Numerical simulation for different densities multi-phase fluids with an energy law preserving method

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Abstract. In this paper, we present a numerical investigation for simulating fluid-fluid interface of isothermal multi-phase fluids with a phase field model. Unlike the previous work, we use continuous finite element method to compute the governing equations and get a discrete energy law equation with a special designed scheme which is almost the same as the continuous energy law. We deal with the stability in pressure by using a penalty formulation to rewrite the continuity condition. The accuracy of calculation is examined by numerical simulation of coalescence of two kissing bubbles. And the accuracy of the discrete energy law is validated as the error in the energy law of numerical examples falls below $10^{-10}$ and this energy law at the discrete level is preserved at each time step.

1. Introduction

Multi-phase fluids have been widely applied in biology, chemistry, physics and engineering, such as the application of nan fluids in cooling equipment’s, boiling tube in nuclear power station and liquid-vapor separator and so on [2]. Multiphase fluids have attracted more and more attention to investigate the mechanism of flows for satisfying the high-speed developing technology.

There are two kinds of theoretical models named sharp interface model and phase field model widely used for multi-phase fluids with clear interface. Sharp interface model [3] uses the single phase fluid model to simulate each phase and treats the interface as the boundary which makes the jump of boundary conditions exists at the interface due to the different property parameters of different phase. As boundary conditions at interface not continuous any more, it adds the difficulty in the computing of the system. Many people investigate multi-phase fluids numerically with sharp interface model as this model is closer to the reality [4], even though they have to deal with the jump condition.

Compared with sharp interface, phase field model which is also called diffuse interface model not considering the interface as the boundary introduces the hypothesis in the continuity of interface. It has thickness between one phase to the other at the interface and the physical property parameters of different phases such as density, viscosity change continuously during the interface. It also avoids the appearance of jump of boundary conditions and treats the multi-phase fluids as one fluid with different material properties. An order parameter is applied to identify different phase which is mostly uniform.
in the bulk energy and this also makes the numerical calculation more easily [5]. In recent years, numerical results with phase field model are better than sharp interface model like the droplet coalescence, pinch off risings and deformations in shear flows.

In addition, there are more and more available numerical methods used to solve the phase field model including spectral method [6], moving mesh method [7], finite element method [8] and finite difference method. A physical energy law usually exists in the phase field model and the energy stable scheme can make a better result. H. Yu and X. Yang developed two efficient and unconditionally energy stable numerical schemes for Navier Stokes Cahn Hilliard and got an energy law at discrete level but inequality [9]. Actually, the preservation of energy law turns out to be important in designing a numerical method as the preserving energy law method can produce the correct solution even though a rapid change or singularity occurs in the computation. An energy law equality at discrete level for the variable density two-phase flow model is obtained by Guo et al. [10] with continuous finite element method due to a special temporal scheme. In addition, the difference between the numerical solution obtained by preserving energy law method with a relatively coarse mesh and numerical results obtained by other methods with finer grid is almost zero.

In this paper, we develop an energy law preserving continuous finite element method for the variable density two-phase flow model proposed by Abels et al. [1]. A special temporal scheme is designed to discretize the weak form of Navier-Stokes-Cahn-Hilliard equations to obtain a discrete energy law equality based on the work in [10].

2. Multi-phase model, weak form and energy law

The model for the vary density multi-phase fluids proposed by Abels et al. [1] is composed of Navier Stokes equations and Cahn-Hilliard models as follows:

\[ \frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = \nabla \cdot (M \nabla \mu) \]

(1)

\[ \nabla \cdot \mathbf{v} = 0 \]

(2)

\[ \frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) = -\nabla p + \eta \Delta \mathbf{v} + \mu \nabla \phi \cdot \nabla \cdot (\mathbf{J} \otimes \mathbf{v}) \]

(3)

\[ \mu = \sigma \varepsilon^{-1} \psi'(\phi) - \sigma \varepsilon \Delta \phi \]

(4)

With boundary conditions of \( \mathbf{v} = 0, \partial_n \phi = 0, \partial_n \mu = 0 \). Here \( \mathbf{v} = (v_1, v_2) \) represents the velocity of the mixture, \( \rho \) is the hydrostatic pressure and \( \phi \) is the order parameter used to mark different phases ( \( \phi = 1 \): fluid 1; \( \phi = -1 \): fluid 2). \( \eta, M, \sigma, \varepsilon, \mu \) Denote fluid viscosity, phenomenological mobility, physical surface tensor, interface thickness and chemical potential, respectively. The density \( \rho \) and mass flux \( \mathbf{J} \) due to the variable density has the expression of \( \rho = ((\rho_1 + \rho_2) + (\rho_1 - \rho_2)\phi)/2 \) and \( \mathbf{J} = (\rho_1 - \rho_2)M \nabla \mu/2 \) where \( \rho_1, \rho_2 \) represent the fluid density of each phase before mixed, respectively.

