Two Important Partial Differential Equations in Phase Field Problems

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November, 2022

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Phase field models

Let us consider the flow of viscous, incompressible, immiscible two fluid systems. Suppose the system has an unstable initial state thus the interface of the two materials gradually evolves, governed by some explicit or implicit mechanism.

Figure: Evolution of interface

The phase field model uses level set method to formulate the system. Hereafter we denote the evolving interface as Γ_t.

Level set method

As its name indicates, the main idea of the level set formulation/method is to represent the hypersurface Γ_t as a zero-level set of a function u in $\mathbb{R}^{d+1}$, that is

$$\Gamma_t := \{x(t) \in \Omega; u(x(t), t) = 0\}, \tag{1}$$

then to evolve the level set function u, instead of the interface Γ_t. By using this method, we transfer a hypersurface in $\mathbb{R}^d$ into a cross section of a evolving surface in $\mathbb{R}^{d+1}$. In order to obtain an appropriate formulation for $u(\cdot, t)$, we formally differentiate the equation $u(x(t), t) = 0$ with respect to t, while treating $x = x(t)$ as an implicit function, and using the chain rule to get

$$\frac{\partial u}{\partial t} + \nabla u \cdot \frac{dx}{dt} = \frac{\partial u}{\partial t} + \nabla u \cdot V = 0, \tag{2}$$

where $V = \dfrac{dx}{dt}$ is the velocity of the surface.

Level set method

Equation (2) is called the level set equation, and it is determined by the velocity field V and the initial condition u_0 such that

$$\Gamma_0 = \left\{ x \in \mathbb{R}^{d+1}; u_0(x) = 0 \right\}.$$

Since the evolution of surface is driven by some physical or geometric laws that are directly contained in the information of surface velocity V, therefore, we need to specify the velocity to represent different geometric laws. In general, the surface velocity can be written in the following form:

$$V_n(t) = F_{\text{int}}(\lambda_1, \ldots, \lambda_d) + F_{\text{ext}} \quad \text{on } \Gamma_t \tag{3}$$

where $V_n(t) := V(t) \cdot n$ is the normal velocity on the surface Γ_t, $\lambda_1, \cdots \lambda_d$ are the principle curvatures of the surface and F_{ext} denotes the external or source function.

Geometric laws

Example1

The simplest and most commonly used is the mean-curvature flow, whose geometric law is

$$F_{\text{int}} = H := \sum_{j=1}^{d} \lambda_j, \quad F_{\text{ext}} \equiv 0. \tag{4}$$

The mean-curvature flow describes the most efficient way for a surface to shrink its area, namely, it minimizes $\frac{d}{dt}|\Gamma_t|$.

Geometric laws

Example2

The following law is called the Hele-Shaw flow

$$F_{\mathrm{int}} = 0, \quad F_{\mathrm{ext}} = \frac{1}{2}\left[\frac{\partial w}{\partial n}\right]_{\Gamma_t} \tag{5}$$

where w is the solution of

$$\begin{aligned} \Delta w = 0 \ \ &in\ \Omega \backslash \Gamma_t, \\ w = \sigma H \ \ &on\ \Gamma_t. \end{aligned} \tag{6}$$

The Hele-Shaw flow says that the normal velocity of the interface equals the jump of the normal derivative of the pressure field w across the interface. Again, H stands for the mean curvature.

Introduction to Allen-Cahn equation

The main idea of the phase field method is to seek a phase field function u^ε such that the interface lies in the narrow region

$$\Gamma_t \subset Q_t^\varepsilon := \left\{ x(t) \in \mathbb{R}^{d+1} : |u^\varepsilon(x(t),t)| \leq 1 - \mathcal{O}(\varepsilon) \right\}. \tag{7}$$

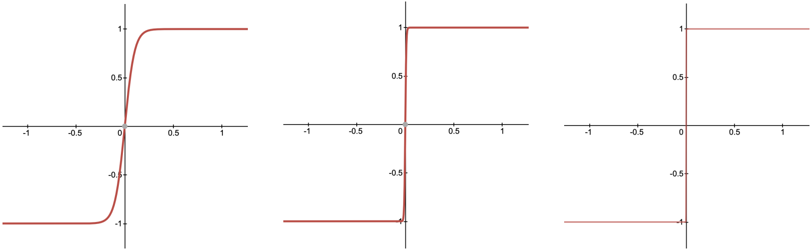
Here ε is a small constant to control the width of Q_t^ε. u^ε is expect to be a function that takes two distinct value $+1$ and -1 to represent two phases, with a smooth change between $+1$ and -1 within Q_t^ε. Approximately, the zero level set

$$\Gamma_t^\varepsilon := \left\{ x\overline{(t)} \in \mathbf{R}^{d+1}; u^\varepsilon(x(t),t) = 0 \right\}$$

is often chosen to represent Γ_t.

