PRISMS-PF Application Formulation: additive_manufacturing

This example application implements a simple set of governing equations for isotropic solidification and grain growth, with an accompanying temperature evolution equation. The model is a simplified version of the one in the following publication:
Phase-field modeling of grain evolutions in additive manufacturing from nucleation, growth, to coarsening, Yang, M., Wang, L. & Yan, W., *npj Comput Mater* 7, 56 (2021).

Consider a free energy expression of the form:

$$F = \int_{\Omega} \left(f_{\text{phase}} + f_{\text{grain}} + f_{\text{gradient}} \right) dV \tag{1}$$

where f_{phase} and f_{grain} represent contributions to the free energy density due to interfaces between the liquid and the solid phases, and contributions from the grain boundary interfaces, respectively. f_{gradient} captures the gradient contributions from the inter-grain and inter-state interfaces.

$$f_{\text{phase}} = m_p \left\{ (1-\xi)^2 \phi + \xi^2 (1-\phi) \right\} \tag{2}$$

$$f_{\text{grain}} = m_g \left\{ \sum_{i=1}^{n} \left(\frac{\eta_i^4}{4} - \frac{\eta_i^2}{2} \right) + \gamma \sum_{i=1}^{n} \sum_{j\neq i} \eta_i^2 \eta_j^2 + \frac{1}{4} (1-\xi)^2 \sum_{i=1}^{n} \eta_i^2 \right\} \tag{3}$$

$$f_{\text{gradient}} = \frac{\kappa_p}{2} (\nabla \xi)^2 + \frac{\kappa_g}{2} (\nabla \eta_i)^2 \tag{4}$$

where η_i is one of N structural order parameters that describe the solid grains, ξ is am order parameter that describes solid/liquid states; $\xi = 0$ in the liquid state and $\xi = 1$ in the solid state. γ is the grain interaction coefficient, and κ is the gradient energy coefficient.

1 Variational treatment

The driving force for grain evolution is determined by the variational derivative of the total energy with respect to each order parameter:

$$\mu_g = \frac{\delta F}{\delta \eta_i} = m_g \left(-\eta_i + \eta_i^3 + 2\gamma \eta_i \sum_{j\neq i}^{N} \eta_j^2 + 2\eta_i (1-\xi)^2 \right) - \kappa_g \nabla^2 \eta_i \tag{5}$$

$$\mu_p = \frac{\delta F}{\delta \xi} = m_p \left(-2(1-\xi)\phi + 2\xi(1-\phi) \right) + m_g \left(-2(1-\xi) \sum_{i=1}^{n} \eta_i^2 \right) - \kappa_p \nabla^2 \xi \tag{6}$$

2 Kinetics

The order parameter for each grain is unconserved, and thus their evolution can be described by Allen-Cahn equations:

$$\frac{\partial \eta_i}{\partial t} = -L_g \mu_g = L_g \left(m_g \left(-\eta_i + \eta_i^3 + 2\gamma \eta_i \sum_{j \neq i}^{N} \eta_j^2 + 2\eta_i \left(1-\xi\right)^2 \right) - \kappa_g \nabla^2 \eta_i \right) \tag{7}$$

where L_g is the constant grain boundary mobility.

Similarly, the liquis/solid order parameter, ξ, is unconserved:

$$\frac{\partial \xi}{\partial t} = -L_p \mu_p = -L_g \left(m_p \left(-2\left(1-\xi\right)\phi + 2\xi\left(1-\phi\right)\right) + m_g \left(-2\left(1-\xi\right) \sum_{i=1}^{n} \eta_i^2 \right) - \kappa_p \nabla^2 \xi \right) \tag{8}$$

Additionally in this application, a transient temperature evolution equation (Heat Equation) is solved:

$$\frac{\partial T}{\partial t} = -\boldsymbol{\nabla} \cdot \left(-D \ \boldsymbol{\nabla} T\right) \tag{9}$$

