PRISMS-PF Application Formulation: grainGrowth

This example application implements a simple set of governing equations for isotropic grain growth. The model is a simplified version of the one in the following publication:
Simulating recrystallization in titanium using the phase field method, S.P. Gentry and K. Thornton, *IOP Conf. Series: Materials Science and Engineering* 89 (2015) 012024.

Consider a free energy expression of the form:

$$\Pi(\eta_i, \boldsymbol{\nabla}\eta_i) = \int_\Omega \left[\sum_{i=1}^{N} \left(-\frac{1}{2}\eta_i^2 + \frac{1}{4}\eta_i^4 \right) + \alpha \sum_{i=1}^{N} \sum_{j>i}^{N} \eta_i^2 \eta_j^2 + \frac{1}{4} \right] + \frac{\kappa}{2} \sum_{i=1}^{N} |\nabla \eta_i|^2 \; dV \tag{1}$$

where η_i is one of N structural order parameters, α 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:

$$\mu = \frac{\delta \Pi}{\delta \eta_i} = \left(-\eta_i + \eta_i^3 + 2\alpha\eta_i \sum_{j\neq i}^{N} \eta_j^2 - \kappa\nabla^2\eta_i \right) \tag{2}$$

2 Kinetics

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

$$\frac{\partial \eta_i}{\partial t} = -L\mu = \left(-\eta_i + \eta_i^3 + 2\alpha\eta_i \sum_{j\neq i}^{N} \eta_j^2 - \kappa\nabla^2\eta_i \right) \tag{3}$$

where L is the constant mobility.

3 Time discretization

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

$$\eta_i^{n+1} = \eta_i^n - \Delta t L \;\; \left(-\eta_i^n + (\eta_i^n)^3 + 2\alpha\eta_i^n \sum_{j\neq i}^{N} (\eta_j^n)^2 - \kappa\nabla^2\eta_i^n \right) \tag{4}$$

4 Weak formulation

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

$$\int_\Omega w\eta_i^{n+1}\ dV = \int_\Omega w\eta_i^n - w\Delta t L\ \left(-\eta_i^n + (\eta_i^n)^3 + 2\alpha\eta_i^n \sum_{j\neq i}^{N} (\eta_j^n)^2 - \kappa\nabla^2\eta_i^n\right)\ dV \tag{5}$$

$$= \int_\Omega w\underbrace{(\eta^n - \Delta t L\ \left(-\eta_i^n + (\eta_i^n)^3 + 2\alpha\eta_i^n \sum_{j\neq i}^{N} (\eta_j^n)^2\right)}_{r_{\eta_i}} + \nabla w \underbrace{(-\Delta t L\kappa)\ \cdot (\nabla\eta_i^n)}_{r_{\eta_i x}}\ dV \quad [\kappa\nabla\eta_i \cdot n = 0 \text{ on } \partial\Omega] \tag{6}$$

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