

PRISMS PhaseField Allen-Cahn Dynamics

Consider a free energy expression of the form:

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

where η is the structural order parameter, and κ is the gradient length scale parameter.

1 Variational treatment

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

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

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

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

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

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

2 Kinetics

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

$$\frac{\partial\eta}{\partial t} = -M (f_{,\eta} - \kappa \Delta\eta) \quad (6)$$

where M is the constant mobility.

3 Time discretization

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

$$\eta^{n+1} = \eta^n - \Delta t M (f_{,\eta}^n - \kappa \Delta\eta^n) \quad (7)$$

4 Weak formulation

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

$$\int_{\Omega} w \eta^{n+1} dV = \int_{\Omega} w \eta^n - w \Delta t M (f_{,\eta}^n - \kappa \Delta \eta^n) dV \quad (8)$$

$$= \int_{\Omega} w \underbrace{(\eta^n - \Delta t M f_{,\eta}^n)}_{r_{\eta}} + \nabla w \underbrace{(-\Delta t M \kappa)}_{r_{\eta x}} \cdot (\nabla \eta^n) dV \quad [\kappa \nabla \eta \cdot n = 0 \quad \text{on} \quad \partial \Omega] \quad (9)$$

The above values of r_{η} and $r_{\eta x}$ are used to define the residuals in the following parameters file:
applications/allenCahn/parameters.h