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A phase-field fluid modeling and computation with interfacial profile correction term

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ABSTRACT

We present a new phase-field fluid model and computation with minimized Cahn–Hilliard (CH) dynamics. Using the CH equation, the internal structure of the interface layer is determined by explicit smoothing flow discontinuities. This method greatly simplifies gridding, discretization, and handling of topological changes. The original CH equation, however, has intrinsic dynamics such as interface length minimization, i.e., the motion by minus the Laplacian of the mean curvature. When the CH equation is applied to the modeling of multiphase fluid flows, we want to minimize its interface length minimization property. The surface tension formulation also requires the multiphase fluid interface to be a hyperbolic tangent profile. Typically, under the advection of flow, the interfacial transition is not a hyperbolic tangent profile, i.e., it is too compressed or sharpened. Even though the original CH dynamics conserves the total mass, the enclosed area obtained by its interface is not preserved. To overcome these shortcomings, we propose a modified CH equation with an interfacial profile correction term. Several numerical examples are presented to show the accuracy of the proposed method. The numerical results demonstrate that the proposed modified CH equation preserves the enclosed area better than the original CH equation.

1. Introduction

We present a phase-field fluid model and computation with minimized Cahn–Hilliard (CH) dynamics. The original CH equation was introduced to model spinodal decomposition in binary alloys [1] and arises from the Helmholtz free energy functional

$$\mathcal{E}_{\mathrm{CH}}(\phi) = \int_{\Omega} \left(F(\phi) + \frac{\epsilon^2}{2} |\nabla \phi|^2 \right) d\mathbf{x},$$

where $\Omega \subset \mathbb{R}^d$ (d is the space dimension), $F(\phi) = 0.25(\phi^2 - 1)^2$, and ϵ is a positive constant. The quantity $\phi(\mathbf{x}, t)$ is defined as the difference between the mole fractions of binary mixtures. The CH equation takes the form

$$\frac{\partial \phi}{\partial t}(\mathbf{x}, t) = M \Delta \mu(\mathbf{x}, t), \mathbf{x} \in \Omega, 0 < t \leq T, \tag{1}$$

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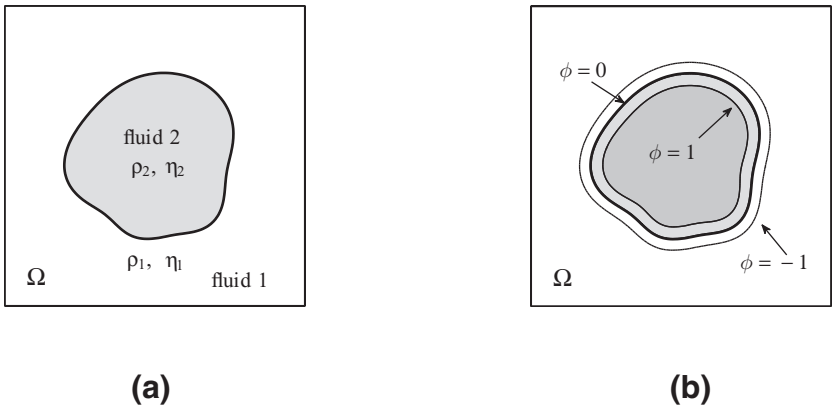

Fig. 1. Schematic illustration of the computational problem. (a) Two fluids. (b) Phase-field.

$$\mu(\mathbf{x},t) = F'(\phi(\mathbf{x},t)) - \epsilon^2\Delta\phi(\mathbf{x},t), \tag{2}$$

$$\mathbf{n}\cdot\nabla\mu(\mathbf{x},t) = 0, \mathbf{x}\in\partial\Omega, \tag{3}$$

