

Multiphase KKS model with crystal plasticity in Moose

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1 Introduction

This document contain notes on the implementation of the phase field model presented in [1] in Moose. The following special notation of volume and surface integrals will be used, in accordance with the official Moose documentation;

$$\int a \cdot b \, dV = (a, b), \quad \int a \cdot b \, dS = \langle a, b \rangle \quad (1)$$

The sets of phase field variables and phase compositions are denoted $\boldsymbol{\eta}$ and \boldsymbol{x} , respectively. The global concentration field is denoted c and h denotes the switching functions. The phase fields, phase compositions and the global concentration are all dimensionless fields in the range $[0, 1]$.

2 Model

2.1 Free energy

The free energy is given by

$$F = f^{ch}(\boldsymbol{\eta}, \boldsymbol{x}) + f^{int}(\boldsymbol{\eta}) + f^d(\boldsymbol{\eta}, \dots), \quad (2) \quad \{\{\text{eq:F}\}\}$$

with f^{ch} and f^{int} representing the chemical and interface energies respectively. f^d represents the contribution from any other physics included in the model e.g. deformation, temperature, electric field etc.

Here we take

$$f^{ch} = \sum_i h_i(\boldsymbol{\eta}) f_i(x_i, \boldsymbol{\eta}), \quad (3) \quad \{\{\text{eq:fch}\}\}$$

with $f_i(x_i, \boldsymbol{\eta}) = \frac{G_i(x_i)}{V^m}$ where G_i is a representation of the Gibbs energy of phase i and V^m denotes the molar volume which is assumed to be constant. The interface energy is taken as

$$f^{int} = m \left(\sum_i \left(\frac{\eta_i^4}{4} - \frac{\eta_i^2}{2} \right) + \sum_i \sum_{j \neq i} \frac{\beta}{2} \eta_i^2 \eta_j^2 + \frac{1}{4} \right) + \frac{\alpha}{2} \sum_i (\nabla \eta_i)^2, \quad (4) \quad \{\text{eq:fint}\}$$

with m , α and β being parameters.

The energy due to deformation is taken as

$$f^d = \sum_i h_i f_i^d \quad (5)$$

where

$$f_i^d = \frac{1}{2} \mathbf{T}_i : \mathbf{E}_i^e \quad (6)$$

for the elastic phases (Cu and Cu₆Sn₅). For the phases where plasticity is included (Sn) the deformation energy is

$$f_i^d = \frac{1}{2} \mathbf{T}_i : \mathbf{E}_i^e + \frac{1}{2} Q_i \sum_{\alpha}^n \sum_{\beta}^n q_{\alpha\beta} s_i^{\alpha} s_i^{\beta} \quad (7)$$

where \mathbf{T} is the second Piola-Kirchoff stress tensor, \mathbf{E}^e is the elastic Green strain tensor, Q is a hardening parameter, and s^{α} is the slip resistance on the α slip system and the sum is taken over all n slip systems. More details on the mechanical model are given in Section 2.5.

2.2 Governing equations

2.2.1 KKS conditions

KKS models require the chemical potential to be equal in all coexisting phases, i.e.

$$\frac{\partial F}{\partial c} = \frac{\partial f_1^{ch}}{\partial x_1} + \frac{\partial f_1^d}{\partial x_1} = \dots = \frac{\partial f_n^{ch}}{\partial x_n} + \frac{\partial f_n^d}{\partial x_n} = \mu_1 \dots = \mu_n. \quad (8) \quad \{\text{eq:KKS}\}$$

Furthermore, mass conservation is fulfilled by

$$c = \sum_i h_i x_i. \quad (9) \quad \{\text{eq:mass}\}$$

Q should be related to something in the equations for γ or s

2.2.2 Cahn-Hilliard equation

The evolution of the concentration field follows the Cahn-Hilliard equation

$$\frac{\partial c}{\partial t} = \nabla \cdot M(\boldsymbol{\eta}, c) \nabla \frac{\delta F}{\delta c} = \nabla \cdot M(\boldsymbol{\eta}, c) \nabla \left(\frac{\partial F}{\partial c} - \nabla \cdot \frac{\partial F}{\partial \nabla c} \right), \quad (10) \quad \{\{\text{eq:CH1}\}\}$$

where M is the mobility. Since there is no dependence on ∇c in the free energy the divergence term of Eq. (10) vanishes.¹