Please to see more details in [10] for the finite element space, the weak form reads: Find \( \mathbf{v} \in W^{1,3}, p \in L^2_0, \phi, \mu \in W^{1,3} \) such that

\[ \int_{\Omega} \left( \frac{\partial \phi}{\partial t} \phi + (\mathbf{v} \cdot \nabla \phi) \phi + M \nabla \mu \cdot \nabla \phi \right) dx = 0 \quad \forall \psi \in W^{1,3} \]

(5)

\[ \int_{\Omega} (\mu \chi - \sigma \varepsilon^{-1} \psi' \chi - \sigma \varepsilon \nabla \phi \cdot \nabla \chi) dx = 0 \quad \forall \chi \in W^{1,3} \]

(6)
\[ \int_\Omega (V \cdot v) q dx = 0 \quad \forall q \in L_0^2 \]  
\[ \int_\Omega \left( \frac{\partial (\rho v)}{\partial t} \cdot u + V \cdot (\rho v \otimes v) \cdot u - p(V \cdot u) + \eta \nabla v : \nabla u - \mu \nabla \phi \cdot u + \nabla (J \otimes v) \cdot u \right) dx = 0 \quad \forall u \in W^{1,1} \]  

We take \( \phi = \mu, u = v, q = p, \chi = \partial \phi / \partial t \) into equation (5)-(8) and the weak form becomes
\[ \int_\Omega \left( \frac{\partial \phi}{\partial t} \mu + (V \cdot \nabla \phi) \mu + M |V \mu|^2 \right) dx = 0 \]  
\[ \int_\Omega \left( \mu \frac{\partial \phi}{\partial t} - \sigma \varepsilon^{-1} \frac{\partial \psi}{\partial t} - \sigma \varepsilon \frac{\partial}{\partial t} \left( |\nabla \phi|^2 \right) \right) dx = 0 \]  
\[ \int_\Omega (p \nabla \cdot v) dx = 0 \]  
\[ \int_\Omega \left( \frac{\partial}{\partial t} \left( \frac{|\nabla \phi|^2}{2} - p(V \cdot v) + \eta |\nabla v|^2 - \mu \nabla \phi \cdot v \right) \right) dx = 0 \quad \text{due to } \frac{\partial p}{\partial t} + V \cdot (\rho v + J) = 0 \]  

And the continuous energy law derived from the equation (9) - (10) + (11) + (12):
\[ \frac{\partial}{\partial t} \left( \frac{1}{2} \| V \phi \|^2 + \frac{\sigma}{2} \| \nabla \phi \|^2 + \sigma \varepsilon^{-1} \int_\Omega \psi^2 dx \right) = - \left( \eta \| \nabla \phi \|^2 + M \| V \mu \|^2 \right) \]  

3. Special finite element scheme and discrete energy law

In the computation of the system, we rewrite equation (2) with \( \nabla \cdot v + \delta p = 0 \) with \( \delta = 10^{-6} \) as the penalty treatment to increase the stability of pressure. The special finite element scheme called preserving energy law method and the fully discretized weak form are given as follows:
\[ \int_\Omega \left( \nabla \cdot \left( \sqrt{\rho + \delta} \right)^{n+1/2} \right) q dx = 0 \]  
\[ \int_\Omega \left( \sqrt{\rho_h + \delta} \right)^{n+1} \cdot u + \left( \rho_h^{n+1/2} \left( \sqrt{\rho_h} \right)^{n+1} + J_h^{n+1/2} \right) \cdot \nabla \left( \sqrt{\rho_h} \right)^{n+1} \cdot u + \frac{1}{2} \nabla \left( \rho_h^{n+1/2} \left( \sqrt{\rho_h} \right)^{n+1} + J_h^{n+1/2} \right) \left( \sqrt{\rho_h} \right)^{n+1} \cdot u \]  
\[ - \rho_h^{n+1/2} (V \cdot u) + \eta \nabla \left( \sqrt{\rho_h} \right)^{n+1} \cdot \nabla u - \mu_h^{n+1/2} \nabla \phi_h^{n+1/2} \cdot u \right) dx = 0 \]  
\[ \int_\Omega \left( \phi_h^{n+1} \phi + \left( \sqrt{\rho_h} \right)^{n+1} \cdot \nabla \phi_h^{n+1/2} \phi + M \nabla \left( \phi_h^{n+1/2} + c \phi_h^{n+1/2} \right) \cdot \nabla \phi \right) dx = 0 \]  
\[ \int_\Omega \left( \mu_h^{n+1/2} \chi - \frac{\sigma}{\varepsilon} \nabla \left( \phi_h^{n+1} \phi \right) + \sigma \varepsilon \nabla \phi_h^{n+1/2} \cdot \nabla \chi \right) dx = 0 \]  

