# Functional derivative and Allen Cahn eq and Cahn Hilliard eq

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## 1 Introduction

In this note, we will introduce the derivation of AC and CH eqs in terms of gradient flow. The note is organized as follows: In section (**??**), we clarify what is gradient flow in a given space/norm. Then, we derive Allen Cahn eq and Cahn Hilliard eq.

### 1.1 Functional derivative and First variation

One of the most central problems in the calculus is to maximize or minimize a given real valued function of a single variable. If $f$ is a given function defined in an open interval $I$, then, $f$ has a local (or relative) minimum at a point $x_0$ in $I$ if $f(x_0) \leq f(x)$ for all $x$, satisfying $|x - x_0| \leq \delta$ for some $\delta$. If $f$ has a local minimum at $x_0$ in $I$ and $f$ is differentiable in $I$, then it is well known that

$$f'(x_0) = 0 \tag{1}$$

where the prime denotes the ordinary derivative of $f$. Condition (1) is called a necessary condition for a local minimum. If (1) holds, we say $f$ is **stationary** at $x_0$ and that $x_0$ is an **critical point** of $f$. The calculus of variations deals with generalizations of this problem from the calculus. Rather than find conditions under which functions have extreme values, the calculus of variations deals with extremizing general quantities called functionals.

Let $A$ be a set of functions, then a functional on $A$ is denoted $J : A \to \mathbf{R}$. A fundamental problem of the calculus of variations can be stated as follows: Given a functional $J$ and a well-defined set of functions $A$, determine which functions in $A$ affords a (local) minimum (or maximum) value to $J$. The set $A$ is called the set of **admissible functions**. The problem of extremizing a functional $J$ over the set $A$ is called a variational problem.

#### 1.1.1 Motivation of Derivatives of Functionals

For a variational problem we assume the set of admissible functions $A$ is a subset of a normed linear space $V$. Then the set $A$ can inherit the norm and algebraic properties of the space $V$. Therefore the notions of local minima and maxima make sense. If $J : A \to \mathbf{R}$ is a functional on $A$, where $A \subseteq V$ and $V$ is a normed linear space with norm $||\cdot||$, then $J$ has a local minimum at $y_0 \in A$, provided $J(y_0) \leq J(y)$ for all $y \in A$ with $||y - y_0|| < d$, for some positive number $d$. We call $y_0$ an extremal of $J$ and say $J$ is stationary at $y_0$.

To motivate the definition of a derivative of a functional, let us rewrite the limit definition of derivative of a function $f$ at $x_0$ as

$$f(x_0 + \Delta x) - f(x_0) = f'(x_0)\Delta x + o(\Delta x). \tag{2}$$

The differential of $f$ at $x_0$, defined by $df(x_0, \Delta x) = f'(x_0)\Delta x$, is the linear part in the increment $\Delta x$ of the total change $\Delta f \equiv f(x_0 + \Delta x) - f(x_0)$. That is

$$\Delta f = df(x_0, \Delta x) + o(\Delta x). \tag{3}$$

Let $y_0 \in A$. To increment $y_0$ we fix an element $h \in V$ such that $y_0 + \epsilon h \in A$ for all $\epsilon \in R$ sufficiently small. The increment $\epsilon h$ is called the **variation** of the function $y_0$ and is often denoted by $\delta y_0$; that is $\delta y_0 \equiv \epsilon h$. Then we define the total change in the functional $J$ due to the change $\epsilon h$ in $y_0$ by

$$\Delta J = J(y_0 + \epsilon h) - J(y_0). \tag{4}$$

Our goal is to calculate the linear part w.r.t $\epsilon$ of this change. To this end, we define the ordinary function

$$\mathcal{J}(\epsilon) \equiv J(y_0 + \epsilon h), \tag{5}$$

which is a function of a real variable $\epsilon$ defined by evaluating the functional $J$ on the one parameter family of functions $y_0 + \epsilon h$. Assuming $\mathcal{J}$ is sufficiently differentiable in $\epsilon$, we have

$$\Delta J = \mathcal{J}(\epsilon) - \mathcal{J}(0) = \mathcal{J}'(0)\epsilon + o(\epsilon). \tag{6}$$

Therefore, $\mathcal{J}'(0)\epsilon$ is like a differential for the functional $\mathcal{J}$, being the linear part (or lowest order) of the increment $\Delta J$.

