

PRISMS PhaseField

Globally Conserved Allen-Cahn Dynamics

This application performs a phase field simulation of Allen-Cahn dynamics subject to global (as opposed to local) conservation. Global conservation implies that $\int_{\Omega} \eta dV$, where Ω is the volume of the system, is constant in time.

Note: This application needs to run with **uniform mesh** in order for the calculation of the chemical potential to be accurate.

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

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

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

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

where $f_{,\eta} = \partial f / \partial \eta$. 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

The Parabolic PDE for Allen-Cahn dynamics is given by:

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

where M is the constant mobility. However, Eq. (6) does not ensure global conservation of η . In order to achieve global conservation we can add a spatially-uniform term, A , to the RHS of (6) that effectively offsets the total change in η such that $\int_{\Omega} \partial \eta / \partial t dV = 0$:

$$\frac{\partial \eta}{\partial t} = -M \mu + A. \quad (7)$$

Applying the global conservation constraint to Eq. (7), we obtain

$$\int_{\Omega} \frac{\partial \eta}{\partial t} dV = - \int_{\Omega} (M\mu - A) dV = 0. \quad (8)$$

Since A is spatially uniform and M is a constant, A given by

$$A = \frac{M}{V} \int_{\Omega} \mu dV. \quad (9)$$

Substituting A from Eq. (9) into Eq. (7) we get

$$\frac{\partial \eta}{\partial t} = -M(\mu - \bar{\mu}), \quad (10)$$

where $\bar{\mu} = (1/V) \int_{\Omega} \mu dV$.

3 Time discretization

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

$$\eta^{n+1} = \eta^n - \Delta t M(\mu^n - \bar{\mu}^n) \quad (11)$$

and

$$\mu^{n+1} = f_{,\eta}^n - \kappa \Delta \eta^n. \quad (12)$$

4 Weak formulation

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

$$\int_{\Omega} w \eta^{n+1} dV = \int_{\Omega} w \underbrace{[\eta^n - \Delta t M(\mu^n - \bar{\mu}^n)]}_{r_{\eta}} dV \quad (13)$$

and

$$\int_{\Omega} w \mu^{n+1} dV = \int_{\Omega} [w f_{,\eta}^n - w \kappa \Delta \eta^n] dV \quad (14)$$

$$= \int_{\Omega} w \underbrace{(f_{,\eta}^n)}_{r_{\mu}} + \nabla w \cdot \underbrace{(\kappa \nabla \eta^n)}_{r_{\mu x}} dV, \quad (15)$$

where the reference chemical potential $\bar{\mu}^n$ for time step n in Eq. (13) is calculated as

$$\bar{\mu}^n = \frac{1}{V} \int_{\Omega} \mu^n dV. \quad (16)$$

The above values of r_{η} , r_{μ} , and $r_{\mu x}$ are used to define the residuals in the following parameters file:
applications/allenCahn_conserved/equations.cc