PRISMS PhaseField
Coupled Cahn-Hilliard and Allen-Cahn Dynamics

Consider a free energy expression of the form:

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

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:

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

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

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:

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

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

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:

$$\eta^{n+1} = \eta^n - \Delta t M_\eta\ ((f^n_{\beta,c} - f^n_{\alpha,c})H^n_{,\eta} - \kappa\Delta\eta^n) \tag{8}$$

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

4 Weak formulation

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

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

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

and

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

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

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*