Using Eq. (2), Eq. (3) and Eq. (4) the derivative become

$$\frac{\partial F}{\partial c} = \frac{\partial f^{ch}}{\partial c} + \frac{\partial f^d}{\partial c} = \sum_i h_i \frac{\partial f_i}{\partial x_i} \frac{\partial x_i}{\partial c} + \cancel{\frac{\partial h_i}{\partial c} f_i}^0 + \frac{\partial f^d}{\partial c}. \quad (11) \quad \{\{\text{eq:dFdc1}\}\}$$

By taking the derivative of the mass conservation Eq. (9) we get

$$\frac{\partial c}{\partial c} = \sum_i h_i \frac{\partial x_i}{\partial c} = 1. \quad (12)$$

Inserting into Eq. (11) and taking into account Eq. (8) we end up with

$$\frac{\partial F}{\partial c} = \mu, \quad (13)$$

where we can arbitrarily choose $\mu = \mu_i$ based on the KKS condition. With this Eq. (10) can be written as

$$\frac{\partial c}{\partial t} = \nabla \cdot M(\boldsymbol{\eta}, c) \nabla \mu_i \quad (14) \quad \{\{\text{eq:CH}\}\}$$

The mobility M is taken as

$$M = \sum_i h_i \frac{D_i}{\frac{d^2 f_i}{dx_i^2}}. \quad (15)$$

The units of Eq. (14) are

$$\frac{1}{s} = \frac{1}{m} \frac{\frac{m^2}{s}}{\frac{J}{m^3}} \frac{1}{m} \frac{J}{m^3} = \frac{1}{s}. \quad (16)$$

¹This is only true for KKS models, in other multiphase models a term like $\kappa(\nabla c)^2$ is included. This term will make the Cahn-Hilliard a fourth order PDE.

This only works if $\frac{\partial f_i}{\partial x_i} = 0$

2.2.3 Allen-Cahn equation

The evolution of each order parameter field follow the Allen-Cahn equation

$$\begin{aligned}\frac{\partial \eta_i}{\partial t} &= -L(\boldsymbol{\eta}) \frac{\delta F}{\delta \eta_i} + \xi(\mathbf{x}, t) = -L \left(\frac{\partial F}{\partial \eta_i} - \nabla \cdot \frac{\partial F}{\partial \nabla \eta_i} \right) + \xi(\mathbf{x}, t) \\ &= -L \left(\frac{\partial f^{ch}}{\partial \eta_i} + \frac{\partial f^{int}}{\partial \eta_i} + \frac{\partial f^d}{\partial \eta_i} - \nabla \cdot \frac{\partial f^{int}}{\partial \nabla \eta_i} - \nabla \cdot \frac{\partial f^d}{\partial \nabla \eta_i} \right) + \xi(\mathbf{x}, t),\end{aligned}\quad (17) \quad \{\text{eq:AC1}\}$$

where $\xi(\mathbf{x}, t)$ is a Langevin force term used to simulate nucleation, see Section 2.3. The derivatives of the interface energy are easy to calculate from Eq. (4)

$$\frac{\partial f^{int}}{\partial \eta_i} - \nabla \cdot \frac{\partial f^{int}}{\partial \nabla \eta_i} = m \left(\eta_i^3 - \eta_i + 2\beta \eta_i \sum_{j \neq i} \eta_j^2 \right) - \nabla \cdot \alpha \nabla \eta_i. \quad (18)$$

The derivative of the chemical energy is

$$\frac{\partial f^{ch}}{\partial \eta_i} = \sum_j \left(\frac{\partial h_j}{\partial \eta_i} f_j + h_j \frac{\partial f_j}{\partial \eta_i} \right), \quad (19) \quad \{\text{eq:dfchdeta}\}$$

where

$$h_j \frac{\partial f_j}{\partial \eta_i} = h_j \underbrace{\frac{\partial f_j}{\partial G_j} \frac{\partial G_j}{\partial x_j} \frac{\partial x_j}{\partial h_j} \frac{\partial h_j}{\partial \eta_i}}_{\mu_j} = \mu_j h_j \frac{\partial x_j}{\partial h_j} \frac{\partial h_j}{\partial \eta_i}. \quad (20) \quad \{\text{eq:dfjdetai}\}$$