Introduction to Allen-Cahn equation

For the Allen-Cahn equation, we heuristically postulate that $u^\varepsilon(x,t) := \tanh\left(\frac{d(x)}{\sqrt{2}\varepsilon}\right)$ since the tanh function matches well with the desired profile for the phase function u^ε. Note that $d(x)$ is the signed distance function between x and Γ_t. The heuristic formulation only provides geometric information near the interface Γ_t.



(a) $\tanh(\frac{x}{0.1})$ (b) $\tanh(\frac{x}{0.01})$ (c) $\tanh(\frac{x}{0.001})$

Figure: tanh functions

Introduction to the Allen-Cahn equation

Using the heuristic formulation, we have the following relation for the surface Γ_t that

$$
\begin{aligned}
\nabla u^\varepsilon(x) &= \frac{\tanh\left(\frac{d(x)}{\sqrt{2}\varepsilon}\right)}{\sqrt{2}\varepsilon}\nabla d(x) \\
D^2 d(x) &= \frac{\sqrt{2}\varepsilon}{1-\left(u^\varepsilon(x)\right)^2}\left(D^2 u^\varepsilon(x) + \frac{2u^\varepsilon(x)}{1-\left(u^\varepsilon(x)\right)^2}\nabla u^\varepsilon(x)\otimes\nabla u^\varepsilon(x)\right)
\end{aligned}
\tag{8}
$$

By the definition of mean curvature, we have also

$$
H = \operatorname{tr}\left(D^2 d(x)\right) = \frac{\sqrt{2}\varepsilon}{1-\left(u^\varepsilon(x)\right)^2}\left(\Delta u^\varepsilon(x) + \frac{1}{\varepsilon^2}\left(u^\varepsilon(x) - \left(u^\varepsilon(x)\right)^3\right)\right)
\tag{9}
$$

Introduction to the Allen-Cahn equation

Now we show that the Allen-Cahn equation can be derived using the mean-curvature flow (4). Differentiate $u^\varepsilon(x,t)=0$ with respect to t and treat $x=x(t)$ as a implicit function, we have

$$0=\frac{\partial u^\varepsilon}{\partial t}+\nabla u^\varepsilon\cdot V=\frac{\partial u^\varepsilon}{\partial t}-|\nabla u^\varepsilon|\,V_n=\frac{\partial u^\varepsilon}{\partial t}-|\nabla u^\varepsilon|\,H \qquad (10)$$

Here we have used the facts that $V=\frac{dx(t)}{dt}$ and $n=-\frac{\nabla u^e}{|\nabla u^\varepsilon}$. Next we combine (8-10) to obtain the Allen-Cahn equation:

$$\frac{\partial u^\varepsilon}{\partial t}-\Delta u^\varepsilon+\frac{1}{\varepsilon^2}\left((u^\varepsilon)^3-u^\varepsilon\right)=0. \qquad (11)$$

Next we will show prove that equation (11) can also be derived using the energetic approach. Before that, we firstly review the definition of functional/variational derivatives.

Introduction to the Allen-Cahn equation

Definition1

Let E be a Banach space and $I : E \to \mathbb{R}$ be a functional defined on E. If for any u, φ, the following limit

$$I'(u, \varphi) := \lim_{t \to 0} \frac{I(u + t\varphi) - I(u)}{t} \tag{12}$$

exits, then (12) is called the Gâteaux derivative of I at $u \in E$.

Definition2

Let E be a Banach space and $I : E \to \mathbb{R}$ be a functional defined on E. Suppose I is Gâteaux differentiable at $u \in E$ with $I'(u, \cdot) \in E^*$, and such that

$$I(u + \varphi) = I(u) + I'(u, \varphi) + o(\|\varphi\|), \quad \varphi \in E, \tag{13}$$

then we say that I is Frechet differentiable at u.