Where
\[ \sqrt{\rho_h^{n+1/2}} = \left( \sqrt{\rho_h^{n+1}} + \sqrt{\rho_h^n} \right) / 2, \rho_h^{n+1/2} = (\rho_h^{n+1} + \rho_h^n) / 2, \left( \sqrt{\rho_h} \right)_h^{n+1} = \left( \sqrt{\rho_h^{n+1}} v_h^n + \sqrt{\rho_h^n} v_h^n \right) / \left( \sqrt{\rho_h^{n+1}} + \sqrt{\rho_h^n} \right) \]
\[ \mu_h^{n+1/2} = \frac{\mu_h^{n+1} + \mu_h^*}{2}, \phi_h^{n+1/2} = \frac{\phi_h^{n+1} + \phi_h^*}{2}, \rho_h^{n+1/2} = \frac{\rho_h^{n+1} + \rho_h^*}{2}, \left(\rho^*_h v_h^{n+1} - \rho_h^* v_h^*\right)/\Delta t, \]
\[ \rho_h^{n+1} = \frac{\rho_1 + \rho_2}{2} + (\rho_2 - \rho_1) \phi_h^{n+1}/2, \psi(\phi_h^{n+1}, \phi_i^*) = \left(\phi_h^{n+1} - \phi_i^*\right)^2 - 2\left(\phi_h^{n+1} + \phi_i^*\right)/4, \phi_i^{n+1} = \phi_h^{n+1} - \phi_i^* / \Delta t, \]
\[ J_h^{n+1/2} = (J_h^{n+1} + J_i^*)/2. \]

Still, we take \( \varphi = \mu^{n+1/2}, u = (\sqrt{\rho v})_{h}^{n+1}, \xi = \left(\phi_h^{n+1} - \phi_i^*\right)/\Delta t, q = p_h^{n+1/2} \) into equation (14)-(17) and we get the energy law at discrete level as
\[ \frac{E^{n+1} - E^n}{\Delta t} = -\left(\eta \left\| \nabla (\sqrt{\rho v})_{h}^{n+1} \right\|_H^2 + \beta \left\| \rho_h^{n+1/2} \right\|_L^2 + M \left\| \nabla \mu^{n+1/2} \right\|_L^2 \right) \] (18)

Where \( E = \left\| \rho_h^{n+1/2} \right\|_L^2 / 2 + 4\epsilon \left\| \nabla \phi_h^{n+1/2} \right\|_L^2 / 2 + B \int_\Omega \sigma \left(\phi_h^{n+1/2} - 1\right)^2 / 4\epsilon d\Omega \) the total free energy at time \( i \).

Compared with equation (13), equation (18) is almost the same as it obviously.

4. Numerical example and discussion
In this section, we compute coalescence of kissing bubbles as the numerical example. We use 64 \times 32 relative coarse grid to discretize the computing domain and the value of some parameters are \( \rho_1 = 1, \rho_2 = 10, \eta_1 = 0.01, \eta_2 = 0.06, M = 0.0005, \sigma = 1.96, \epsilon = 0.01, c = 0.5, \Delta t = 10^{-5} \). Figure 1 shows the interface structure of kissing bubble at different time. As the value of \( \phi \) varies from -1 to 1 at the vicinity of the interface, the result would show the thickness apparently according to the different color and here we choose \( \phi = 0 \) to show in Figure 1. The dentate interface due to the relative coarse grid comes out in the initial time, but the interface becomes smooth with the preserving energy method. As the interface of kissing bubbles overlapped, they coalesce into one large bubble and become an elliptical bubble due to the surface tension. The result for the velocity field is shown in Figure 2. Compared the result in [10], they agreed well and also validate the accuracy of the numerical solution.
Figure 1. The evolution of interface ($\phi = 0$) for two kissing bubbles at time $t = 0, 0.03, 0.1, 0.15$. 
Figure 2. The velocity field for two kissing bubbles at time $t = 0.03, 0.1, 0.15$.

We also examine the time evolution of the total free energy and the energy law at discrete level defined in equation (18). The total free energy is shown in Figure 3 (a) and the decreasing result match with the equation (18). The result in Figure 3 (b) shows the error in the discrete energy law (equation (18)). The discrete energy law can be preserved at each time and the accuracy of equation (18) can be validated as the error in the discrete energy law falls down to $10^{-10}$.

Figure 3. a: The evolution of total free energy; b: The error in the discrete energy law.
5. Conclusion
In this paper, we numerically investigate fluid-fluid interface of isothermal multi-phase fluids with a preserving energy law finite element method. The Navier-Stokes-Cahn-Hilliard equations are discretized by this method and a discrete energy law which is almost the same as the continuous energy law is derived. This discrete energy law equality of this phase model is never established before with finite element method. With the examination of numerical simulation of two kissing bubble, velocity field, the evolution of total free energy and the error in the energy law, the accuracy of the preserving energy law method and the discrete energy law equality are validated apparently.

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