Using that $\frac{\partial c}{\partial \eta_i} = 0$, equation Eq. (9) then gives

$$\begin{aligned}\frac{\partial c}{\partial \eta_i} &= \sum_j \left(\frac{\partial h_j}{\partial \eta_i} x_j + h_j \frac{\partial x_j}{\partial h_j} \frac{\partial h_j}{\partial \eta_i} \right) = \sum_j \frac{\partial h_j}{\partial \eta_i} \left(x_j + h_j \frac{\partial x_j}{\partial h_j} \right) = 0 \\ &\iff \sum_j h_j \frac{\partial x_j}{\partial h_j} \frac{\partial h_j}{\partial \eta_i} = - \sum_j \frac{\partial h_j}{\partial \eta_i} x_j.\end{aligned}\quad (21)$$

Only works for $\frac{\partial f_i^d}{\partial x_i} = 0$

By making use of the KKS condition Eq. (19) can then be written

$$\frac{\partial f^{ch}}{\partial \eta_i} = \sum_j \frac{\partial h_j}{\partial \eta_i} (f_j - \mu_j x_j) \quad (22)$$

For the deformation energy we get

$$\frac{\partial f^d}{\partial \eta_i} = \sum_j \frac{\partial h_j}{\partial \eta_i} f_j^d + h_j \cancel{\frac{\partial f_j^d}{\partial \eta_i}} \quad (23)$$

for $\frac{\partial f^d}{\partial x_i} = 0$

Equation Eq. (17) now becomes

$$\frac{\partial \eta_i}{\partial t} = -L \left(\sum_j \frac{\partial h_j}{\partial \eta_i} (f_j - \mu_j x_j + f_j^d) + m \left(\eta_i^3 - \eta_i + 2\beta \eta_i \sum_{j \neq i} \eta_j^2 \right) - \nabla \cdot \alpha \nabla \eta_i \right) + \xi(\mathbf{x}, t). \quad (24) \quad \{\text{eq:AC}\}$$

The mobility L is taken as

$$L(\boldsymbol{\eta}) = \frac{\sum_i \sum_{j \neq i} L_{ij} \eta_i^2 \eta_j^2}{\sum_i \sum_{j \neq i} \eta_i^2 \eta_j^2}. \quad (25)$$

L_{ij} is taken as

$$L_{ij} = \frac{2m}{3\alpha (x_i^{eq} - x_j^{eq})^2} \frac{M_i + M_j}{2}, \quad (26) \quad \{\text{eq:lab}\}$$

where $M_i = \frac{D_i}{\frac{d^2 f_i}{dx_i^2}}$ and $M_j = \frac{D_j}{\frac{d^2 f_j}{dx_j^2}}$ are the mobilities and x_i^{eq} and x_j^{eq} are the equilibrium molar fractions of phases i and j respectively.

The units of Eq. (24) are

$$\frac{1}{s} = \frac{\frac{J}{m^3} \frac{m^2}{s}}{\frac{J}{m} \frac{J}{m^3}} \frac{J}{m^3} = \frac{1}{s}. \quad (27)$$

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2.3 Nucleation

Nucleation of the intermetallic phases is achieved using the so called Langevin force approach where a small pertubation, ξ , is added to the Allen-Cahn equations to initiate the evolution of the phase fields. Following [2] the perturbation is taken as

$$\xi(\mathbf{x}, t) = \sqrt{\frac{2k_B T L}{\lambda^d \Delta t}} \rho, \quad (28)$$

where k_B is the Boltzmann constant, T is temperature, λ is the grid spacing, d is the dimensionality of the grid (1, 2 or 3 for 1D, 2D or 3D), Δt is the timestep, and ρ is a random number drawn from a Gaussian distribution that satisfies $\langle \rho_i \rangle = 0$ and $\langle \rho_i \rho_j \rangle = \delta_{ij}$.

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2.4 Non-constant molar volume

I'm not sure it is possible to easily remove the assumption of constant molar volume. It is certainly not as easy as I thought before. For non-constant molar volume Eq. (9) becomes $c = \sum_i h_i \frac{x_i}{V_i^m}$ which converts c to units of mol m^{-3} . The problem is that the free energy is formulated in units of J m^{-3} , which means that $\frac{\partial F}{\partial c}$ get the units J mol^{-1} . I don't think this is good neither for the KKS conditions nor for the Cahn-Hilliard equation. Perhaps we can formulate the Eq. (14) as

$$\frac{1}{V^m} \frac{\partial c}{\partial t} = \nabla \cdot M(\boldsymbol{\eta}, c) \nabla \mu_i \quad (29)$$

together with the mass balance in Eq. (9) and still have c dimensionless. Then the question is how to choose V^m ?

