Quiz Assignment on Variational Derivatives and the Cahn-Hilliard Equation

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Instructions

Answer all questions with detailed steps and justifications. Simplify expressions wherever possible.

Problem 1: Variational Derivative of a Functional

Given a functional of the form

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

where Ω is the domain, compute the variational derivative $\frac{\delta F}{\delta \phi}$ explicitly in terms of $f(\phi, \nabla\phi)$.

Problem 2: Functional Derivative of a Phase-Field Free Energy

Consider the double-well potential function

$$f(\phi) = \lambda(\phi^2 - 1)^2, \tag{2}$$

where λ is a constant.

(a) Sketch the function $f(\phi)$, its first derivative $\frac{df}{d\phi}$, and its second derivative $\frac{d^2 f}{d\phi^2}$ as a function of ϕ.

(b) Using Python and Matplotlib, write a script to plot these functions. A sample script is provided below:

```
import numpy as np
import matplotlib.pyplot as plt

phi = np.linspace(-2, 2, 100)
lambda_val = 1
f_phi = lambda_val * (phi**2 - 1)**2
df_phi = 4 * lambda_val * phi * (phi**2 - 1)
```

```
d2f_phi = 4 * lambda_val * (3*phi**2 - 1)

plt.figure(figsize=(10,4))
plt.subplot(1,3,1)
plt.plot(phi, f_phi, label='$f(\phi)$')
plt.xlabel('$\phi$')
plt.legend()

plt.subplot(1,3,2)
plt.plot(phi, df_phi, label='$df/d\phi$', color='r')
plt.xlabel('$\phi$')
plt.legend()

plt.subplot(1,3,3)
plt.plot(phi, d2f_phi, label='$d^2f/d\phi^2$', color='g')
plt.xlabel('$\phi$')
plt.legend()

plt.tight_layout()
plt.show()
```

(c) Consider the phase-field free energy functional

$$F[\phi] = \int_{\Omega} \left[\frac{\kappa}{2} (\nabla \phi)^2 + f(\phi) \right] dV. \tag{3}$$

Compute the functional derivative $\frac{\delta F}{\delta \phi}$.

(d) Discuss the physical interpretation of each term in the result.

Case Study 1: Derivation of the Cahn-Hilliard Equation

The Cahn-Hilliard equation describes phase separation in a conserved order parameter system. Consider the free energy functional

$$F[\phi] = \int_{\Omega} \left[\frac{\kappa}{2} (\nabla \phi)^2 + f(\phi) \right] dV, \tag{4}$$

where ϕ is a conserved order parameter.

(a) Compute the chemical potential $\mu = \frac{\delta F}{\delta \phi}$.

(b) Apply the conservation law

$$\frac{\partial \phi}{\partial t} = \nabla \cdot (M \nabla \mu), \tag{5}$$

where M is the mobility, to derive the Cahn-Hilliard equation.

Case Study 2: Boundary Conditions in the Cahn-Hilliard Equation

Boundary conditions play a crucial role in determining the evolution of phase separation. Consider the following common types of boundary conditions:

- **No-flux boundary condition:** $\mathbf{n} \cdot \nabla\mu = 0$ ensures that there is no transport of ϕ across the boundary.
- **Dirichlet boundary condition:** Specifies a fixed value of ϕ on the boundary, such as $\phi(\mathbf{x}) = \phi_0$.
- **Neumann boundary condition:** Ensures that the derivative of ϕ normal to the boundary is specified.
- **Periodic boundary condition:** Assumes that ϕ and its derivatives repeat at the boundaries, i.e., $\phi(x + L) = \phi(x)$.

(a) Derive the necessary boundary conditions for the system. (b) Discuss the physical significance of these boundary conditions in the context of phase separation. (c) Explain how periodic boundary conditions influence the numerical implementation of the Cahn-Hilliard equation.

Problem 5: Interpretation of the Cahn-Hilliard Equation

(a) Explain the role of the diffusion term and the term $\nabla^2(\frac{df}{d\phi})$ in the Cahn-Hilliard equation.
(b) How does the Cahn-Hilliard equation differ from the diffusion equation:

$$\frac{\partial\phi}{\partial t} = \nabla \cdot D\nabla\phi. \tag{6}$$

(c) Do a Google search to find applications of the Cahn-Hilliard equation in various fields of science and engineering, including fluid dynamics, image processing, pattern recognition, microelectronic packaging, manufacturing processes, and so on. Write a short summary of this. More credits will be given to those summaries that list more unique applications.

Problem 6: Computing Variational Derivatives using SymPy

(a) Write a Python script using SymPy to compute the functional derivative of the phase-field free energy functional:

$$F[\phi] = \int_\Omega \left[\frac{\kappa}{2}(\nabla\phi)^2 + f(\phi)\right] dV. \tag{7}$$

(b) Extend the script to verify the variational derivative of a more complex functional, such as:

$$F[\phi] = \int_{\Omega} \left[\frac{\kappa}{2} (\nabla \phi)^2 + \lambda (\phi^2 - 1)^2 \right] dV. \tag{8}$$

One can use the SymPy notebook posted in the classroom to calculate the variational derivatives using computer algebra.

End of Assignment