**Definition** Let $J : A \to \mathbf{R}$ be a functional on $A$, where $A \subseteq V$, $V$ a normed linear space. Let $y_0 \in A$ and $h \in V$ such that $y_0 + \epsilon h \in A$ for all $\epsilon$ sufficiently small. Then the first variation (also the Gateaux derivative) if $J$ at $y_0$ in the direction of $h$ is defined by

$$\delta J(y_0, h) \equiv \lim_{\epsilon \to 0} \frac{J(y + \epsilon h) - J(y)}{\epsilon} \equiv \mathcal{J}'(0) \equiv \left. \frac{d}{d\epsilon} J(y_0 + \epsilon h) \right|_{\epsilon=0}, \tag{7}$$

provided the derivative exists. Such a direction $h$ for eq((7)) exists is called an **admissible variation** at $y_0$.

There is an analogy of $\delta J$ with a directional derivative. Let $f(\mathbf{x})$ be a real valued function defined for $\mathbf{x} = (x, y) \in R^2$, and let $\mathbf{n} = (n_1, n_2)$ be a unit vector. Then the derivative of $f$ at $\mathbf{x}_0 = (x_0, y_0)$ in the direction $\mathbf{n}$ is defined by

$$D_n f(\mathbf{x}) \equiv \lim_{\epsilon \to 0} \frac{f(\mathbf{x}_0 + \epsilon \mathbf{n}) - f(\mathbf{x}_0)}{\epsilon}.$$

### 1.1.2 First variation and functional derivative

Let the first variation/differential of functional be $\delta J(y_0, h)$ and $\frac{\delta J}{\delta y_0(\mathbf{x})}$ be functional derivative. The functional derivative $\frac{\delta J}{\delta y_0(\mathbf{x})}$ is the functional such that eq.((8)) is validate for arbitrary function $h(\mathbf{x})$.

$$\delta J(y_0, h) \equiv \left. \frac{d}{d\epsilon} J(y_0 + \epsilon h) \right|_{\epsilon=0} = \int \frac{\delta J[y_0(\mathbf{x})]}{\delta y_0(\mathbf{x})} h(\mathbf{x}) d\mathbf{x} = \left( \frac{\delta J[y_0(\mathbf{x})]}{\delta y_0(\mathbf{x})}, h(\mathbf{x}) \right), \tag{8}$$

Hence, the first variation is a generalization of directional derivative and the functional derivative is a generalization of gradient. And eq.(8) states the relationship between directional derivative and gradient. When the functional $J$ is defined on Banach space, then, the functional derivative is called Frechet derivative.

### 1.1.3 First Example

Compute the first variation of

$$J(y) = \int_a^b y y' dx \tag{9}$$

From the definition above,

$$\begin{aligned}
\delta J(y, h) &= \left. \frac{d}{d\epsilon} J(y + \epsilon h) \right|_{\epsilon \to 0} && (10) \\
&= \left. \frac{d}{d\epsilon} \int_a^b (y + \epsilon h)(y' + \epsilon h') dx \right|_{\epsilon \to 0} && (11) \\
&= \left. \frac{d}{d\epsilon} \int_a^b y y' + \epsilon y h' + \epsilon h y' + \epsilon^2 h h' dx \right|_{\epsilon \to 0} && (12) \\
&= \left. \int_a^b y h' + h y' + 2\epsilon h h' dx \right|_{\epsilon \to 0} && (13) \\
&= \int_a^b y h' + h y' dx. && (14)
\end{aligned}$$

### 1.1.4 Second example

Let $A = \{y \in C^2[a,b] \quad | \quad y(a) = y_0, y(b) = y_1\}$ Compute the functional derivative of the functional defined on $A$,

$$J(y) = \int_a^b L(x, y, y')dx, \tag{15}$$

where $y \in C^2[a,b]$ and $y(a) = y_0, y(b) = y_1$. $L$ is given, twice continuously differentiable function on $[a,b] \times R^2$. , then, $y \in A$ and $h \in C^2[a,b]$ and $h(a) = h(b) = 0$, then $y + \epsilon h \in A$. Then, by the definition of functional derivative, we get

$$\begin{aligned}
\delta J(y,h) \equiv & \left.\frac{d}{d\epsilon} J(y + \epsilon h)\right|_{\epsilon \to 0} \\
= & \left.\frac{d}{d\epsilon} \int_a^b L(x, y + \epsilon h, y' + \epsilon h')dx\right|_{\epsilon \to 0} \\
= & \left.\int_a^b \frac{\partial L(x, y + \epsilon h, y' + \epsilon h')}{\partial y} h + \frac{\partial L(x, y + \epsilon h, y' + \epsilon h')}{\partial y'} h' dx\right|_{\epsilon \to 0} \\
= & \int_a^b \frac{\partial L(x, y, y')}{\partial y} h + \frac{\partial L(x, y, y')}{\partial y'} h' dx \\
= & \int_a^b Ł_y h dx - \int_a^b h \frac{d}{dx} L_{y'} dx + L_{y'} h|_a^b \quad \text{integration by parts} \\
= & \int_a^b \left( L_y(x, y, y') - \frac{d}{dx} L_{y'}(x, y, y') \right) h dx
\end{aligned}$$

To get the functional derivative, we need the following **the fundamental lemma of calculus of variations**:

If $f(x) \in C[a,b]$ and if

$$\int_a^b f(x)h(x)dx = 0 \tag{16}$$

for every $h \in C^2[a,b]$ with $h(a) = h(b) = 0$, then, $f(x) = 0$ for $x \in [a,b]$.

