Quiz Assignment
MS5033

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Problem 1: Variational Derivative of a Functional

$$F[\phi] = \int_\Omega [f(\phi, \nabla\phi)]dV \tag{1}$$

Pertub ϕ by $\delta\phi$ such that $\phi \to \phi + \delta\phi$ and $\nabla\phi \to \nabla\phi + \nabla\delta\phi$.

$$\begin{aligned} F[\phi + \delta\phi] &= \int_\Omega [f(\phi + \delta\phi, \nabla\phi + \nabla\delta\phi)]dV \\ &= \int_\Omega [f(\phi, \nabla\phi) + \delta\phi\frac{\partial f}{\partial\phi} + \nabla\delta\phi \cdot \frac{\partial f}{\partial\nabla\phi}]dV \end{aligned} \tag{2}$$

Subtracting (1) from (2) we get,

$$\begin{aligned} \delta F &= F[\phi + \delta\phi] - F[\phi] \\ &= \int_\Omega [\delta\phi\frac{\partial f}{\partial\phi} + \nabla\delta\phi \cdot \frac{\partial f}{\partial\nabla\phi}]dV \end{aligned} \tag{3}$$

Using integration by parts on the second term in (3),

$$\begin{aligned} \delta F &= \int_\Omega [\delta\phi\frac{\partial f}{\partial\phi}]dV + [\frac{\partial f}{\partial\nabla\phi}\delta\phi]_{\partial\Omega} - \int_\Omega [\nabla \cdot \frac{\partial f}{\partial\nabla\phi}\delta\phi]dV \\ &= \int_\Omega [\delta\phi\frac{\partial f}{\partial\phi} - \nabla \cdot \frac{\partial f}{\partial\nabla\phi}\delta\phi]dV \\ &= \int_\Omega [\frac{\partial f}{\partial\phi} - \nabla \cdot \frac{\partial f}{\partial\nabla\phi}]\delta\phi dV \end{aligned} \tag{4}$$

In (4), as $\delta\phi$ is zero at the boundary, the second term vanishes.
For stationary condition, integral must hold for all variations $\delta\phi$.

$$\boxed{\frac{\partial F}{\partial\phi} = \frac{\partial f}{\partial\phi} - \nabla \cdot \frac{\partial f}{\partial\nabla\phi}} \tag{5}$$

Problem 2: Functional Derivative of Phase-Field Free Energy

Part (a)

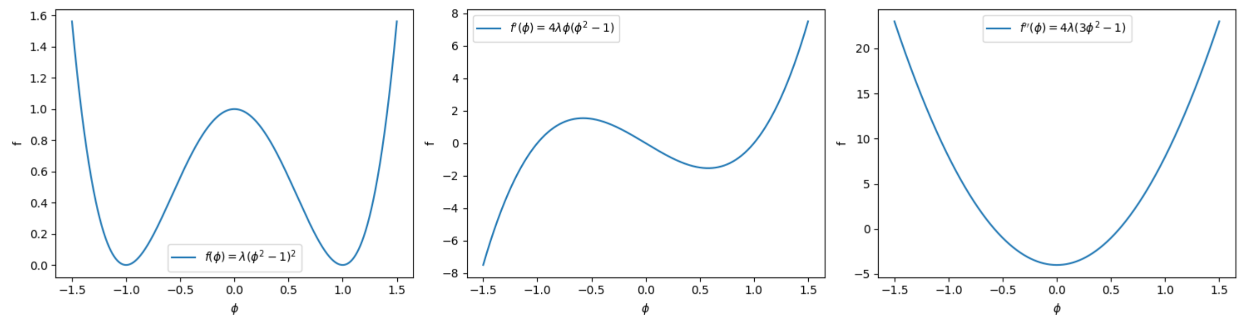

Figure 1: Function and its derivatives separately

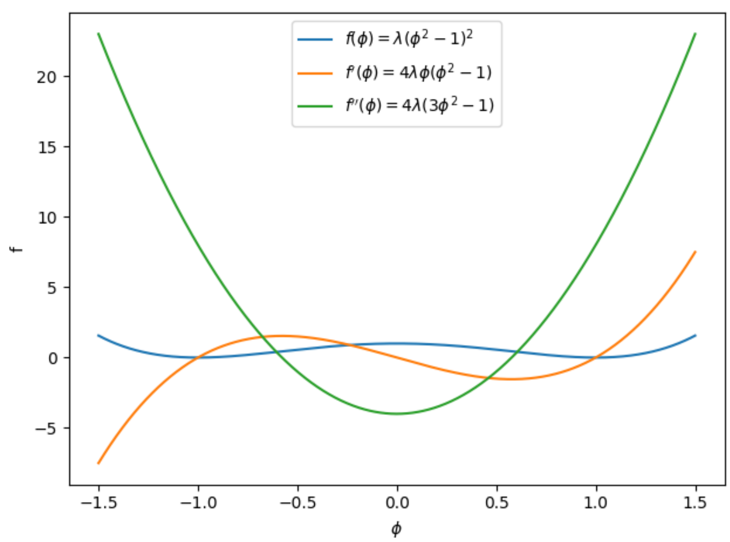

Figure 2: Function and its derivatives combined

Part (b)

Refer to the python notebook for the code implementation.