where M is the positive constant mobility and $\mathbf{n}$ is the outward normal vector at the boundary. The CH equation can be derived from a constrained gradient flow in the $\dot{H}^{-1}$ Hilbert space. It guarantees that the total free energy $\mathcal{E}_{\mathrm{CH}}(\phi)$ decreases in time t [2]. The solution $\phi(\mathbf{x}, t)$ to Eqs. (1)–(3) possesses the properties that the total mass is conserved, i.e., $d(\int_\Omega \phi d\mathbf{x})/dt = 0$, and the total energy $\mathcal{E}_{\mathrm{CH}}(t)$ decreases with time. Governing equations for the flow are obtained by coupling the momentum and CH equations. The CH equation has been successfully applied to a wide range of problems in materials science [5,6], biology [7,8], image processing [9,10], surface/volume reconstruction [11], and fluid dynamics [12–23,25–44] (see the recent review paper [32] and the references therein). Using the CH equation, the internal structure of the interface layer can be determined by explicit smoothing flow discontinuities. This method greatly simplifies gridding, discretization, and handling of topological changes. The momentum equation is a modified Navier–Stokes equation:

$$\rho(\phi)(\mathbf{u}_t + \mathbf{u}\cdot\nabla\mathbf{u}) = -\nabla p + \nabla\cdot(\eta(\phi)(\nabla\mathbf{u} + \nabla\mathbf{u}^T)) + \sigma\mathbf{SF}(\phi) + \rho(\phi)\mathbf{g}, \tag{4}$$

$$\nabla\cdot\mathbf{u} = 0, \tag{5}$$

where $\mathbf{u}$ is the velocity, p is the pressure, σ is the surface tension coefficient, and $\mathbf{g} = (0, -g)$ is the gravity. The density $\rho(\phi)$ and viscosity $\eta(\phi)$ are assumed to be linearly related to the concentration ϕ:

$$\rho(\phi) = \rho_1(1-\phi)/2 + \rho_2(1+\phi)/2 \quad \text{and} \quad \eta(\phi) = \eta_1(1-\phi)/2 + \eta_2(1+\phi)/2,$$

where ρ_1 and ρ_2 are the densities of fluid 1 and fluid 2, respectively. η_1 and η_2 are the viscosities of fluid 1 and fluid 2, respectively. A schematic illustration of the computational problem is shown in Fig. 1.

The interfacial force $\mathbf{SF}(\phi)$ satisfying the Laplace–Young condition is defined as $\mathbf{SF}(\phi) = -\kappa(\phi)\delta(\phi)\mathbf{n}_s(\phi)$, where $\mathbf{n}_s(\phi)$ is the outward unit normal vector to the interface of the two phases, $\kappa(\phi)$ is the mean curvature, and $\delta(\phi)$ is the surface Dirac-delta distribution. Furthermore, $\mathbf{n}_s$, κ and δ are given by $\mathbf{n}_s = -\nabla\phi/|\nabla\phi|$, $\kappa = \nabla\cdot\mathbf{n}_s$, and $\delta = \epsilon\alpha|\nabla\phi|^2$ [3], respectively. The CH dynamics is characterized by transition layers between two phases with an equilibrium profile [4]:

$$\phi^{eq}(r) = \tanh(r/(\sqrt{2}\epsilon)). \tag{6}$$

The local coordinate r is from the outside of the surface to the inside normally and is zero at the interface. With the equilibrium composition profile, α can be computed as $\alpha = 3\sqrt{2}/4$ by solving $\epsilon\alpha\int_{-\infty}^{\infty}(\phi_r^{eq})^2 dr = 1$. Thus, the interface of the two phases should be a hyperbolic tangent profile to accurately calculate the surface tension force. However, when an advection term is added, the interface of the two phases may not be a hyperbolic tangent profile. The original CH equation has intrinsic dynamics such as interface length minimization, i.e., the motion by minus the Laplacian of the mean curvature [45]. Thus, when the CH equation is applied to model multiphase fluid flows, we want to minimize its interface length minimization property. In practice, when a large time step or coarse grid is used, the interface length minimization property of the CH equation is significant. Furthermore, although the CH dynamics conserves the total mass over the entire domain, it typically does not preserve the area enclosed by the interface of the two phases. Yue et al. [46] noted that the equilibrium solution of the CH equation is similar to, but not equal to a hyperbolic tangent profile; the solution to the CH equation is in $[-1+\beta, 1+\beta]$, where β is a small value related to the thickness ϵ, the volume of the whole computational domain and drop. This is because the total energy can be reduced by shrinking the drop while simultaneously shifting the bulk ϕ slightly away from the initial values (see Fig. 2). Therefore, the CH