

PRISMS PhaseField Anisotropy (with Coupled CH-AC Dynamics)

Consider a free energy expression of the form:

$$\Pi(c, \eta, \nabla\eta) = \int_{\Omega} (f_{\alpha}(1-H) + f_{\beta}H) + \frac{1}{2}|\gamma(\mathbf{n})\nabla\eta|^2 dV \quad (1)$$

where f_{α} and f_{β} are the free energy densities corresponding to α and β phases, respectively, and are functions of composition c . H is a function of the structural order parameter η . The interface normal vector \mathbf{n} is given by

$$\mathbf{n} = \frac{\nabla\eta}{|\nabla\eta|} \quad (2)$$

for $\nabla\eta \neq \mathbf{0}$, and $\mathbf{n} = \mathbf{0}$ when $\nabla\eta = \mathbf{0}$.

1 Variational treatment

Following standard variational arguments (see Cahn-Hilliard formulation), we obtain the chemical potentials:

$$\mu_c = (f_{\alpha,c}(1-H) + f_{\beta,c}H) \quad (3)$$

$$\mu_{\eta} = (f_{\beta,c} - f_{\alpha,c})H_{,\eta} - \nabla \cdot \mathbf{m} \quad (4)$$

The component of the anisotropic gradient \mathbf{m} are given by

$$m_i = \gamma(\mathbf{n}) \left(\nabla\eta + |\nabla\eta|(\delta_{ij} - n_i n_j) \frac{\partial\gamma(\mathbf{n})}{n_j} \right), \quad (5)$$

where δ_{ij} is the Kronecker delta.

2 Kinetics

Now the PDE for Cahn-Hilliard dynamics is given by:

$$\frac{\partial c}{\partial t} = -\nabla \cdot (-M_c \nabla \mu_c) \quad (6)$$

$$= M_c \nabla \cdot (\nabla(f_{\alpha,c}(1-H) + f_{\beta,c}H)) \quad (7)$$

and the PDE for Allen-Cahn dynamics is given by:

$$\frac{\partial \eta}{\partial t} = -M_{\eta} \mu_{\eta} \quad (8)$$

$$= -M_{\eta} ((f_{\beta,c} - f_{\alpha,c})H_{,\eta} - \nabla \cdot \mathbf{m}) \quad (9)$$

where M_c and M_{η} are the constant mobilities.

3 Time discretization

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

$$\eta^{n+1} = \eta^n - \Delta t M_\eta ((f_{\beta,c}^n - f_{\alpha,c}^n) H_{,\eta}^n - \nabla \cdot \mathbf{m}^n) \quad (10)$$

$$c^{n+1} = c^n + \Delta t M_\eta \nabla \cdot (\nabla (f_{\alpha,c}^n (1 - H^n) + f_{\beta,c}^n H^n)) \quad (11)$$

4 Weak formulation

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

$$\int_{\Omega} w \eta^{n+1} dV = \int_{\Omega} w \eta^n - w \Delta t M_\eta ((f_{\beta,c}^n - f_{\alpha,c}^n) H_{,\eta}^n - \kappa \Delta \eta^n) dV \quad (12)$$

$$= \int_{\Omega} w \left(\underbrace{\eta^n - \Delta t M_\eta ((f_{\beta,c}^n - f_{\alpha,c}^n) H_{,\eta}^n)}_{r_\eta} \right) + \nabla w \cdot \underbrace{(-\Delta t M_\eta) \mathbf{m}^n}_{r_{\eta x}} dV \quad (13)$$

and

$$\int_{\Omega} w c^{n+1} dV = \int_{\Omega} w c^n + w \Delta t M_c \nabla \cdot (\nabla (f_{\alpha,c}^n (1 - H^n) + f_{\beta,c}^n H^n)) dV \quad (14)$$

$$= \int_{\Omega} w \underbrace{c^n}_{r_c} + \nabla w \underbrace{(-\Delta t M_c) [(f_{\alpha,cc}^n (1 - H^n) + f_{\beta,cc}^n H^n) \nabla c + ((f_{\beta,c}^n - f_{\alpha,c}^n) H_{,\eta}^n \nabla \eta)]}_{r_{cx}} dV \quad (15)$$

The above values of r_η , $r_{\eta x}$, r_c and r_{cx} are used to define the residuals in the following equations file:
applications/CHAC_anisotropy/equations.h