Then, by this Lemma and the definition of functional derivative, we get

$$\left( \frac{\delta J[y(x)]}{\delta y(x)}, h \right) = \delta J(y,h) = \int_a^b \left( L_y(x, y, y') - \frac{d}{dx} L_{y'}(x, y, y') \right) h dx \tag{17}$$

$$\Rightarrow \frac{\delta J[y(x)]}{\delta y(x)} = L_y(x, y, y') - \frac{d}{dx} L_{y'}(x, y, y') \tag{18}$$

### 1.1.5 Third Example

Let the functional defined on a set of multi-variant functions as

$$J[y] = \int L(\mathbf{x}, y(\mathbf{x}), \nabla y(\mathbf{x}))d\mathbf{x}, \tag{19}$$

Then, one can obtain the functional derivative of it as follows,

$$\begin{aligned}
\delta J(y,h) = & \left.\frac{d}{d\epsilon} \int L(\mathbf{x}, y + \epsilon h, \nabla(y + \epsilon h))d\mathbf{x}\right|_{\epsilon \to 0} \\
= & \int \frac{\partial L}{\partial y} h + \frac{\partial L}{\partial \nabla y} \cdot \nabla h d\mathbf{x} \\
= & \int \frac{\partial L}{\partial y} h d\mathbf{x} + \nabla \cdot \left( \frac{\partial L}{\partial \nabla y} h \right) - \nabla \cdot \frac{\partial L}{\partial \nabla y} h d\mathbf{x} \quad \text{product rule of divergence} \\
= & \int \left( \frac{\partial L}{\partial y} - \nabla \cdot \frac{\partial L}{\partial \nabla y} \right) h d\mathbf{x} \quad \text{divergence theorem and } h \text{ is arbitrary, then, set } h = 0 \text{ on boundary} \\
\Rightarrow \frac{\delta J[y(\mathbf{x})]}{\delta y} = & \frac{\partial L}{\partial y} - \nabla \cdot \frac{\partial L}{\partial \nabla y} \quad \textbf{fundamental lemma of calculus of variations}
\end{aligned}$$

### 1.1.6 Integration by parts/Greens' formulas

**product rule of divergence**

$$\nabla \cdot (\mathbf{u}v) = (\nabla \cdot \mathbf{u})v + \mathbf{u} \cdot \nabla v \tag{20}$$

$$\nabla \cdot (u\nabla v) = \nabla u \cdot \nabla v + u\Delta v \tag{21}$$

$$\nabla \cdot (v\nabla u) = \nabla u \cdot \nabla v + v\Delta u \tag{22}$$

Let (21)-(22), we have

$$u\Delta v - v\Delta u = \nabla \cdot (u\nabla v) - \nabla \cdot (v\nabla u) \tag{23}$$

Now, apply divergence theorem on the right hand side of (23), we end up with

$$\int_\Omega u\Delta v - v\Delta u d\mathbf{x} = \int_{\partial\Omega} u\mathbf{n} \cdot \nabla v - v\mathbf{n} \cdot \nabla u dS \tag{24}$$

### 1.1.7 Forth Example

Let the functional defined on a set of multi-variant functions as

$$J[y] = \int L(\mathbf{x}, y(\mathbf{x}), \nabla y(\mathbf{x}), \Delta y) d\mathbf{x}, \tag{25}$$

Then, one can obtain the functional derivative of it as follows,

$$\begin{aligned}
\delta J(y,h) &= \frac{d}{d\epsilon} \int L(\mathbf{x}, y+\epsilon h, \nabla(y+\epsilon h)) d\mathbf{x} \Big|_{\epsilon \to 0} \\
&= \int \frac{\partial L}{\partial y} h + \frac{\partial L}{\partial \nabla y} \cdot \nabla h d\mathbf{x} \\
&= \int \frac{\partial L}{\partial y} h d\mathbf{x} + \nabla \cdot \left( \frac{\partial L}{\partial \nabla y} h \right) - \nabla \cdot \frac{\partial L}{\partial \nabla y} h d\mathbf{x} \quad \text{product rule of divergence} \\
&= \int \left( \frac{\partial L}{\partial y} - \nabla \cdot \frac{\partial L}{\partial \nabla y} \right) h d\mathbf{x} \quad \text{divergence theorem and } h \text{ is arbitrary, then, set } h = 0 \text{ on boundary} \\
\Rightarrow \frac{\delta J[y(\mathbf{x})]}{\delta y} &= \frac{\partial L}{\partial y} - \nabla \cdot \frac{\partial L}{\partial \nabla y} \quad \textbf{fundamental lemma of calculus of variations}
\end{aligned}$$

