Phase Field Tutorial 1: Exercise Results

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Problem 1. Suppose there are three functions:$\phi, \psi : \mathbb{R}^3 \to \mathbb{R}$ and $\mathbf{f} : \mathbb{R} \to \mathbb{R}^3$. Please prove the following indentities:

$$\nabla (\phi\psi) = \phi\nabla\psi + \psi\nabla\phi$$

$$\nabla \cdot (\phi\mathbf{f}) = \nabla\phi \cdot \mathbf{f} + \phi\nabla \cdot \mathbf{f}.$$

Proof. By the definition of the ∇:

$$\nabla = \begin{bmatrix} \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial x_3} \end{bmatrix} = \left[\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}\right]^{\mathsf{T}},$$

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thus we have:

$$
\begin{aligned}
\nabla(\phi\psi) &= \left[\frac{\partial(\phi\psi)}{\partial x_1}, \frac{\partial(\phi\psi)}{\partial x_2}, \frac{\partial(\phi\psi)}{\partial x_3}\right]^{\mathsf{T}} \\
&= \left[\frac{\partial \phi}{\partial x_1}\psi + \phi\frac{\partial \psi}{\partial x_1}, \frac{\partial \phi}{\partial x_2}\psi + \phi\frac{\partial \psi}{\partial x_2}, \frac{\partial \phi}{\partial x_3}\psi + \phi\frac{\partial \psi}{\partial x_3}\right]^{\mathsf{T}} \\
&= \left[\psi\frac{\partial \phi}{\partial x_1}, \psi\frac{\partial \phi}{\partial x_2}, \psi\frac{\partial \phi}{\partial x_3}\right]^{\mathsf{T}} + \left[\phi\frac{\partial \psi}{\partial x_1}, \phi\frac{\partial \psi}{\partial x_2}, \phi\frac{\partial \psi}{\partial x_3}\right]^{\mathsf{T}} \\
&= \psi\left[\frac{\partial \phi}{\partial x_1}, \frac{\partial \phi}{\partial x_2}, \frac{\partial \phi}{\partial x_3}\right]^{\mathsf{T}} + \phi\left[\frac{\partial \psi}{\partial x_1}, \frac{\partial \psi}{\partial x_2}, \frac{\partial \psi}{\partial x_3}\right]^{\mathsf{T}} \\
&= \phi\nabla\psi + \psi\nabla\phi,
\end{aligned}
$$

and:

$$
\begin{aligned}
\nabla\cdot(\phi\mathbf{f}) &= \left[\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}\right]^{\mathsf{T}} \cdot [\phi f_1, \phi f_2, \phi f_3]^{\mathsf{T}} \\
&= \frac{\partial}{\partial x_1}\phi f_1 + \frac{\partial}{\partial x_2}\phi f_2 + \frac{\partial}{\partial x_3}\phi f_3 \\
&= \frac{\partial \phi}{\partial x_1} f_1 + \frac{\partial f_1}{\partial x_1}\phi + \frac{\partial \phi}{\partial x_2} f_2 + \frac{\partial f_2}{\partial x_2}\phi + \frac{\partial \phi}{\partial x_3} f_3 + \frac{\partial f_3}{\partial x_3}\phi \\
&= \left(\frac{\partial \phi}{\partial x_1} f_1 + \frac{\partial \phi}{\partial x_2} f_2 + \frac{\partial \phi}{\partial x_3} f_3\right) + \left(\phi\frac{\partial f_1}{\partial x_1} + \phi\frac{\partial f_2}{\partial x_2} + \phi\frac{\partial f_3}{\partial x_3}\right) \\
&= \nabla\phi\cdot\mathbf{f} + \phi\nabla\cdot\mathbf{f},
\end{aligned}
$$

□

PROBLEM 2. Please try to subsitute the following free energy functional into Cahn-Hilliard equation get the gonvering equation:

$$
F(x, c, \nabla c) = \int_\Omega f(c) + \frac{\kappa}{2}(\nabla c)^2 \,\mathrm{d}v.
$$