Another way is maybe to formulate the energies in J mol^{-1} but then I guess the mesh will represent a certain number of moles instead of a certain volume?

2.5 Crystal plasticity

{sec:crypla}

The crystal plasticity model implemented in Moose is from Zhao et al. [3]. The deformation gradient \mathbf{F} is decomposed into an elastic part \mathbf{F}^e and a plastic part \mathbf{F}^p according to

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p. \quad (30)$$

The evolution of the plastic velocity gradient is given by

$$\dot{\mathbf{F}}^p \mathbf{F}^{p-1} = \sum_{\alpha}^n \dot{\gamma}^{\alpha} \mathbf{m}^{\alpha} \otimes \mathbf{n}^{\alpha}, \quad (31)$$

where $\dot{\gamma}^{\alpha}$, \mathbf{m}^{α} , and \mathbf{n}^{α} denotes the slip rate, slip direction, and slip plane normal on slip system α . The flow rule for the slip rate is

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left| \frac{\tau^{\alpha}}{s^{\alpha}} \right|^{1/m} \text{sgn}(\tau^{\alpha}) \quad (32)$$

where γ_0 is a reference slip rate, τ^{α} is the resolved shear stress, s^{α} is the slip resistance, and m controls the strain rate sensitivity. The evolution of the slip resistance is described by

$$\dot{s}^{\alpha} = \sum_{\beta}^n h^{\alpha\beta} |\dot{\gamma}^{\beta}|, \quad (33)$$

with the hardening matrix taken as

$$h^{\alpha\beta} = q^{\alpha\beta} h_0 \left| 1 - \frac{s^\beta}{s_s} \right|^c \operatorname{sgn}\left(1 - \frac{s^\beta}{s_s}\right), \quad (34)$$

where s_s is the saturation value for the slip resistance, h_0 and c are constants, and $q_{\alpha\beta} = 1 + 0.4\delta_{\alpha\beta}$ controls the ratio between self ($\alpha = \beta$) and cross ($\alpha \neq \beta$) hardening.

2.6 Weak form residual equations

The weak form of the residual equation for η_i is constructed from Eq. (17) by multiplication with a test function ψ and integrating over the domain:

$$\begin{aligned} \mathbf{R}_{\eta_i} &= \left(\frac{\partial \eta_i}{\partial t}, \psi \right) + \left(L \left(\frac{\partial f^{ch}}{\partial \eta_i} + \frac{\partial f^{int}}{\partial \eta_i} + \frac{\partial f^d}{\partial \eta_i} \right), \psi \right) - (L \nabla \cdot \alpha \nabla \eta_i, \psi) - (\xi, \psi) \\ &= \left(\frac{\partial \eta_i}{\partial t}, \psi \right) + \left(L \left(\frac{\partial f^{ch}}{\partial \eta_i} + \frac{\partial f^{int}}{\partial \eta_i} + \frac{\partial f^d}{\partial \eta_i} \right), \psi \right) + (\alpha \nabla \eta_i, \nabla L \psi) \\ &\quad - (\xi, \psi) - \langle (\alpha \nabla \eta_i) \cdot \mathbf{n}, L \psi \rangle = \mathbf{0}, \end{aligned} \quad (35)$$

with the divergence theorem used on the gradient term. Inserting the derivatives calculated above gives

$$\begin{aligned} \mathbf{R}_{\eta_i} &= \left(\frac{\partial \eta_i}{\partial t}, \psi \right) + \left(L \sum_j \frac{\partial h_j}{\partial \eta_i} f_j, \psi \right) - \left(L \frac{\partial h_j}{\partial \eta_i} \mu_j x_j, \psi \right) \\ &\quad + \left(L m \left(\eta_i^3 - \eta_i + 2\beta \eta_i \sum_{j \neq i} \eta_j^2 \right), \psi \right) + \left(L \sum_j \frac{\partial h_j}{\partial \eta_i} f_j^d, \psi \right) \\ &\quad + (\alpha \nabla \eta_i, \nabla L \psi) - \langle (\alpha \nabla \eta_i) \cdot \mathbf{n}, L \psi \rangle - (\xi, \psi) = \mathbf{0} \end{aligned} \quad (36)$$