### 1.1.8 Fifth Example

Let the functional defined on a set of multi-variant functions as

$$J[y] = \int L(\mathbf{x}, y(\mathbf{x}), \nabla y(\mathbf{x}), \nabla\nabla y(x)) d\mathbf{x}, \tag{26}$$

Then, one can obtain the functional derivative of it as follows,

$$\begin{aligned}
\delta J(y,h) &= \frac{d}{d\epsilon} \int L(\mathbf{x}, y+\epsilon h, \nabla(y+\epsilon h), \nabla\nabla(y+\epsilon h)) d\mathbf{x} \Big|_{\epsilon \to 0} \\
&= \int \frac{\partial L}{\partial y} h + \frac{\partial L}{\partial \nabla y} \cdot \nabla h + \frac{\partial L}{\partial \nabla\nabla y} : \nabla\nabla h d\mathbf{x} \\
&= \int \frac{\partial L}{\partial y} h d\mathbf{x} + \nabla \cdot \left( \frac{\partial L}{\partial \nabla y} h \right) - \nabla \cdot \frac{\partial L}{\partial \nabla y} h + \frac{\partial L}{\partial \nabla\nabla y} : \nabla\nabla h d\mathbf{x} \quad \text{product rule of divergence} \\
&= \int \left( \frac{\partial L}{\partial y} - \nabla \cdot \frac{\partial L}{\partial \nabla y} \right) h d\mathbf{x} \quad \text{divergence theorem and } h \text{ is arbitrary, then, set } h = 0 \text{ on boundary} \\
\Rightarrow \frac{\delta J[y(\mathbf{x})]}{\delta y} &= \frac{\partial L}{\partial y} - \nabla \cdot \frac{\partial L}{\partial \nabla y} \quad \textbf{fundamental lemma of calculus of variations}
\end{aligned}$$

### 1.1.9 Chain rule of functional derivative

# 2 Euler-Lagrange equation

The following theorem provides a necessary condition for a local minimum in variation of calculus which is a generalization version of Fermat lemma in calculus.

**Theorem 1** *Let $V$ be a linear norm space with norm $||\cdot||$ $J : A \to R$ be a functional, $A \subseteq V$. If $y_0 \in A$ provides a local minimum for $J$ relative to norm $||\cdot||$, then*

$$\delta J(y_0, h) = 0 \tag{27}$$

*for all **admissible variations** $h$.*

The fact that eq.(27) often allows us to eliminate $h$ from the condition and obtain an equation just in terms of $y_0$, which can be solved for $y_0$.

## 2.1 Example

For the same problem stated in Example (1.1.4), we have

$$\delta J(y, h) = \int_a^b \left( L_y(x, y, y') - \frac{d}{dx} L_{y'}(x, y, y') \right) h dx \tag{28}$$

To find the local minimum of functional $J$, we could set the first variation to be zero based on the above theorem. Hence, we have

$$\int_a^b \left( L_y(x, y, y') - \frac{d}{dx} L_{y'}(x, y, y') \right) h dx = 0 \tag{29}$$

Then, if we assume proper admission set for $h$, based on the fundamental lemma of calculus of variations, we obtain the so called Euler-Lagrange equation:

$$L_y(x, y, y') - \frac{d}{dx} L_{y'}(x, y, y') = 0 \tag{30}$$

## 2.2 Dirichlet Boundary Conditions

Let $A = \{y \in C^2[a, b] | y(a) = y_0, y(b) = y_1\}$ denote the admission function class, then try to find a local minimum for functional

$$J[y] = \int_a^b L(x, y, y') dx \tag{31}$$

let $y \in A$, and $h \in C^2[a, b]$ with $h(a) = h(b) = 0$, so that $y + \epsilon h \in A$ is an admission function, then by Theorem (1), we have

