PRISMS PhaseField
Allen-Cahn Dynamics

Consider a free energy expression of the form:

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

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 from $\eta + \epsilon w$, we have

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

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

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

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

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

2 Kinetics

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

$$\frac{\partial\eta}{\partial t} = -M \; \left(f_{,\eta} - \kappa\Delta\eta\right) \tag{6}$$

where M is the constant mobility.

3 Time discretization

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

$$\eta^{n+1} = \eta^{n} - \Delta t M \; \left(f^{n}_{,\eta} - \kappa\Delta\eta^{n}\right) \tag{7}$$

4 Weak formulation

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

$$\int_\Omega w\eta^{n+1}\ dV = \int_\Omega w\eta^n - w\Delta tM\ (f^n_{,\eta} - \kappa\Delta\eta^n)\ dV \tag{8}$$

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

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