Phase field models and their numerical methods

1. Background and equations

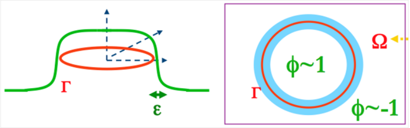
August 14, 2019

Phase field model

Phase field model is one of the *diffuse interface methods* and used to describe morphological evolution of patterns.

- An implicit surface representation:
  sharp interfaces $\rightarrow$ diffuse interfaces by phase field functions.
- Phase field function:

$$\phi(x) = \tanh \frac{d(x, \Gamma)}{\sqrt{2}\varepsilon}$$



Advantages:

- Interface with different topology is described by a single level set function;
- A single set of equations to be solved throughout the domain, no need to track interface.

Phase field model: A simple example

Membrane: Hydrophilic (mix) V.S. Hydrophobic (de-mix).
For example: oil and water, could be labeled by the phase function

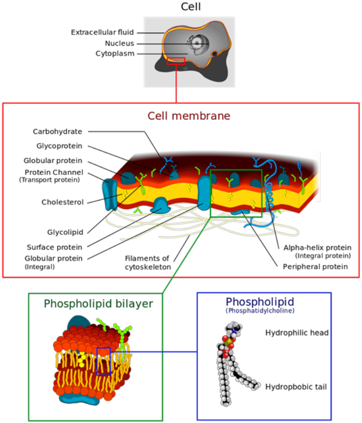
$$\phi(x) = \begin{cases} 1, & \text{fluid 1 (oil)}, \\ -1, & \text{fluid 2 (water)}. \end{cases} \tag{1}$$

Consider the free energy

$$E(\phi) = \int_\Omega e(\phi(x))\,\mathrm{d}x, \tag{2}$$

where $e(\phi)$ is the energy density.

Intuitively, it is reasonable to assume that *if* $e(\phi) \to 0$, *then* ϕ *tends to a constant state*. So $e(\phi)$ should consist of $\nabla\phi$ to decrease the potential energy and force the whole system to the steady states.



Phase field model: A simple example (continued)

$$E(\phi) = \int_\Omega e(\phi(x))dx.$$

Intuitively,

- if $e(\phi) \to 0$, then ϕ tends to a constant state;
- $e(\phi)$ consists of the derivatives of ϕ.

A good choice is

$$e(\phi) = \lambda\Big(|\nabla\phi|^2 + \frac{1}{2\varepsilon^2}(\phi^2-1)^2\Big), \tag{3}$$

where λ is the scale of free energy, and ε is the interface width.
Now we write our free energy as

$$E(\phi) = \int_\Omega \Big(\frac{1}{2}|\nabla\phi|^2 + \frac{1}{4\varepsilon^2}(\phi^2-1)^2\Big)dx. \tag{4}$$

Phase field model: A simple example (continued)

Free energy functional:

$$E(\phi) = \int_\Omega \Big(\frac{1}{2} |\nabla \phi|^2 + \frac{1}{4\varepsilon^2} (\phi^2 - 1)^2 \Big) dx.$$

Euler-Lagrange equation of E:

$$\phi_t = -\frac{\delta E(\phi)}{\delta \phi}, \tag{5}$$

where

$$\frac{\delta E(\phi)}{\delta \phi} = -\Delta \phi + \frac{1}{\varepsilon^2} (\phi^3 - \phi). \tag{6}$$

The 2nd order equation (5) with (6) gives the *Allen-Cahn equation*.

Phase field model: A simple example (continued)

Free energy functional:

$$E(\phi) = \int_{\Omega} \left(\frac{1}{2} |\nabla \phi|^2 + \frac{1}{4\varepsilon^2} (\phi^2 - 1)^2 \right) dx.$$

According to the mass conservation law

$$\phi_t = -\nabla \cdot J,$$

and the Fick's law

$$J = -M(\phi) \nabla \frac{\delta E(\phi)}{\delta \phi},$$

we can obtain

$$\phi_t = \nabla \cdot \left(M(\phi) \nabla \frac{\delta E(\phi)}{\delta \phi} \right), \tag{7}$$

where $M(\phi)$ is the phase-dependent mobility.

The 4th order equation (7) with (6) gives the *Cahn-Hilliard equation*.

Gradient flow

Phase field models are often given by *gradient flows* with respect to some free energy functionals.

Suppose

$$E(\phi) = \int G(\phi, \nabla\phi, \Delta\phi)dx, \tag{8}$$

the variational derivative is defined via

$$\left(\frac{\delta E(\phi)}{\delta \phi}, \psi\right)_{L^2} = \frac{\mathrm{d}}{\mathrm{d}s} E(\phi + \lambda\psi)\Big|_{\lambda=0}, \quad \forall \psi \in L^2. \tag{9}$$

Boundary conditions:
homogenous Dirichlet, homogenous Neumann, or periodic.