$$\begin{aligned}
\delta J(y, h) \equiv & \left. \frac{d}{d\epsilon} J(y + \epsilon h) \right|_{\epsilon \to 0} = 0 \\
= & \left. \frac{d}{d\epsilon} \int_a^b L(x, y + \epsilon h, y' + \epsilon h') dx \right|_{\epsilon \to 0} \\
= & \left. \int_a^b \frac{\partial L(x, y + \epsilon h, y' + \epsilon h')}{\partial y} h + \frac{\partial L(x, y + \epsilon h, y' + \epsilon h')}{\partial y'} h' dx \right|_{\epsilon \to 0} \\
= & \int_a^b \frac{\partial L(x, y, y')}{\partial y} h + \frac{\partial L(x, y, y')}{\partial y'} h' dx \\
= & \int_a^b \text{Ł}_y h dx - \int_a^b h \frac{d}{dx} L_{y'} dx + L_{y'} h|_a^b \quad \text{integration by parts} \\
= & \int_a^b \left( L_y(x, y, y') - \frac{d}{dx} L_{y'}(x, y, y') \right) h dx = 0 \quad \textbf{zero B.C on } h \\
\Rightarrow & L_y(x, y, y') - \frac{d}{dx} L_{y'}(x, y, y') = 0 \quad \textbf{fundamental lemma of calculus of variations}
\end{aligned}$$

Hence, if a function $y$ provides a local minimum for th functional $J$ on $A$ and the Dirichlet boundary condition is built into the admission function class $A$,

$$J[y] = \int_a^b L(x, y, y') dx \tag{32}$$

then, $y$ must satisfy the differential equation

$$L_y(x, y, y') - \frac{d}{dx} L_{y'}(x, y, y') = 0. \tag{33}$$

This equation is called the **Euler equation** or **Euler-Lagrange equation**. It is a second order ODE since

$$\begin{aligned} & L_y(x,y,y') - \frac{d}{dx} L_{y'}(x,y,y') = 0 \\ & = L_y(x,y,y') - L_{y'x}(x,y,y') - L_{y'y}(x,y,y')y' - L_{y'y'}(x,y,y)y'' = 0. \end{aligned}$$

Hence, from the above variational problem, we end up with the ODE with Dirichlet boundary conditions which is built into the admission function class.

## 2.3 Neumann Boundary Conditions

Let $A = C^2[a,b]$ denote the admission function class with boundary free, then try to find a local minimum for functional

$$J[y] = \int_a^b L(x,y,y')dx \tag{34}$$

let $y \in A$, and $h \in C^2[a,b]$, so that $y + \epsilon h \in A$ is an admission function, then by Theorem (1), we have

$$\begin{aligned} \delta J(y,h) \equiv & \left. \frac{d}{d\epsilon} J(y+\epsilon h) \right|_{\epsilon \to 0} = 0 \\ = & \left. \frac{d}{d\epsilon} \int_a^b L(x, y+\epsilon h, y'+\epsilon h')dx \right|_{\epsilon \to 0} \\ = & \left. \int_a^b \frac{\partial L(x,y+\epsilon h, y'+\epsilon h')}{\partial y} h + \frac{\partial L(x,y+\epsilon h, y'+\epsilon h')}{\partial y'} h' dx \right|_{\epsilon \to 0} \\ = & \int_a^b \frac{\partial L(x,y,y')}{\partial y} h + \frac{\partial L(x,y,y')}{\partial y'} h' dx \\ = & \int_a^b Ł_y h dx - \int_a^b h \frac{d}{dx} L_{y'} dx + L_{y'} h|_a^b \quad \text{integration by parts} \end{aligned}$$

By theorem (1), we know

$$\int_a^b Ł_y h dx - \int_a^b h \frac{d}{dx} L_{y'} dx + L_{y'} h|_a^b = 0$$

for all $h \in C^2[a,b]$, then, it must hold for $h$ with $h(a) = h(b) = 0$, then,

$$\begin{aligned} & \Rightarrow \int_a^b \left( L_y(x,y,y') - \frac{d}{dx} L_{y'}(x,y,y') \right) h dx = 0 \quad \textbf{zero B.C on } h \\ & \Rightarrow L_y(x,y,y') - \frac{d}{dx} L_{y'}(x,y,y') = 0 \quad \textbf{fundamental lemma of calculus of variations} \end{aligned}$$

Hence, $y$ must satisfy the Euler-Lagrange equation.

Now, consider the boundary conditions.