The Cahn-Hilliard equation Eq. (14) can be solved in two ways. Either you can solve it directly using the residual

$$\begin{aligned} \mathbf{R}_c &= \left(\frac{\partial c}{\partial t}, \psi \right) - (\nabla \cdot M \nabla \mu, \psi) = \\ &\quad \left(\frac{\partial c}{\partial t}, \psi \right) + (M \nabla \mu, \nabla \psi) - \langle M \nabla \mu \cdot \mathbf{n}, \psi \rangle = \mathbf{0}. \end{aligned} \quad (37)$$

This seems to be fairly straight forward, but for some reason it is “not fully implemented” in Moose. Instead, the equation is split into two and solved

for the concentration c as well as for the chemical potential μ . The residuals for this are

$$\mathbf{R}_\mu = \left(\frac{\partial c}{\partial t}, \psi \right) + (M \nabla \mu, \nabla \psi) - \langle M \nabla \mu \cdot \mathbf{n}, \psi \rangle = \mathbf{0} \quad (38)$$

$$\mathbf{R}_c = \left(\frac{\partial F}{\partial c} - \mu, \psi \right) = \mathbf{0}. \quad (39)$$

The residual for the mechanical equilibrium equations are given by

$$\left(\rho_0 \frac{d^2 \mathbf{u}}{dt^2}, \psi \right) - (\boldsymbol{\sigma}, \nabla \psi) + \langle \boldsymbol{\sigma} \cdot \mathbf{n}, \psi \rangle = \mathbf{0}, \quad (40)$$

where \mathbf{u} denotes displacements and $\boldsymbol{\sigma} = \sum_j h_j \boldsymbol{\sigma}_j$ is the global Cauchy stress calculated from the stress in each phase.

3 Implementation

This section describes the input file used to run the simulation. Moose input files consists of different blocks which together defines the model. All necessary blocks are described below.

3.1 Mesh

The mesh block can be used to create meshes of simple geometries. It can also be used to read the mesh from a file. A rectangular 2D mesh is created like this:

```
[Mesh]
  type = GeneratedMesh
  dim = 2
  nx = 100
  ny = 10
  xmax = 0.304 # Length
  ymax = 0.0257 # Height
  displacements = 'disp_x disp_y'
[] .
```

By specifying the displacements in the mesh block results can be visualized in the deformed configuration. For this to work the displacement variables must be called `disp_`.

3.2 Variables

The `Variables` block declares the variables of the model. A variables is defined like this:

```
[Variables]
# concentration Sn
[./c] # Variable name
      order = FIRST
      family = LAGRANGE
[../]
[]
```

To solve the model the following variables are needed: c , μ , x_i , η_i , u_x , u_y , and u_z i.e. a 3D simulation with three grains of different phases contains 11 variables.

3.3 ICs and BCs

Initial conditions can be set in the `ICs` block. For simple initial conditions the type `FunctionIC` can be used. The following code will initiate the variable η_{imc} as a ring with radius 8 centered at (20, 20).

```
[ICs]
[./eta2] #Cu6Sn5
      variable = eta_imc
      type = FunctionIC
      function = 'r:=sqrt((x-20)^2+(y-20)^2);if(r>8&r<=16,1,0)'
[../]
[]
```

There are some more complicated initial conditions already implemented but probably I'll have to make something myself.

Boundary conditions are set in the `BCs` block using a very similar syntax as the `ICs`.

3.4 Kernels

In Moose each part of the residual equations are implemented in separate kernels. Each kernel is responsible for evaluating the residual and (optionally) calculate the Jacobian. For each of the Allen-Cahn equations the kernels in Table 1 is needed. For the Cahn-Hilliard equation and the KKS conditions the kernels in Table 2 are needed.

