

PRISMS PhaseField

Coupled Cahn-Hilliard and Allen-Cahn Dynamics

Consider a free energy expression of the form:

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

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 . Note that we don't have the gradient terms for the composition, i.e, ∇c terms, unlike classical Cahn-Hilliard formulation.

1 Variational treatment

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

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

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

2 Kinetics

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

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

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

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

$$\frac{\partial \eta}{\partial t} = -M_{\eta} \mu_{\eta} \quad (6)$$

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

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:

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

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

4 Weak formulation

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

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

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

and

$$\begin{aligned} \int_{\Omega} w c^{n+1} dV &= \int_{\Omega} w c^n + w \Delta t M_c \nabla \cdot (\nabla (f_{\alpha,c}^n (1 - H^{n+1}) + f_{\beta,c}^n H^{n+1})) dV \\ &= \int_{\Omega} w \underbrace{c^n}_{r_c} + \underbrace{\nabla w (-\Delta t M_c) [(f_{\alpha,cc}^n (1 - H^{n+1}) + f_{\beta,cc}^n H^{n+1}) \nabla c + ((f_{\beta,c}^n - f_{\alpha,c}^n) H_{,\eta}^{n+1} \nabla \eta)]}_{r_{cx}} dV \end{aligned} \quad (12)$$

(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