Part (c)

$$F[\phi] = \int_\Omega [\frac{\kappa}{2}(\nabla\phi)^2 + f(\phi)]dV$$

Here, $f(\phi, \nabla\phi) = \frac{\kappa}{2}(\nabla\phi)^2 + f(\phi)$.
We know that,

$$\begin{aligned}\frac{\partial F}{\partial \phi} &= \frac{\partial f}{\partial \phi} - \nabla \cdot \frac{\partial f}{\partial \nabla\phi} \\ &= \frac{\partial f}{\partial \phi} - \nabla \cdot \frac{\partial(\frac{\kappa}{2}(\nabla\phi)^2)}{\partial \nabla\phi}\end{aligned}$$

$$\boxed{\frac{\partial F}{\partial \phi} = \frac{\partial f}{\partial \phi} - \nabla \cdot \kappa \nabla\phi}$$

Part (d)

$\frac{\partial f}{\partial \phi}$: local energy density of the phase-field variable ϕ. Represents phase separation behavior using a double-well potential $f(\phi)$.

$\nabla \cdot \kappa\nabla\phi$: Introduces diffusion of the phase-field variable ϕ with a diffusivity κ. Acts as a smoothing term, ensuring that ϕ transitions gradually between phases.

Case Study 1: Derivation of the Cahn-Hillard Equation

Part (a)

$$F[\phi] = \int_\Omega [\frac{\kappa}{2}(\nabla\phi)^2 + f(\phi)]dV$$

Here, $f(\phi, \nabla\phi) = \frac{\kappa}{2}(\nabla\phi)^2 + f(\phi)$.
We know that,

$$\begin{aligned}\frac{\partial F}{\partial \phi} &= \frac{\partial f}{\partial \phi} - \nabla \cdot \frac{\partial f}{\partial \nabla\phi} \\ &= \frac{\partial f}{\partial \phi} - \nabla \cdot \frac{\partial(\frac{\kappa}{2}(\nabla\phi)^2)}{\partial \nabla\phi}\end{aligned}$$

$$\boxed{\mu = \frac{\partial F}{\partial \phi} = \frac{\partial f}{\partial \phi} - \nabla \cdot \kappa \nabla\phi}$$

Part (b)

By conservative law,

$$\frac{\partial \phi}{\partial t} = \nabla \cdot (M\nabla\mu)$$

$$\boxed{\frac{\partial \phi}{\partial t} = \nabla \cdot (M\nabla(\frac{\partial f}{\partial \phi} - \nabla \cdot \kappa\nabla\phi))}$$

Case Study 2: Boundary Conditions in Cahn-Hillard Equation

Part (a)

Consider the Cahn-Hillard equation,

$$\frac{\partial \phi}{\partial t} = \nabla \cdot (M\nabla(\frac{\partial f}{\partial \phi} - \nabla \cdot \kappa \nabla \phi))$$

where $F[\phi] = \int_\Omega [\frac{\kappa}{2}(\nabla \phi)^2 + f(\phi)]dV$.
Variational principle by considering first variation of $F[\phi]$,

$$\delta F = \int_\Omega [\delta \phi \frac{\partial f}{\partial \phi} - \nabla \cdot \kappa \nabla \delta \phi]dV + \int_{\partial \Omega} [\kappa \nabla \phi \cdot \delta \phi]dS$$

- **No-flux boundary condition**: $n \cdot \nabla \phi = 0$ at $\partial \Omega$. This ensures no transport of ϕ across the boundary. As $\mu = \frac{\partial f}{\partial \phi} - \nabla \cdot \kappa \nabla \phi$, imples $\nabla \cdot (\nabla f' - \nabla \cdot \kappa \nabla \phi) = 0$.
- **Dirichlet boundary condition**: $\phi = \phi_0$ at $\partial \Omega$. This ensures a fixed value of ϕ at the boundary.
- **Neumann boundary condition**: $\nabla \phi \cdot n = g$ at $\partial \Omega$. This ensures a fixed flux of ϕ at the boundary.
- **Periodic boundary condition**: Ensures that ϕ and its derivatives repeat across boundaries, often used for systems without explicit boundaries: $\phi(x) = \phi(x + L)$, and $\nabla \phi(x) = \nabla \phi(x + L)$.

