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Optimal mass transport-based adaptive mesh method for phase-field models of two-phase fluid flows

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ABSTRACT

In this paper, we present an efficient adaptive mesh method for solving phase-field model of a mixture of two-phase incompressible fluid flows. The adaptive mesh is generated by a coordinate transformation that is determined as the solution of the classical problem of the optimal mass transportation, also known as Monge–Kantorovich problem (MKP). The numerical solution of the MKP is computed by taking the gradient of the steady state solution of a parabolic Monge–Ampère equation (PMAE). Several numerical experiments are conducted to demonstrate the performance of the PMAE method for solving phase-field models. The numerical results illustrate that the adaptive mesh computed with PMAE method captures well the moving interface of the phase-field function.

1. Introduction

Phase-field method has recently become popular within the materials science and engineering communities because it avoids some of the problems associated with the sharp interface models, e.g. the complexity of the numerical simulation of sharp interface models in particular in the events of merging or pinch-off over the course of phase transformation (for more details, e.g. see [1–3]). Phase-field method maintains a continuous transition between the two sides of the interface. Several numerical methods have been proposed to solve the phase-field models on a fixed uniform grid, for example see [4–6]. However, using a uniform mesh to accurately resolve the spatial derivatives of the phase function at the thin moving interface requires an extremely fine mesh, and as a result the computations become prohibitively expensive and inefficient. For these problems, it becomes critical to use adaptive mesh methods in order to approximate the spatial derivatives more accurately and reduce the computational cost. There are two approaches for mesh adaptation, the first is h-method which involves local refinement or coarsening of the spatial mesh by adding or removing points based on a posterior error estimates. The second approach is the r-method or moving mesh method which uses a fixed number of mesh points that are continuously redistributed so that they are sufficiently concentrated in regions of large physical solution variations. The mesh concentration is controlled by some measure of the solution variation or error which is called the adaptation function (or monitor function). In this work, we use the second approach to generate the adaptive mesh for phase-field models of two-phase incompressible fluid flows.

For standard moving mesh methods, the mesh redistribution is done by constructing a continuous time-dependent coordinate transformation,

$$\boldsymbol{x} = \boldsymbol{x}(\boldsymbol{\xi}, t), \quad \boldsymbol{\xi} \in \Omega_c, \ \boldsymbol{x} \in \Omega \tag{1.1}$$

where Ω_c is the logical or computational domain and Ω is the physical domain. The adaptive mesh is then obtained as the image of a given fixed uniform grid in Ω_c. In one spatial dimension, the transformation $\boldsymbol{x} = \boldsymbol{x}(\boldsymbol{\xi}, t)$ is typically determined by

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the equidistribution principle where a measure of the solution variation or error is equally distributed over each subinterval of the physical domain Ω (see [7–9] and the references therein for more details). In practice, the so called adaptation (or monitor) function $\rho(\boldsymbol{x}, t)$ is used as a measure of the physical solution variation or error. In higher dimensions, one needs an extra set of constraints to uniquely determine the coordinate transformation that generates the adaptive mesh. Over the last decade several moving mesh methods have been developed for two- and three-dimensional problems (for example, see [10–15]).

Shen and Yang [16] applied a variational moving mesh PDE method of [17,18] with spectral method for the Allen–Cahn equations. In [19], a finite element moving mesh method is used for the Allen–Cahn phase-field model.

In this paper, we propose the PMAE method [15] to solve the modified Allen–Cahn phase-field model more efficiently. The PMAE method is based on solving a parabolic Monge–Ampère equation. In [15], we show that the parabolic Monge–Ampére equation converges to the unique solution of the L^2 optimal mass transfer, also known as L^2 Monge–Kantorovich problem (MKP) [20–22].

The rest of the paper is organized as follows. In Section 2 we describe the phase-field model of two-phase incompressible fluid flows. In Section 3, we present the PMAE adaptive grid method to solve the modified Allen–Cahn phase-field model. Several numerical experiments are given in Section 4 to demonstrate the accuracy and effectiveness of the PMAE adaptive grid method for solving the phase-field model. In Section 5, we give some concluding remarks.