We substitute the Euler-Lagrange equation into the above expression of $\delta J(y,h)$, we get

$$L_{y'}(b, y(b), y'(b))h(b) - L_{y'}(a, y(a), y'(a))h(a) = 0 \tag{35}$$

for all $h \in C^2[a,b]$, then, it must hold for $h$ with $h(a) = 0$, then,

$$\Rightarrow L_{y'}(b, y(b), y'(b))h(b) = 0 \tag{36}$$

hold for all $h(b)$, then

$$\Rightarrow L_{y'}(b, y(b), y'(b)) = 0 \tag{37}$$

Similarly, we have the equation holds for $h$ with $h(b) = 0$,

$$L_{y'}(b, y(b), y'(b))h(b) - L_{y'}(a, y(a), y'(a))h(a) = 0 \tag{38}$$

then,

$$\Rightarrow L_{y'}(a, y(a), y'(a))h(a) = 0 \tag{39}$$

holds for any $h(a)$, hence, we get

$$\Rightarrow L_{y'}(a, y(a), y'(a)) = 0 \tag{40}$$

Hence, we end up with ODE with neumann boundary conditions.

### 2.4 Robin Boundary Conditions

Let $A = C^2[a,b]$ denote the admission function class, then try to find the stationary point of functional

$$J[y] = \int_a^b L(x,y,y')dx \tag{41}$$

# 3 What is free energy?

**This section will be updated soon.**

# 4 Gradient flow

check ref.bib for two references.

A general gradient flow model is given by

$$\frac{\partial \Phi}{\partial t} = \mathcal{G}\frac{\delta E}{\delta \Phi}, \quad \mathbf{x} \in \Omega, \tag{42}$$

where $\Phi = (\phi_1, ..., \phi_d)^T$ is the state variable vector, $\mathcal{G}$ is the $d \times d$ mobility matrix operator which can depend on $\Phi$, E is the free energy functional, and $\frac{\delta E}{\delta \Phi}$ is the variational derivative of the free energy functional with respect to the state variable, known as the chemical potential. The triple $(\Phi, \mathcal{G}, E)$ uniquely defines the gradient flow model. For model ((42)) to be thermodynamically consistent, the time rate of change of the free energy must be non-increasing:

$$\frac{dE}{dt} = (\frac{\delta E}{\delta \Phi}, \frac{\partial \Phi}{\partial t}) = (\frac{\delta E}{\delta \Phi}, \mathcal{G}\frac{\delta E}{\delta \Phi}) \leq 0, \tag{43}$$

where the inner product is defined by $(\mathbf{f}, \mathbf{g}) = \sum_{i=1}^d \int_\Omega f_i g_i d\mathbf{x}, \quad \forall \mathbf{f}, \mathbf{g} \in (L^2(\Omega))^d$, which requires $\mathcal{G}$ to be negative semi-definite. The $L^2$ norm is defined as $||\mathbf{f}||^2 = \sqrt{(\mathbf{f}, \mathbf{f})}$. Note that the energy dissipation law ((43)) holds only for suitable boundary conditions. Such boundary conditions include periodic boundary conditions and the other boundary conditions that make the boundary integrals resulted from the integration by parts vanish in the calculation of variational derivatives.

**Justify the first eq sign in eq.**(43) for 1D case with functional defined by up to second order spatial derivatives.

**Example 1.** Let $J[u] = \int_a^b f(x, u(t,x), u'(t,x))dx, x \in R, t \in R^+$, then, to compute the time derivative of $J$, we have

$$\begin{aligned}
\frac{d}{dt}J[u] &= \frac{d}{dt}\int_a^b f(x, u(t,x), u'(t,x))dx \\
&= \int_a^b f_u u_t + f_{u'}u_t' dx \quad \text{chain rule} \\
&= \int_a^b f_u u_t - \frac{d}{dx}f_{u'}u_t dx + f_{u'}u_t|_{x=a}^{x=b} \quad \text{Integration by parts for the last term} \\
&= \int_a^b \left(f_u - \frac{d}{dx}f_{u'}\right)u_t dx \quad \textbf{proper boundary conditions to eliminate boundary terms on } u \\
&= \left(\frac{\delta J}{\delta u}, u_t\right) \quad \textbf{by definition of first variation}
\end{aligned}$$

**Example 2.** Let $J[u] = \int_a^b f(x, u(t,x), u'(t,x), u''(t,x))dx$, then, to compute the time derivative of $J$, we have