Gradient flow (continued)

L^2 gradient flow:

$$\phi_t = -\frac{\delta E(\phi)}{\delta \phi}. \tag{10}$$

Energy decay:

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \left(\frac{\delta E}{\delta \phi}, \frac{\partial \phi}{\partial t}\right)_{L^2} = -\left\|\frac{\partial \phi}{\partial t}\right\|^2 \leq 0. \tag{11}$$

Example:
Allen-Cahn equation is the L^2 gradient flow w.r.t. the energy (4).

Gradient flow (continued)

H^{-1} gradient flow:

$$\phi_t = \Delta \frac{\delta E(\phi)}{\delta \phi}. \tag{12}$$

Energy decay:

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \left(\frac{\delta E}{\delta \phi}, \frac{\partial \phi}{\partial t} \right)_{L^2} = - \left\| \nabla \frac{\partial \phi}{\partial t} \right\|^2 \leq 0. \tag{13}$$

Mass conservation:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \phi(x,t) dx = \int_\Omega \Delta \frac{\delta E}{\delta \phi} dx = \int_{\partial\Omega} \frac{\partial}{\partial n} \frac{\delta E}{\delta \phi} dl = 0. \tag{14}$$

Example:
Cahn-Hilliard equation (with constant mobility) is the H^{-1} gradient flow w.r.t. the energy (4).

More examples of phase field models

- Allen-Cahn equation (2nd order);
- Cahn-Hilliard equation (4th order);

- *Swift-Hohenberg model* (4th order);
- *phase field crystal model* (6th order);
- *Epitaxial growth models* (4th order);
- Peng-Robinson equation of state;
- Ginzburg-Landau model for superconductivity;
- ......

Swift-Hohenberg and phase field crystal models

Consider the energy functional

$$E(\phi) = \int \Big(\frac{1}{4}\phi^4 + \frac{1-\varepsilon}{2}\phi^2 - |\nabla\phi|^2 + \frac{1}{2}|\Delta\phi|^2\Big)dx. \tag{15}$$

The L^2 gradient flow of E gives the *Swift-Hohenberg (SH) model*

$$\phi_t = -\phi^3 - (1-\varepsilon)\phi - 2\Delta\phi - \Delta^2\phi. \tag{16}$$

The H^{-1} gradient flow of E gives the *phase field crystal (PFC) model*

$$\phi_t = \Delta(\phi^3 + (1-\varepsilon)\phi + 2\Delta\phi + \Delta^2\phi). \tag{17}$$

Epitaxial growth models

Consider the energy functionals

$$E_1(\phi) = \int \Big(\frac{1}{4}(|\nabla\phi|^2 - 1)^2 + \frac{\varepsilon^2}{2}|\Delta\phi|^2\Big)dx, \tag{18}$$

$$E_2(\phi) = \int \Big(-\frac{1}{2}\ln(1 + |\nabla\phi|^2) + \frac{\varepsilon^2}{2}|\Delta\phi|^2\Big)dx. \tag{19}$$

The L^2 gradient flow of E_1 reads

$$\phi_t = -\nabla\cdot[(1 - |\nabla\phi|^2)\nabla\phi] - \varepsilon^2\Delta^2\phi, \tag{20}$$

which is called the epitaxial growth model *with slope selection*.
The L^2 gradient flow of E_2 reads

$$\phi_t = -\nabla\cdot\left(\frac{\nabla\phi}{1 + |\nabla\phi|^2}\right) - \varepsilon^2\Delta^2\phi, \tag{21}$$

which is called the epitaxial growth model *without slope selection*.

Epitaxial growth models (continued)

Epitaxial growth model with slope selection:

$$\phi_t = -\nabla \cdot [(1 - |\nabla\phi|^2)\nabla\phi] - \varepsilon^2\Delta^2\phi. \tag{22}$$

Epitaxial growth model without slope selection:

$$\phi_t = -\nabla \cdot \left(\frac{\nabla\phi}{1 + |\nabla\phi|^2}\right) - \varepsilon^2\Delta^2\phi. \tag{23}$$

Remark:

- Consider (22) in 1-D case.
  Let $\psi = \phi_x$, then ψ satisfies the Cahn-Hilliard equation.
- When $|\nabla\phi|$ is small, it holds $(1 + |\nabla\phi|^2)^{-1} \approx 1 - |\nabla\phi|^2$.
  That means (22) is an approximation of (23) for small $|\nabla\phi|$.