2. Phase-field model for a mixture of two incompressible fluids

We study a phase-field model of a mixture of two-phase flows as described in [16]. To this end, consider a physical domain $\Omega \subset \mathbb{R}^d, d = 2,$ or 3 that is filled with a mixture of two incompressible viscous fluids separated by a thin free moving interface. The interface is described by a phase-field function $\phi(\boldsymbol{x}, t)$ defined on the physical domain Ω. On the interface $\phi(\boldsymbol{x}, t) = 0$, on one side of the interface $\phi(\boldsymbol{x}, t) = 1$, and on the other side $\phi(\boldsymbol{x}, t) = -1$. Therefore, at any given time the interface is formed by the points $x \in \Omega$ that satisfy $\phi(\boldsymbol{x}, t) = 0$. The time evolution of the phase function ϕ is governed by the Allen–Cahn equation given as the gradient flow [2,4]

$$\phi_t + \boldsymbol{u} \cdot \nabla\phi = -\gamma \frac{\partial W}{\partial \phi} = \gamma \left(\Delta\phi - \frac{1}{\hat{\eta}^2}\phi(\phi^2 - 1) \right) \tag{2.1}$$

where $\boldsymbol{u}$ is the velocity of the fluids, γ is the time relaxation parameter and $W(\phi)$ is the elastic (mixing) energy functional for the interaction between the two fluids defined as

$$W(\phi, \nabla\phi) = \int_\Omega \left(\frac{1}{2} |\nabla\phi|^2 + F(\phi) \right) dx, \tag{2.2}$$

where

$$F(\phi) = \frac{1}{4\hat{\eta}^2} \left(\phi^2 - 1\right)^2, \tag{2.3}$$

is the double-well potential of the mixing energy and $\hat{\eta}$ is the width of the mixing layer.

The original phase-field model (2.1) does not conserve the volume fraction. Shen and Yang [16] introduce the modified Allen–Cahn phase-field model (also see[23])

$$\phi_t + \boldsymbol{u} \cdot \nabla\phi = \gamma \left(\Delta\phi - \frac{1}{\hat{\eta}^2}\phi(\phi^2 - 1) + \hat{\xi}(t) \right), \tag{2.4a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \phi \mathrm{d}\boldsymbol{x} = 0, \tag{2.4b}$$

where $\hat{\xi}(t)$ is the Lagrange multiplier introduced so that the volume fraction, defined as $\int_\Omega \phi \mathrm{d}\boldsymbol{x}$, is conserved by the constraint (2.4b).

In this work, we consider a mixture of two incompressible fluid flows with the same constant densities, $\rho_1 = \rho_2 = 1$ and same viscosity constants. The time evolution of the fluid flow is then governed by the incompressible Navier–Stokes equations and the continuity equation [4,24]

$$\boldsymbol{u}_t + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} - \nu\Delta\boldsymbol{u} + \nabla p + \lambda\nabla \cdot (\nabla\phi \otimes \nabla\phi) = g(x), \tag{2.5a}$$

$$\nabla \cdot \boldsymbol{u} = 0, \tag{2.5b}$$

where p is the pressure, g is the external body force, ν is the kinematic viscosity constant, $\nabla\phi \otimes \nabla\phi$ is the stress tensor product, where $\nabla \cdot (\nabla\phi \otimes \nabla\phi) = \Delta\phi\nabla\phi + \frac{1}{2}\nabla(|\nabla\phi|^2)$, and λ corresponds to the surface tension.

The system of equations (2.4) and (2.5) is supplied with the initial conditions

$$\phi(\boldsymbol{x}, 0) = \phi_0(\boldsymbol{x}), \qquad \boldsymbol{u}(\boldsymbol{x}, 0) = \boldsymbol{u}_0(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega, \tag{2.6}$$

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