Were D is the thermal diffusivity

3 Time discretization

Considering forward Euler explicit time stepping, we have the time discretized kinetics equation:

$$\eta_i^{n+1} = \eta_i^n - \Delta t L_g \ \left(m_g \left(-\eta_i + \eta_i^3 + 2\gamma \eta_i \sum_{j \neq i}^{N} \eta_j^2 + 2\eta_i \left(1-\xi\right)^2 \right) - \kappa_g \nabla^2 \eta_i \right) \tag{10}$$

$$\xi^{n+1} = \xi^n - \Delta t L_p \ \left(m_p \left(-2\left(1-\xi\right)\phi + 2\xi\left(1-\phi\right)\right) + m_g \left(-2\left(1-\xi\right) \sum_{i=1}^{n} \eta_i^2 \right) - \kappa_p \nabla^2 \xi \right) \tag{11}$$

$$T^{n+1} = T^n + \left(\Delta t D\right) \ \Delta T^n \tag{12}$$

4 Weak formulation

In the weak formulation, considering an arbitrary variation w, the above equation can be expressed as a residual equation:

$$\int_\Omega w \eta_i^{n+1} \ dV = \int_\Omega w \eta_i^n - w \Delta t L_g \ \left(m_g \left(-\eta_i + \eta_i^3 + 2\gamma \eta_i \sum_{j \neq i}^{N} \eta_j^2 + 2\eta_i \left(1-\xi\right)^2 \right) - \kappa_g \nabla^2 \eta_i \right) \ dV \tag{13}$$

$$= \int_\Omega w \underbrace{(\eta^n - \Delta t L_g \ m_g \left(-\eta_i + \eta_i^3 + 2\gamma \eta_i \sum_{j \neq i}^{N} \eta_j^2 + 2\eta_i \left(1-\xi\right)^2 \right)}_{r_{\eta_i}} + \boldsymbol{\nabla} w \underbrace{\left(-\Delta t L_g \kappa_g\right) \ \cdot \left(\boldsymbol{\nabla} \eta_i^n\right)}_{r_{\eta_i x}} \ dV \quad [\kappa_g \boldsymbol{\nabla} \eta_i \cdot n \tag{14}$$

$$\int_\Omega w \xi^{n+1} \; dV = \int_\Omega w \xi^n - w \Delta t L_p \; \left(m_p \left(-2\left(1-\xi\right)\phi + 2\xi\left(1-\phi\right)\right) + m_g \left(-2\left(1-\xi\right) \sum_{i=1}^{n} \eta_i^2 \right) - \kappa_p \nabla^2 \xi \right) \; dV \tag{15}$$

$$= \int_\Omega w \underbrace{(\eta^n - \Delta t L_p \; \left(m_p \left(-2\left(1-\xi\right)\phi + 2\xi\left(1-\phi\right)\right) + m_g \left(-2\left(1-\xi\right) \sum_{i=1}^{n} \eta_i^2 \right) \right)}_{r_{\eta_i}} + \nabla w \underbrace{\left(-\Delta t L_p \kappa_p\right) \; \cdot \left(\nabla \xi^n\right)}_{r_{\xi x}} \tag{16}$$

$$\int_\Omega w T^{n+1} \; dV = \int_\Omega w T^n + w(\Delta t D)\Delta T^n \tag{17}$$

$$= \int_\Omega w(T^n) - \nabla w \cdot (\Delta t D) \nabla T^n \; dV + \int_{\partial\Omega} w(\Delta t D) \nabla T^n \cdot n \; dS \tag{18}$$

$$= \int_\Omega w(T^n) - \nabla w \cdot (\Delta t D) \nabla T^n \; dV + \int_{\partial\Omega} w(\Delta t D) j^n \; dS \tag{19}$$

$$= \int_\Omega w(\underbrace{T^n}_{r_c}) + \nabla w \cdot \underbrace{(-\Delta t D) \nabla T^n}_{r_{cx}} \; dV \quad \text{[assuming flux } j = 0\text{]} \tag{20}$$

The above values of r_{η_i} and $r_{\eta_i x}$ are used to define the residuals in the following parameters file: *applications/additivemanufacturing/equations.h*