PRISMS PhaseField
Coupled Cahn-Hilliard and Allen-Cahn Dynamics

Consider a free energy expression of the form:

$$\Pi(c, \eta, \boldsymbol{\nabla}\eta) = \int_\Omega \left(f_\alpha(1 - H) + f_\beta H \right) + \frac{\kappa}{2} \boldsymbol{\nabla}\eta \cdot \boldsymbol{\nabla}\eta \; dV \tag{1}$$

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. Note that we don't have the gradient terms for the composition, i.e, $\boldsymbol{\nabla}c$ terms, unlike classical Cahn-Hillard formulation.

1 Variational treatment

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

$$\mu_c = (f_{\alpha,c}(1 - H) + f_{\beta,c}H) \tag{2}$$

$$\mu_\eta = (f_{\beta,c} - f_{\alpha,c})H_{,\eta} - \kappa\Delta\eta \tag{3}$$

2 Kinetics

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

$$\frac{\partial c}{\partial t} = -\boldsymbol{\nabla} \cdot (-M_c\boldsymbol{\nabla}\mu_c) \tag{4}$$

$$= M_c \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}(f_{\alpha,c}(1 - H) + f_{\beta,c}H)) \tag{5}$$

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

$$\frac{\partial \eta}{\partial t} = -M_\eta\mu_\eta \tag{6}$$

$$= -M_\eta \left((f_{\beta,c} - f_{\alpha,c})H_{,\eta} - \kappa\Delta\eta \right) \tag{7}$$

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:

$$\eta^{n+1} = \eta^n - \Delta t M_\eta \left((f_{\beta,c}^n - f_{\alpha,c}^n)H_{,\eta}^n - \kappa\Delta\eta^n \right) \tag{8}$$

$$c^{n+1} = c^n + \Delta t M_\eta \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}(f_{\alpha,c}^n(1 - H^n) + f_{\beta,c}^n H^n)) \tag{9}$$

4 Weak formulation

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

$$\int_\Omega w\eta^{n+1} \ dV = \int_\Omega w\eta^n - w\Delta t M_\eta \ ((f_{\beta,c}^n - f_{\alpha,c}^n)H_{,\eta}^n - \kappa\Delta\eta^n) \ dV \tag{10}$$

$$= \int_\Omega w \left(\underbrace{\eta^n - \Delta t M_\eta \ ((f_{\beta,c}^n - f_{\alpha,c}^n)H_{,\eta}^n)}_{r_\eta} \right) + \boldsymbol{\nabla} w \cdot \underbrace{(-\Delta t M_\eta \kappa)\boldsymbol{\nabla}\eta^n}_{r_{\eta x}} \ dV \tag{11}$$

and

$$\int_\Omega wc^{n+1} \ dV = \int_\Omega wc^n + w\Delta t M_c \ \boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}(f_{\alpha,c}^n(1 - H^n) + f_{\beta,c}^n H^n)) \ dV \tag{12}$$

$$= \int_\Omega w \underbrace{c^n}_{r_c} + \boldsymbol{\nabla} w \underbrace{(-\Delta t M_c) \ [\ (f_{\alpha,cc}^n(1 - H^n) + f_{\beta,cc}^n H^n)\boldsymbol{\nabla}c + \ ((f_{\beta,c}^n - f_{\alpha,c}^n)H_{,\eta}^n\boldsymbol{\nabla}\eta)]}_{r_{cx}} \ dV \tag{13}$$

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