

PRISMS PhaseField Cahn-Hilliard Dynamics (Mixed-Formulation)

Consider a free energy expression of the form:

$$\Pi(c, \nabla c) = \int_{\Omega} f(c) + \frac{\kappa}{2} \nabla c \cdot \nabla c \, dV \quad (1)$$

where c is the composition, and κ is the gradient length scale parameter.

1 Variational treatment

Considering variations on the primal field c of the form $c + \epsilon w$, we have

$$\delta\Pi = \frac{d}{d\epsilon} \int_{\Omega} f(c + \epsilon w) + \frac{\kappa}{2} \nabla(c + \epsilon w) \cdot \nabla(c + \epsilon w) \, dV \Big|_{\epsilon=0} \quad (2)$$

$$= \int_{\Omega} w f_{,c} + \kappa \nabla w \nabla c \, dV \quad (3)$$

$$= \int_{\Omega} w (f_{,c} - \kappa \Delta c) \, dV + \int_{\partial\Omega} w \kappa \nabla c \cdot n \, dS \quad (4)$$

Assuming $\kappa \nabla c \cdot n = 0$, and using standard variational arguments on the equation $\delta\Pi = 0$ we have the expression for chemical potential as

$$\mu = f_{,c} - \kappa \Delta c \quad (5)$$

2 Kinetics

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

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

$$= -M \nabla \cdot (-\nabla (f_{,c} - \kappa \Delta c)) \quad (7)$$

where M is the constant mobility. This equation can be split into two equations as follow:

$$\mu = f_{,c} - \kappa \Delta c \quad (8)$$

$$\frac{\partial c}{\partial t} = M \nabla \cdot (\nabla \mu) \quad (9)$$

3 Time discretization

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

$$\mu^{n+1} = f_{,c}^n - \kappa \Delta c^n \quad (10)$$

$$c^{n+1} = c^n + \Delta t M \nabla \cdot (\nabla \mu^n) \quad (11)$$

4 Weak formulation

In the weak formulation, considering an arbitrary variation w , the above equations can be expressed as residual equations representing a mixed (split) formulation:

$$\int_{\Omega} w \mu^{n+1} dV = \int_{\Omega} w f_{,c}^n - w \kappa \Delta c^n dV \quad (12)$$

$$= \int_{\Omega} w \underbrace{f_{,c}^n}_{r_{mu}} + \nabla w \cdot \underbrace{\kappa \nabla c^n}_{r_{mux}} dV \quad (13)$$

and

$$\int_{\Omega} w c^{n+1} dV = \int_{\Omega} w c^n + w \Delta t M \nabla \cdot (\nabla \mu^n) dV \quad (14)$$

$$= \int_{\Omega} w \underbrace{c^n}_{r_c} + \nabla w \cdot \underbrace{(-\Delta t M)}_{r_{cx}} \cdot (\nabla \mu^n) dV \quad [\text{neglecting boundary flux}] \quad (15)$$

The above values of r_{mu} , r_{mux} , r_c and r_{cx} are used to define the residuals in the following parameters file:

applications/cahnHilliard/parameters.h