Table 1: Kernels needed for the Allen-Cahn equation

{tab:AC}

| Residual term | Parameters | Kernel name |
|---|-------------|--|
| $\left(\frac{\partial \eta_i}{\partial t}, \psi\right)$ | | <code>TimeDerivative</code> |
| $\left(L \sum_j \frac{\partial h_j}{\partial \eta_i} f_j + w \frac{\partial g}{\partial \eta_i}, \psi\right)$ | $L, w = 0$ | <code>KKSMultiACBulkF²</code> |
| $-\left(L \frac{\partial h_j}{\partial \eta_i} \mu_j x_j, \psi\right)$ | L | <code>KKSMultiACBulkC</code> |
| $\left(L \frac{\partial f^d}{\partial \eta_i}, \psi\right)$ | | |
| $\left(L m \left(\eta_i^3 - \eta_i + 2\beta \eta_i \sum_{j \neq i} \eta_j^2\right), \psi\right)$ | m, β | <code>ACGrGrMulti</code> |
| $(\alpha \nabla \eta_i, \nabla L \psi)$ | L, α | <code>ACInterface</code> |
| (ξ, ψ) | | <code>LangevinNoise</code> |

Table 2: Kernels needed for the split version of the Cahn-Hilliard equation and the KKS conditions

{tab:CH}

| Residual term | Parameters | Kernel name |
|--|------------|---|
| $\left(\frac{\partial c}{\partial t}, \psi\right)$ | | <code>CoupledTimeDerivative</code> |
| $(M \nabla \mu, \nabla \psi)$ | M | <code>SplitCHWRes</code> |
| $\left(\frac{\partial F}{\partial c} - \mu, \psi\right)$ | | <code>KKSSplitCHCRes</code> |
| $\mu = \mu_i = \mu_j$ | | <code>KKSPHaseChemicalPotential</code> |
| $c = \sum_i h_i x_i$ | | <code>KKSMultiPhaseConcentration</code> |

3.5 Materials

The free energies and the switching functions are defined in the `Materials` block of the input file. The chemical free energy of each phase can be described using the type `DerivativeParsedMaterial`. This type uses automatic differentiation to calculate the derivatives.

```
[Materials]
  [./fch_cu] #Chemical energy Cu phase
    type = DerivativeParsedMaterial
    f_name = fch_cu
    args = 'c_cu'
    function = '20*(c_cu-0.1)^2'
  [./]
[]
```

²This kernel includes a double well that can be use to constrain the order parameters to $[0, 1]$, turn off the double well by setting $w = 0$.

The switching functions are set like

```
[./h_cu]
    type = SwitchingFunctionMultiPhaseMaterial
    h_name = h_cu
    all_etas = 'eta_cu eta_imc eta_sn'
    phase_etas = eta_cu
[../]
```

The same switching function can be used to describe all grain of the same phase (I think).

The materials block can also be used to define constants. For example

```
[./constants]
    type = GenericConstantMaterial
    prop_names = 'L kappa gamma mu tgrad_corr_mult'
    prop_values = '1. 0.5 0.5 1. 0.'
[../]
```

3.6 Executioner, Preconditioning and Outputs

The parameters of the solver are set in the **Executioner**, **Preconditioning** and **Outputs** blocks, here you can also set options for the behavior of the underlying PETSc commands. The blocks can look something like this

```
[Executioner]
    type = Transient
    solve_type = 'PJFNK'
    petsc_options_iname = '-pc_type -sub_pc_type -sub_pc_factor_shift_type'
    petsc_options_value = 'asm          ilu          nonzero'
    l_max_its = 30
    nl_max_its = 10
    l_tol = 1.0e-4
    nl_rel_tol = 1.0e-10
    nl_abs_tol = 1.0e-11

    num_steps = 100
    dt = 0.5
[]

[Preconditioning]
    active = 'full'
```

```

[./full]
  type = SMP
  full = true
[../]
[./mydebug]
  type = FDP
  full = true
[../]
[]

[Outputs]
  exodus = true
[]

```

These settings will solve the equations using the Pre-Conditioned Jacobian-Free Newton-Krylow method which is the standard way in Moose. The results will be written to a file that can be viewed in e.g. Peacock or Paraview.

References

- [1] Johan Hektor, Matti Ristinmaa, Håkan Hallberg, Stephen A Hall, and Srinivasan Iyengar. Coupled diffusion-deformation multiphase field model for elastoplastic materials applied to the growth of Cu₆Sn₅. *Acta Materialia*, 108:98–109, 2016.
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- [3] L Zhao, P Chakraborty, MR Tonks, and I Szlufarska. On the plastic driving force of grain boundary migration: A fully coupled phase field and crystal plasticity model. *Computational Materials Science*, 128:320–330, 2017.