PRISMS PhaseField
Allen-Cahn Dynamics (Implicit Solver Formulation)

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Consider a free energy expression of the form:

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

where η is the structural order parameter ($0 < \eta < 1$), and κ is the gradient length scale parameter.

1 Kinetics

The parabolic PDE for Allen-Cahn dynamics is given by

$$\frac{\partial\eta}{\partial t} = -M\frac{\delta\mathcal{F}}{\delta\eta}, \tag{2}$$

where M is the mobility of the interface. The term $\delta\mathcal{F}/\delta\eta$ is obtained by taking the variational derivative of $\mathcal{F}$:

$$\frac{\partial\eta}{\partial t} = -M(f_{,\eta} - \kappa\nabla^2\eta), \tag{3}$$

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

2 Time discretization

Considering fully implicit time stepping, we have the time discretized kinetics equation:

$$\eta^n = \eta^{n-1} - \Delta t M(f^n_{,\eta} - \kappa\nabla^2\eta^n) \tag{4}$$

At each time step, it is assumed that we know η^{n-1} and need to solve for η^n. The approach in PRISMS-PF is to find the solution for η^n iteratively by employing a Newton-Picard scheme.

3 Implicit solver formulation

We denote the values of η for two consecutive Newton iterations as η^n_{j-1} and η^n_j and define

$$\delta\eta^n_j = \eta^n_j - \eta^n_{j-1}. \tag{5}$$

Substituting $\eta^n_j = \eta^n_{j-1} + \delta\eta^n_j$ into Eq. (4), we get

$$\eta^n_{j-1} + \delta\eta^n_j = \eta^{n-1} - \Delta t M\left[f_{,\eta}(\eta^n_{j-1} + \delta\eta^n_j) - \kappa\nabla^2(\eta^n_{j-1} + \delta\eta^n_j)\right] \tag{6}$$

Assuming $\delta\eta^n_j$ is small everywhere, we can expand $f_{,\eta}$ around η^n_{j-1} to first order:

$$f_{,\eta}(\eta^n_{j-1} + \delta\eta^n_j) \simeq f_{,\eta}(\eta^n_{j-1}) + f_{,\eta\eta}(\eta^n_{j-1})\delta\eta^n_j. \tag{7}$$

Substituting in Eq. (6), and rearranging the equation so that all terms proportional to $\delta\eta^n_j$ are on the LHS and remaining terms on the RHS, we get

$$[1 + \Delta t M f_{,\eta\eta}(\eta^n_{j-1})]\delta\eta^n_j - \Delta t M\kappa\nabla^2\delta\eta^n_j = \eta^{n-1} - \eta^n_{j-1} - \Delta t M\left[f_{,\eta}(\eta^n_{j-1}) - \kappa\nabla^2\eta^n_{j-1}\right] \tag{8}$$

4 Solution Scheme

At every time step, the known value η^{n-1} is taken as the initial guess for the Newton scheme, η_0^n. Then, for every Newton iteration, $\delta\eta_j^n$ is found using Eq. (8) and η_j^n is updated using Eq. (5). The Newton scheme converges when the norm of $\delta\eta_j^n$ is smaller than some tolerance value (given by the user) after N steps. At that, η^n is calculated as η_N^n and the scheme is repeated for the next time step.

5 Weak formulation

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