PRISMS PhaseField
Regularized Anisotropy (with Coupled CH-AC Dynamics)

Consider a free energy expression of the form:

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

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. δ is a scalar regularization parameter. The interface normal vector $\mathbf{n}$ is given by

$$\mathbf{n} = \frac{\boldsymbol{\nabla}\eta}{|\boldsymbol{\nabla}\eta|} \tag{2}$$

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

1 Variational treatment

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

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

$$\mu_\eta = (f_{\beta,c} - f_{\alpha,c})H_{,\eta} - \boldsymbol{\nabla}\cdot\mathbf{m} + \delta^2\Delta(\Delta\eta) \tag{4}$$

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

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

where δ_{ij} is the Kronecker delta.

2 Kinetics

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

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

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

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

$$\frac{\partial\eta}{\partial t} = -M_\eta\mu_\eta \tag{8}$$

$$= -M_\eta\ [(f_{\beta,c} - f_{\alpha,c})H_{,\eta} - \boldsymbol{\nabla}\cdot\mathbf{m} + \delta^2\Delta(\Delta\eta)] \tag{9}$$

where M_c and M_η are the constant mobilities. In order that the formulation only includes second order derivatives, an auxiliary field is introduced to break up the biharmonic term:

$$\phi = \Delta\eta \tag{10}$$

and PDE for Allen-Cahn dynamics becomes

$$\frac{\partial \eta}{\partial t} = -M_\eta \ ((f_{\beta,c} - f_{\alpha,c})H_{,\eta} - \mathbf{\nabla} \cdot \mathbf{m}) + \delta^2 \Delta \phi. \tag{11}$$

3 Time discretization

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

$$\phi^{n+1} = \Delta \eta^n \tag{12}$$

$$\eta^{n+1} = \eta^n - \Delta t M_\eta \ ((f^n_{\beta,c} - f^n_{\alpha,c})H^n_{,\eta} - \mathbf{\nabla} \cdot \mathbf{m}^n + \delta^2 \Delta \phi^n) \tag{13}$$

$$c^{n+1} = c^n + \Delta t M_\eta \ \mathbf{\nabla} \cdot (\mathbf{\nabla}(f^n_{\alpha,c}(1 - H^n) + f^n_{\beta,c} H^n)) \tag{14}$$

4 Weak formulation

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

$$\int_\Omega w \phi^{n+1} \ dV = \int_\Omega \mathbf{\nabla} w \cdot \underbrace{\mathbf{\nabla} \eta^n}_{r_{\phi x}} \ dV \tag{15}$$

$$\int_\Omega w \eta^{n+1} \ dV = \int_\Omega w \eta^n - w \Delta t M_\eta \ ((f^n_{\beta,c} - f^n_{\alpha,c})H^n_{,\eta} - \kappa \Delta \eta^n) \ dV \tag{16}$$

$$= \int_\Omega w \left(\underbrace{\eta^n - \Delta t M_\eta \ ((f^n_{\beta,c} - f^n_{\alpha,c})H^n_{,\eta})}_{r_\eta} \right) + \mathbf{\nabla} w \cdot \underbrace{(-\Delta t M_\eta)(\mathbf{m}^n - \delta^2 \phi^n)}_{r_{\eta x}} \ dV \tag{17}$$

and

$$\int_\Omega w c^{n+1} \ dV = \int_\Omega w c^n + w \Delta t M_c \ \mathbf{\nabla} \cdot (\mathbf{\nabla}(f^n_{\alpha,c}(1 - H^n) + f^n_{\beta,c} H^n)) \ dV \tag{18}$$

$$= \int_\Omega w \underbrace{c^n}_{r_c} + \mathbf{\nabla} w \underbrace{(-\Delta t M_c) \ [\ (f^n_{\alpha,cc}(1 - H^n) + f^n_{\beta,cc} H^n) \mathbf{\nabla} c + \ ((f^n_{\beta,c} - f^n_{\alpha,c}) H^n_{,\eta} \mathbf{\nabla} \eta^n)]}_{r_{cx}} \ dV \tag{19}$$

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