PRISMS PhaseField
Cahn-Hilliard Dynamics (Mixed-Formulation)

Consider a free energy expression of the form:

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

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 from $c + \epsilon w$, we have

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

$$= \int_{\Omega} w f_{,c} + \kappa \boldsymbol{\nabla} w \boldsymbol{\nabla} c \ dV \tag{3}$$

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

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

$$\mu = f_{,c} - \kappa \Delta c \tag{5}$$

2 Kinetics

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

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

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

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

$$\mu = f_{,c} - \kappa \Delta c \tag{8}$$

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

3 Time discretization

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

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

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

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:

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

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

and

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

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

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