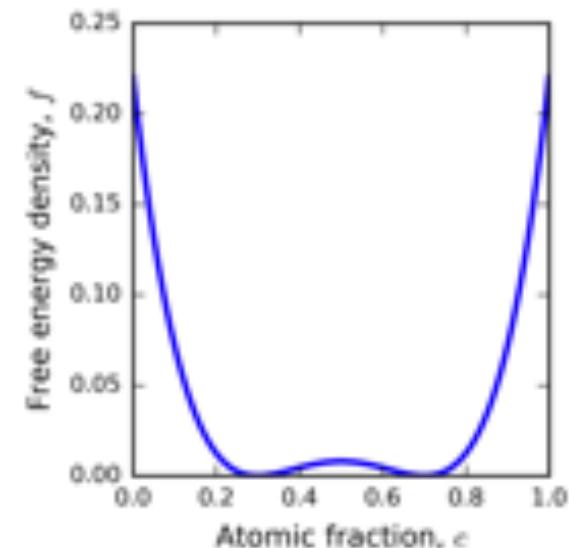
CHiMaD/NIST Spinodal Decomposition Benchmark Problem

One
conserved
order
parameter

$$F = \int_V \left(f_{chem}(c) + \frac{\kappa}{2} |\nabla c|^2 \right) dV$$

$$f_{chem}(c) = \rho_s (c - c_\alpha)^2 (c - c_\beta)^2$$

$$\frac{\partial c}{\partial t} = \nabla \cdot \left\{ M \nabla \left(\frac{\partial f_{chem}}{\partial c} - \kappa \nabla^2 c \right) \right\}$$



Domains
and initial
conditions

Input File Blocks – Mesh and ICs

```
[Mesh]
  type = GeneratedMesh
  xmax = 200
  ymax = 200
  nx = 200
  ny = 200
  dim = 2
[]

[ICs]
  [./c_IC]
    type = FunctionIC
    variable = c
    function = '0.5 + 0.01*(cos(0.105*x)*cos(0.11*y)
                  + (cos(0.13*x)*cos(0.087*y))^2
                  + cos(0.025*x - 0.15*y)*cos(0.07*x - 0.02*y)'
  [..]
[]
```

Input File Blocks – Actions and Materials

```
[Modules]
  [./PhaseField]
    [./Conserved]
      [./c]
        free_energy = F
        kappa = kappa
        mobility = M
        solve_type = FORWARD_SPLIT
      [../../]
    [../../]
  [../../]
[]
```

```
[Materials]
  [./constant_props]
    type = GenericConstantMaterial
    prop_names = 'kappa M'
    prop_values = '2 5'
  [../../]
  [./F_mat]
    type = DerivativeParsedMaterial
    f_name = F
    args = c
    function = 'A*(c-ca)^2*(c-cb)^2'
    constant_names = 'A ca cb'
    constant_expressions = '5 0.3 0.7'
  [../../]
[]
```

Input File Blocks – AuxKernels and BCs

```
[AuxVariables]
[./Fdens]
    order = CONSTANT
    family = MONOMIAL
[...]
[]

[AuxKernels]
[./Fdens]
    type = TotalFreeEnergy
    variable = Fdenc
    interfacial_vars = c
    kappa_names = kappa
    f_name = F
    execute_on = TIMESTEP_END
[...]
[]

[BCs]
[./Periodic]
[./All]
    auto_direction = 'x y'
[...]
[...]
[]
```

Input File Blocks – Preconditioning, Executioner and Outputs

```
[Executioner]
  type = Transient
  solve_type = NEWTON
  scheme = BDF2
  petsc_options_iname = '-pc_type
                        -sub_pc_type
                        -pc_asm_overlap'
  petsc_options_value = 'asm lu 2'
  nl_max_its = 12
  l_max_its = 40
  l_tol = 1e-5
  nl_rel_tol = 1e-6
  end_time = 1e6

[./TimeStepper]
  type = IterationAdaptiveDT
  dt = 0.05
  growth_factor = 1.1
  cutback_factor = 0.8
  optimal_iterations = 6
[...]
[]
```

```
[Preconditioning]
  [./SMP]
    type = SMP
    full = true
  [...]
[]

[Outputs]
  exodus = true
  csv = true
  perf_graph = true
[]
```