Proposition

Given the free energy functional

$$\mathcal{J}(u) := \int_{\Omega} \left(\frac{1}{2} |\nabla u|^2 + \frac{1}{\varepsilon^2} F(u) \right) dx, \quad F(u) := \frac{1}{4} \left(u^2 - 1 \right)^2 \tag{14}$$

then the Allen-Cahn equation can be interpreted as the L^2 gradient flow for $\mathcal{J}$:

$$\frac{\partial u}{\partial t} = -\mathcal{J}'(u) \tag{15}$$

where $\mathcal{J}'(u)$ is the Gâteaux derivative of $\mathcal{J}$ in the L^2 topology.

Proof.

$$
\begin{aligned}
&\delta\mathcal{J}(u) \\
=\ & \frac{d}{ds}\mathcal{J}(u+s\eta)\Big|_{s=0} \\
=\ & \frac{d}{ds}\Big|_{s=0}\int_\Omega \left(\frac{1}{2}(\nabla u + s\nabla\eta)\cdot(\nabla u + s\nabla\eta) + \frac{1}{\varepsilon^2}F(u+s\eta)\right)dx \\
=\ & \frac{d}{ds}\Big|_{s=0}\int_\Omega \left(\frac{1}{2}\nabla u\cdot\nabla u + s\nabla u\cdot\nabla\eta + \frac{1}{2}s^2\nabla\eta\cdot\nabla\eta + \frac{1}{\varepsilon^2}F(u+s\eta)\right)dx \\
=\ & \int_\Omega \left(-\Delta u + \frac{1}{\varepsilon^2}F'(u)\right)\eta dx \\
=\ & \left(-\Delta u + \frac{1}{\varepsilon^2}f(u), \eta\right)_{L_2(\Omega)}.
\end{aligned}
$$

Then by the definition of Gâteaux derivative, it yields (11):

$$\frac{\partial u}{\partial t} = \Delta u - \frac{1}{\varepsilon^2}(u^3 - u)$$

Introduction to the Allen-Cahn equation

Let $E(u, \nabla u) = \frac{1}{2}|\nabla u|^2 + \frac{1}{\varepsilon^2}F(u)$. By applying the definition of functional derivatives, we can also derive the energy law of Allen-Cahn equation.

$$\begin{aligned}
\frac{\partial \mathcal{J}(u)}{\partial t} &= \int_\Omega \frac{\partial}{\partial t} E(u, \nabla u) dx \\
&= \int_\Omega \left(E_u \frac{\partial u}{\partial t} + E_{\nabla u} \cdot \frac{\partial \nabla u}{\partial t} \right) dx \\
&= \int_\Omega \left(E_u - \nabla \cdot E_{\nabla u} \right) \frac{\partial u}{\partial t} dx \\
&= - \left\| \frac{\partial u}{\partial t} \right\|_{L_2(\Omega)}^2
\end{aligned}$$

where we have used the Euler-Lagrangian $\frac{\delta \mathcal{J}}{\delta u} = E_u - \nabla \cdot E_{\nabla u}$.

Introduction to the Cahn-Hilliard equation

The Cahn-Hilliard equation is a forth order problem which is given by

$$\frac{\partial u^\varepsilon}{\partial t} + \Delta\left(\varepsilon \Delta u^\varepsilon - \frac{1}{\varepsilon} f\left(u^\varepsilon\right)\right) = 0. \tag{16}$$

The equation can be derived by the level set method where the geometric law is chosen as the Hele-Shaw flow defined in (5-6). Moreover, the Cahn-Hilliard equation can also be interpreted as the H^{-1} gradient flow of the Cahn–Hilliard free energy $\widehat{\mathcal{J}} := \varepsilon \mathcal{J}$. Recall that the $H^{-1}(\Omega)$ space is defined as the dual space of $H_0^1(\Omega)$, with an inner product

$$(u, v)_{H^{-1}(\Omega)} = \left((-\Delta)^{-1} u, v\right)_{L^2(\Omega)}. \tag{17}$$

