Numerical Method for Phase Field Equations

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1. Mathematical Model

The standard Allen-Cahn energy is given by

$$E(\phi) = \int_\Omega \left\{ \frac{1}{2} |\nabla \phi|^2 + \frac{1}{\epsilon^2} F(\phi) \right\} d\boldsymbol{x}, \tag{1}$$

where $\Omega \subset \mathbf{R}^d$, where $d = 2$ or 3, $\phi : \Omega \to \mathbf{R}$ is the concentration field, ϵ is a constant, and $F(\phi)$ is a given energy potential (e.g. the Ginzburg-Landau double-well potential (Figure.1) $F(\phi) = \frac{1}{4}(\phi^2 - 1)^2$ which has been widely used). In turn, the chemical potential is defined as

$$\mu_{AC} := \delta_\phi E = -\triangle \phi + \frac{1}{\epsilon^2} F'(\phi) = -\triangle \phi + \frac{1}{\epsilon^2} f(\phi). \tag{2}$$

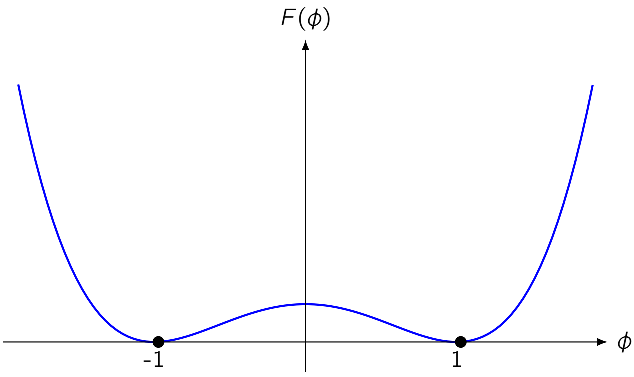

Figure 1. The Ginzburg-Landau double-well potential.

The standard Cahn-Hilliard equation is given by

$$\begin{cases} \phi_t = \triangle \phi - \frac{1}{\epsilon^2} f(\phi), & \text{in } \Omega \times (0, T], \\ \frac{\partial \phi}{\partial n} = 0, & \text{in } \partial\Omega \times (0, T], \\ \phi(\boldsymbol{x}, 0) = \phi_0(\boldsymbol{x}), & \text{in } \Omega \times \{0\}. \end{cases} \tag{3}$$

2. Semi-implicit linearization scheme

2.1. Weak Formulation of Mixed FEM

The mixed weak formulation of (3) is derived as follows:

1. First (3) can be splited as the following system

$$\begin{cases} u_t &= \Delta v, \\ v &= -\varepsilon^2 \Delta u + u^3 - u. \end{cases} \tag{4}$$

2. Then the weak formations for the system is

$$\begin{cases} \int_\Omega u_t \varphi - \int_\Omega \Delta v \varphi &= 0, \\ \int_\Omega v \psi + \varepsilon^2 \int_\Omega \Delta u \psi - \int_\Omega (u^3 - u)\psi &= 0. \end{cases} \tag{5}$$

And integration by parts gives

$$\begin{cases} \int_\Omega u_t\varphi - \int_{\partial\Omega}(\nabla u\cdot \boldsymbol{n})\varphi + \int_\Omega \nabla v\nabla\varphi & = 0 \\ \int_\Omega v\psi + \varepsilon^2\int_{\partial\Omega}(\nabla u\cdot \boldsymbol{n})\psi - \varepsilon^2\int_\Omega \nabla u\nabla\psi - \int_\Omega (u^3-u)\psi & = 0 \end{cases} \tag{6}$$

Applying the boundary conditions $\nabla u\cdot \boldsymbol{n} = \frac{\partial u}{\partial \boldsymbol{n}} = 0$ and $\nabla v\cdot \boldsymbol{n} = \frac{\partial v}{\partial \boldsymbol{n}} = 0$ on $\partial\Omega$ yields

$$\begin{cases} \int_\Omega u_t\varphi + \int_\Omega \nabla v\nabla\varphi & = 0 \\ \int_\Omega v\psi - \varepsilon^2\int_\Omega \nabla u\nabla\psi - \int_\Omega (u^3-u)\psi & = 0 \end{cases} \tag{7}$$

2.2. Time Discretization

1. We use forward-Euler time discretization and substitut u^{n+1} with $au^n + (1-a)u^{n+1}$:

$$\begin{cases} \int_\Omega \frac{u^{n+1}-u^n}{\tau}\varphi + \int_\Omega \nabla v\nabla\varphi & = 0 \\ \int_\Omega v\psi - \varepsilon^2\int_\Omega \nabla u^{n+1}\nabla\psi - \int_\Omega ((u^n)^3 - au^n - (1-a)u^{n+1})\psi & = 0 \end{cases} \tag{8}$$

2. We use backward-Euler time discretization

$$\begin{cases} \int_\Omega \frac{u^{n+1}-u^n}{\tau}\varphi + \nabla v^{n+1}\cdot\nabla\varphi = 0 & \forall\varphi\in H^1 \\ \int_\Omega v^{n+1}\psi - \varepsilon^2\nabla u^{n+1}\cdot\nabla\psi - f'(u^{n+1})\psi = 0 & \forall\psi\in H^1 \end{cases} \tag{9}$$

3. Some numerical Results

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