Notice that the mobility M_{ij} of Cahn-Hilliard equation is considered as a constant:

$$\begin{aligned}\frac{\partial c_i}{\partial t} &= \nabla \cdot M_{ij} \nabla \frac{\delta F}{\delta c_j\left(r, t\right)} \\ &= M \nabla^2 \frac{\delta F}{\delta c_j\left(r, t\right)}.\end{aligned}$$

Solution. The variational derivative of a functional of the following form:

$$J[y] = \int_{\Omega} L(x, y(x), \nabla y(x))\, \mathrm{d}\omega$$

is:

$$\frac{\delta J[y]}{\delta y} = \frac{\partial L}{\partial y} - \nabla \cdot \frac{\partial L}{\partial \nabla y}.$$

Thus, by taking variational derivative of the free energy functional: $F[c] = F(x, c, \nabla c)$, and define free energy density $f_t(x, c, \nabla c) = f(c) + \frac{\kappa}{2}\left(\nabla c\right)^2$, we will get:

$$\begin{aligned}\frac{\delta F}{\delta c_j} &= \frac{\partial f_t}{\partial c_j} - \nabla \cdot \frac{\partial f_t}{\partial \nabla c_j}. \\ &= \frac{\partial f}{\partial c_j} - \nabla \cdot \left(\kappa \nabla c_j\right) \\ &= \frac{\partial f}{\partial c_j} - \kappa \nabla^2 c_j.\end{aligned}$$

So, the final gonvering equation will be:

$$\frac{\partial c_i}{\partial t} = M \nabla^2 \left(\frac{\partial f}{\partial c_j} - \kappa \nabla^2 c_j\right).$$

Note of Problem 2.

1. The variational derivative of a functional F with gradient of function (∇c) as its derivative to the variable (y') should replace $\frac{\mathrm{d}}{\mathrm{d}x}()$ with $\nabla \cdot ()$. You can refer to the Wiki for more information.

2. Take a look at the integrand of the free energy functional, you will find that $\left(\nabla c\right)^2$ should be a scalar. Indeed this is the inner product

of the gradient of concentration. Fortunately, the derivative of $\nabla c \cdot \nabla c$ with respect to the vector ∇c is still $2\nabla c$.

3. There is another way to consider the variational derivative, especially the latter part of the Euler-Lagrange function. Below is from this blog :

$$
\begin{aligned}
\delta F &= \delta \int_\Omega \left(f(c) + \frac{\kappa}{2} (\nabla c)^2 \right) \mathrm{d}\omega \\
&= \delta \int_\Omega \left(f(c) + \frac{\kappa}{2} |\nabla c|^2 \right) \mathrm{d}\omega \\
&= \int_\Omega (\delta f(c) + \kappa\, \delta \partial_i c\, \partial_i c) \, \mathrm{d}\omega \\
&= \int_\Omega \left(\frac{\partial f(c)}{\partial c} \delta c + \kappa\, \partial_i \delta c\, \partial_i c \right) \mathrm{d}\omega \\
&= \int_\Omega \left(\frac{\partial f(c)}{\partial c} \delta c + \kappa \left[\partial_i (\partial_i c \delta c) - \partial_i \partial_i c \delta c \right] \right) \mathrm{d}\omega \\
&= \int_\Omega \left(\frac{\partial f(c)}{\partial c} - \kappa \partial_i \partial_i c \right) \delta c \mathrm{d}\omega + \int_\Omega \kappa \partial_i (\partial_i c \delta c) \, \mathrm{d}\omega \\
&= \int_\Omega \left(\frac{\partial f(c)}{\partial c} - \kappa \partial_{ii} c \right) \delta c \mathrm{d}\omega + \int_{\partial\Omega} \kappa \partial_i c n_i \, \delta c \mathrm{d}\omega \\
&= \int_\Omega \left(\frac{\partial f(c)}{\partial c} - \kappa \nabla^2 c \right) \delta c \mathrm{d}\omega + \int_{\partial\Omega} \kappa \nabla c \cdot \mathbf{n} \, \delta c \mathrm{d}\omega
\end{aligned}
$$

Now as the gradient is perpendicular to the normal vector along the edge of the solving domain $\partial\Omega$, the last term $\nabla c \cdot \mathbf{n}$ should be 0. By this way, we, in another way, obtain the variational derivative of free energy functional.