$$
\begin{aligned}
\frac{d}{dt}J[u] &= \frac{d}{dt}\int_a^b f(x, u(t,x), u'(t,x), u''(t,x))dx \\
&= \int_a^b f_u u_t + f_{u'}u_t' + f_{u''}u_t''dx \quad \text{interchange integral and derivative \& chain rule} \\
&= \int_a^b f_u u_t - \frac{d}{dx}f_{u'}u_t dx + f_{u'}u_t|_{x=a}^{x=b} - \int_a^b \frac{d}{dx}f_{u''}u_t' dx + f_{u''}u_t'|_{x=a}^{x=b} \quad \text{integration by parts twice!} \\
&= \int_a^b f_u u_t - \frac{d}{dx}f_{u'}u_t dx + f_{u'}u_t|_{x=a}^{x=b} + f_{u''}u_t|_{x=a}^{x=b} + \int_a^b \frac{d^2}{d^2x}f_{u''}u_t dx - \frac{d}{dx}f_{u''}u_t|_{x=a}^{x=b} \\
&= \int_a^b \left(f_u - \frac{d}{dx}f_{u'} + \frac{d^2}{d^2x}f_{u''}\right)u_t dx \quad \textbf{proper boundary conditions on } u \textbf{ to eliminate boundary terms} \\
&= \left(\frac{\delta J}{\delta u}, u_t\right)
\end{aligned}
$$

Now, let's show two more example in high dimensional space with up to second spatial derivatives.

**Example 3.** Let $J[u] = \int_a^b f(\mathbf{x}, u(t,\mathbf{x}), \nabla u(t,\mathbf{x}))dx$, where $\mathbf{x} \in \Omega \subset R^n$ then, to compute the time derivative of $J$, we use Einstein summation notation in the following derivation/computation.

$$
\begin{aligned}
\frac{d}{dt}J[u] &= \frac{d}{dt}\int_\Omega f(\mathbf{x}, u(t,\mathbf{x}), \nabla u(t,\mathbf{x}))d\mathbf{x} \\
&= \int_\Omega \frac{\partial f}{\partial u}u_t + \frac{\partial f}{\partial \nabla_i u}\nabla_i u_t d\mathbf{x} \quad \text{chain rule} \\
&= \int_\Omega \frac{\partial f}{\partial u}u_t + \nabla_i\left(\frac{\partial f}{\partial \nabla_i u}u_t\right) - \nabla_i\frac{\partial f}{\partial \nabla_i u}u_t d\mathbf{x} \quad \text{product rule of divergence/derivative for the last term} \\
&= \int_\Omega \left(\frac{\partial f}{\partial u} - \nabla_i\frac{\partial f}{\partial \nabla_i u}\right)u_t d\mathbf{x} + \int_{\partial\Omega} n_i\frac{\partial f}{\partial \nabla_i u}u_t dS \quad \textbf{divergence theorem} \\
&= \int_\Omega \left(\frac{\partial f}{\partial u} - \nabla\cdot\frac{\partial f}{\partial \nabla u}\right)u_t d\mathbf{x} + \int_{\partial\Omega} \mathbf{n}\cdot\frac{\partial f}{\partial \nabla u}u_t dS \\
&= \left(\frac{\delta J}{\delta u}, u_t\right) \quad \textbf{proper B.C. to eliminate boundary terms and by definition of first variation}
\end{aligned}
$$

Note that there are some conditions need to be satisfied by $u$ in the second equal sign when one interchange the order between spatial derivative and time derivative.
Remark: we use Einstein summation notation in the above derivation and it is suggested to write calculations in component and caring assigned indices. (tensor product etc. read the textbook shared by Jun Li)

**Example 4.** Let $J[u] = \int_a^b f(\mathbf{x}, u(t,\mathbf{x}), \nabla u, \nabla\nabla u)dx$, where $\mathbf{x} \in \Omega \subset R^n$ then, to compute the time derivative of $J$, we use Einstein summation notation in the following derivation/computation.