Introduction to the Cahn-Hilliard equation

Since

$$\begin{aligned} \delta\hat{\mathcal{J}} &= \left(-\nabla\cdot(\epsilon\nabla u) + \frac{1}{\epsilon}f(u), \eta\right)_{L_2(\Omega)} \\ &= \left((-\Delta)\left(-\nabla\cdot(\epsilon\nabla u) + \frac{1}{\epsilon}f(u)\right), \eta\right)_{H^{-1}(\Omega)}, \end{aligned}$$

then we have the equation:

$$\begin{aligned} u_t &= -\frac{\delta\hat{\mathcal{J}}(u)}{\delta u}, \quad \text{in } H^{-1}(\Omega) \\ u_t + \Delta\left(\epsilon\Delta u - \frac{1}{\epsilon}f(u)\right) &= 0 \end{aligned} \tag{18}$$

Introduction to the Cahn-Hilliard equation

The H^{-1}-gradient flow structure implies the following energy law:

$$\begin{aligned}\frac{\partial \hat{\mathcal{J}}(u)}{\partial t} &= \int_\Omega \epsilon \left(E_u - \nabla \cdot E_{\nabla u}\right) \frac{\partial u}{\partial t} dx \\ &= \int_\Omega \Delta \left(\epsilon \Delta u - \frac{1}{\epsilon} f(u)\right) \cdot \left(\epsilon \Delta u - \frac{1}{\epsilon} f(u)\right) dx \\ &= -\|\nabla \mu\|^2_{L_2 \Omega}\end{aligned}$$

in which $\mu = \epsilon \Delta u - (1/\epsilon) f(u)$ is often called the chemical potential and there will be a Neumann boundary condition applied on this potential.

Introduction to the Cahn-Hilliard equation

In addition, a degenerate form of the Cahn-Hilliard equation can be interpreted as a "weighted" H^{-1} gradient flow.

$$u_t = -\nabla \cdot \left(b(u) \nabla \frac{\delta \hat{\mathcal{J}}(u)}{\delta u} \right), \quad \text{in } L_2(\Omega) \tag{19}$$

for some $b(u) \geq 0$. The corresponding energy law is then

$$\frac{\partial \hat{\mathcal{J}}(u)}{\partial t} = -\int_\Omega b(u) \nabla \mu \cdot \nabla \mu dx. \tag{20}$$

Convergence analysis for the Allen-Cahn equation

A natural question about the level set method and the formulation of the phase field problem is that whether the narrow region converges to the exact sharp interface. As a matter of fact, we have the following result for the Allen-Cahn equation (11):

Theorem

(Evans et al.(1992)) Let $I \equiv \{(x,t) \in R^n \times (0,\infty) \mid u(x,t) > 0\}$ *and* $O \equiv \{(x,t) \in R^n \times (0,\infty) \mid u(x,t) < 0\}$. *Then*

$$u^\varepsilon \to 1 \quad \textit{uniformly on compact subsets of } I \tag{21}$$

$$u^\varepsilon \to -1 \quad \textit{uniformly on compact subsets of } O \tag{22}$$

$$\mathrm{dist}_H\left(\Gamma_t^\varepsilon, \Gamma_t\right) = O(\varepsilon), \qquad \textit{as } \varepsilon \to 0 \tag{23}$$

Convergence analysis for the Cahn-Hilliard equation

There is also some literature in analysing the convergence of Cahn-Hilliard equation.

Theorem

(Caginalp and Chen (1998)) Consider the generalized Cahn-Hilliard equation

$$\alpha(\varepsilon)\frac{\partial\varphi^{\varepsilon}}{\partial t} = \varepsilon\Delta\varphi^{\varepsilon} - \frac{1}{\varepsilon}f\left(\varphi^{\varepsilon}\right) + s(\varepsilon)u^{\varepsilon}, \tag{24}$$

$$c(\varepsilon)\frac{\partial u^{\varepsilon}}{\partial t} = \Delta u^{\varepsilon} - \frac{\partial\varphi^{\varepsilon}}{\partial t} \tag{25}$$

Then as $\varepsilon \to 0$, $\operatorname{dist}_H\left(\Gamma_t^{\varepsilon}, \Gamma_t\right) \to 0$ *and* $\varphi^{\varepsilon} \longrightarrow \pm 1$ *uniformly in any compact subset of* $\bar{\Omega}_T \backslash \Gamma^0$.

The proof of these two theorems is based on the Sobolev embedding inequalities and the second theorem also used the interpolation inequality in its proof.

Reference.

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