Part (b)

Physical interpretation of the boundary conditions are as follows:

- **No-flux boundary condition**: Used in closed systems where the total amount of ϕ is conserved. It ensures that there is no transport of ϕ across the boundary ensuring mass conservation.
- **Dirichlet boundary condition**: Used when the value of ϕ is known at the boundary. It ensures that the value of ϕ is fixed at the boundary.
- **Neumann boundary condition**: Used when the flux of ϕ is known at the boundary. Controls the rate of phase separation at boundaries, often used in systems with external driving forces.
- **Periodic boundary condition**: Used in systems without explicit boundaries. It ensures that the system is translationally invariant, often used in systems with periodic structures.

Part (c)

Periodic boundary conditions are widely used to approximate infinite systems by eliminating boundary effects.

- Seamless continuation of the phase separation process without artificial walls.
- Effiecient implementation of Fourier transforms for solving the Cahn-Hilliard equation.
- Eliminates the need for explicit boundary conditions, simplifying the problem.

Problem 5: Interpretation of the Cahn-Hillard Equation

Part (a)

Diffusive term $\nabla \cdot (M\nabla\mu)$

- The diffusive term is responsible for the diffusion of the phase-field variable ϕ.
- Unlike regular diffusion, the diffusive term includes chemical potential gradient $\nabla\mu$, which drives phase seperation rather than simple concentration gradient.
- The diffusive term is proportional to the mobility M and the Laplacian of the chemical potential μ. The Laplacian of the chemical potential μ is the driving force for the diffusion of the phase-field variable ϕ.

$\nabla^2 \frac{\partial f}{\partial \phi}$ term

- The higher-order term $-\kappa\nabla^2\phi$ introduces interfacial effects, penalizing sharp gradients and enforcing a smooth transition between phases.
- The bulk free energy density $f(\phi)$ contributes $\frac{\partial f}{\partial \phi}$ dictating the preferred phases.
- This term leads to phase separation with surface tension effects, unlike ordinary diffusion which homogenizes concentration.

Part (b)

- The diffusion equation leads to smooth spreading of ϕ, whereas the Cahn-Hilliard equation leads to phase separation and domain formation due to the higher-order derivative term.
- Diffusion eqaution uses Flick's second law, whereas Cahn-Hilliard equation uses phase separation dynamics.
- The diffusion equation is a linear equation, whereas the Cahn-Hilliard equation is a nonlinear equation.
- The Cahn-Hilliard equation ensures conserved dynamics, meaning the total amount of each phase remains fixed, unlike the diffusion equation.

Part (c)

Application of Cahn-Hillard equation are as follows:

- **Image Impainting:** Image inpainting is the filling in of damaged or missing regions of an image with the use of information from surrounding areas.Let f(x), where x = (x, y), be a given binary image in a domain Ω and $D \subset \Omega$ be the inpainting domain. The image is scaled so that $0 \leq f \leq 1$. Let c(x, t) be a phase-field which is governed by the following modified CH equation:

$$c_t(x,t) = \nabla\mu(x,t) + \lambda(f(x) - c(x,t))$$
$$\mu(x,t) = F'(c(x,t)) - \epsilon^2\nabla^2 c(x,t), \text{where} F(c) = \frac{1}{4}c^2(1-c)^2$$

- **Tumor Growth Simulation:** To provide optimal strategies for treatments, a mathematical modeling is very useful since it gives systematic investigation. Let Ω be a computational domain. Let $\Omega_H, \Omega_V, \Omega_D$ be the healthy, viable, and dead tumor tissues, respectively. The Cahn-Hilliard equation naturally captures the evolution of these phases over time, leading to the formation of distinct tumor boundaries.

- **Spinodal Decomposition:** A system of the CH equations is the leading model of spinodal decomposition in binary alloys. Spinodal decomposition is a process by which a mixture of two materials can separate into distinct regions with different material concentrations.

- **Two Phase Fluid Flows:** In the two-phase fluid flow problem, we use the CH equation for capturing the interface location between two immiscible fluids. The CH equation provides a good mass conservation property. We model the variable quantities such as viscosity and density by using the phase-field. Also, we model the surface tension effect with the phase-field. The velocity field is governed by the modified Navier–Stokes equation.

Problem 6: Computing Variational Derivative using SymPy

Refer to the python notebook for the code implementation.