$$
\begin{aligned}
\frac{d}{dt}J[u] &= \frac{d}{dt}\int_\Omega f(\mathbf{x}, u, \nabla u, \nabla\nabla u)d\mathbf{x} \\
&= \int_\Omega \frac{\partial f}{\partial u}u_t + \frac{\partial f}{\partial \nabla_i u}\nabla_i u_t + \frac{\partial f}{\partial \nabla_i\nabla_j u} : \nabla_i\nabla_j u_t d\mathbf{x} \quad \text{chain rule} \\
&= \int_\Omega \frac{\partial f}{\partial u}u_t - \nabla_i\frac{\partial f}{\partial \nabla_i u}u_t d\mathbf{x} + \int_{\partial\Omega} n_i\left(\frac{\partial f}{\partial \nabla_i u}u_t\right)dS + \int_\Omega \nabla_i\left(\frac{\partial f}{\partial \nabla_i\nabla_j u}\nabla_j u_t\right) - \nabla_i\frac{\partial f}{\partial \nabla_i\nabla_j u}\nabla_j u_t d\mathbf{x} \\
&= \int_\Omega \left(\frac{\partial f}{\partial u} - \nabla\cdot\frac{\partial f}{\partial \nabla u}\right)u_t d\mathbf{x} - \int_\Omega \nabla_i\frac{\partial f}{\partial \nabla_i\nabla_j u}\nabla_j u_t d\mathbf{x} + \int_{\partial\Omega} n_i\frac{\partial f}{\partial \nabla_i\nabla_j u}\nabla_j u_t dS + \int_{\partial\Omega} \mathbf{n}\cdot\frac{\partial f}{\partial \nabla u}u_t dS \quad \textbf{divergence the} \\
&= I_1 - \int_{\partial\Omega} n_j\nabla_i\frac{\partial f}{\partial \nabla_i\nabla_j u}u_t dS + \int_\Omega \nabla_j\nabla_i\frac{\partial f}{\partial \nabla_i\nabla_j u}u_t d\mathbf{x} + \int_{\partial\Omega} n_i\frac{\partial f}{\partial \nabla_i\nabla_j u}\nabla_j u_t dS \quad \text{divergence theorem} \\
&= I_1 + \int_\Omega \nabla\nabla : \frac{\partial f}{\partial \nabla\nabla u}u_t d\mathbf{x} - \int_{\partial\Omega} n\nabla : \frac{\partial f}{\partial \nabla\nabla u}u_t dS + \int_{\partial\Omega} n_i\frac{\partial f}{\partial \nabla_i\nabla_j u}\nabla_j u_t dS
\end{aligned}
$$

Note that we define $I_1$ by the blue terms above it. Now, the issue is how to handle the surface integral with a conventional gradient in it? How do we convert it into someway that we could apply surface divergence theorem?

## 5 Derivation of Allen Cahn equation

check ref.bib for two references.

## 6 Derivation of Cahn Hilliard equation

check ref.bib for two references.

Let us consider the following free energy density functional:

$$E[u] = \frac{\epsilon^2}{2}(\nabla u, \nabla u) + (F(u), 1) = \int_\Omega \left( \frac{\epsilon^2}{2}|\nabla u(x,t)|^2 + F(u(x,t)) \right) dx, \tag{44}$$

where

- $u = u(t,x)$ is the time-dependent quantity of interests;
- $x \in \Omega \in \mathbf{R}^d$ is open, connected and bounded region with Lipschitz boundary;
- $(\cdot,\cdot)$ denotes the $L^2$ inner product on $\Omega$;
- $\epsilon > 0$ represents the interface width of the two phases and $F(u)$ is the associated nonlinear potential function.

The classic Allen-Cahn eq could be viewed as the gradient flow in $L^2$ of eq ((44)):

$$\partial_t u(x,t) = \frac{\delta E}{\delta u} = \epsilon^2 \Delta u(x,t) + f(u(x,t)), x \in \Omega, t > 0 \tag{45}$$

The classic Cahn-Hilliard eq as the gradient flow in $H^{-1}$ of eq ((44)):

$$\partial_t u(x,t) = -\Delta(-\frac{\delta E}{\delta u}) = -\Delta(\epsilon^2 \Delta u(x,t) + f(u(x,t))), x \in \Omega, t > 0 \tag{46}$$

where $f(u) = -F'(u)$.

The energy dissipation law holds for the Allen-Cahn eq ((45)) as

$$\frac{d}{dt}E[u(x,t)] = -\int_\Omega |\partial_t u(x,t)|^2 dx \leq 0 \tag{47}$$

while for the Cahn-Hilliard eq ((46)) it reads

$$\frac{d}{dt}E[u(x,t)] = -\int_\Omega |\nabla \frac{\delta E}{\delta u}|^2 dx \leq 0 \tag{48}$$

**Allen-Cahn equation:**

- satisfies the maximum bound principle(MBP) in the sense that if the initial values are pointwisely bounded by a specific constant in absolute value, then the absolute value of the solution is bounded by the same constant everwhere for all time.
- but fails to conserve the total mass $V(t) := \int_\Omega u(x,t)dt$ along the time.

**Cahn-Hilliard equation:**

- conserve the total mass along the time
- but fails to satisfies the maximum bound principle as AC eq stated above. It may has bound, but not necessarily be bounded by the same constant.

**Some typical potential functions**

- Double-well potential:
$$F(u) = \frac{1}{4}(u^2-1)^2, f(u) = u - u^3 \tag{49}$$
- Flory-Huggins potential:
$$F(u) = \frac{\theta}{2}[(1+u)ln(1+u) + (1-u)ln(1-u)] - \frac{\theta_c}{2}u^2, f(u)\frac{\theta}{2}ln\frac{1-u}{1+u} + \theta_c u \tag{50}$$
with $0 < \theta < \theta_c$, and the bounding constant is the positive root of $f(\rho) = 0$.