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Decoupled Energy Stable Schemes for a Phase-Field Model of Two-Phase Incompressible Flows with Variable Density

Chun Liu · Jie Shen · Xiaofeng Yang

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Abstract We consider in this paper numerical approximations of two-phase incompressible flows with different densities and viscosities. We present a variational derivation for a thermodynamically consistent phase-field model that admits an energy law. Two decoupled time discretization schemes for the coupled nonlinear phase-field model are constructed and shown to be energy stable. Numerical experiments are carried out to validate the model and the schemes for problems with large density and viscosity ratios.

Keywords Phase-field · Two-phase flow · Navier–Stokes · Variable density · Stability · Energy stable schemes

1 Introduction

The interfacial dynamics about immiscible and incompressible two-phase flows have attracted much attention for more than a century. In recent years, the diffuse interface approaches, or sometimes called phase field models, whose origin can be traced back to [39] and [49], have been used extensively with much successes and become one of the major tools to study a variety of interfacial phenomena (cf. [5,24,26,30,31,54] and the recent reviews [27,46]). A particular advantage of these phase-field approaches is that they can often be derived from an energy-based variational formalism (energetic variational approaches), while usually leading to well-posed nonlinear coupled systems that satisfy thermodynamics-consistent

C. Liu
Department of Mathematics, Penn State University, University Park, PA 16802, USA
e-mail: liu@math.psu.edu

J. Shen (✉)
Department of Mathematics, Purdue University, West Lafayette, IN 47907, USA
e-mail: shen@math.purdue.edu

X. Yang
Department of Mathematics, University of South Carolina, Columbia, SC 29208, USA
e-mail: xfyang@math.sc.edu

energy dissipation laws. This makes it possible to carry out mathematical analysis and design numerical schemes which satisfy a corresponding discrete energy dissipation law (cf., for instance, [8,18,29]). It is a remarkably fact that the numerical schemes which do not respect the energy dissipation laws may be "overloaded" with an excessive amount of numerical dissipation near singularities, which in turn lead to large numerical errors, particularly for long time integration [13,19,48,51,52]. For the dynamical solutions of coarse-graining (macroscopic) process described by the Allen–Cahn and Cahn–Hilliard equations in typical phase-field models that undergo rapid changes and physical singularities at the interface, it is especially desirable to design numerical schemes that preserve the energy dissipation law at the discrete level.

One of the main challenges in the phase field models is how to describe the dynamics of the mixture of two fluids with different densities and viscosities. However, most of the analysis and simulation of the phase-field models for two-phase flows have been restricted to the cases with matched density or with small density ratios for which the Boussinesq approximation, where the variable density is replaced by a background constant density value while an external gravitational force is added to model the effect of density difference, can be used (cf. for instance [30]). While the phase-field model with Boussinesq approximation leads to a well-posed dissipative system, their physical validity is based on the assumption that the density ratio between the two phases is relatively small. Hence, they can not be used for two-phase flows with large density ratios. Thus, for the cases with large density ratios, we need to derive physically consistent phase-field models which are also mathematically well-posed.

The challenges and complexities of problems involving the mixtures of different materials lie in their nature of multiscale and sometimes multiphysics. It is the competitions and couplings between these effects which determine the overall properties of the mixtures. A main difficulty in dealing with non-matching densities can be seen in the basic macroscopic (continuum) mass conservation $\rho_t + \mathrm{div}(\rho u) = 0$ and (macroscopic) incompressibility $\mathrm{div} u = 0$. As the density ρ is an macroscopic quantity, it may be different with the direct average from microscopic descriptions, such as from the phase fields. For instance, the mixtures of two incompressible fluids may not be incompressible, for we have to take into consideration of the interaction between two different particles. Various approaches have been proposed in the literature. Traditionally, they can be classified into two categories: incompressible or quasi-incompressible. In the former approach, the *volume averaged velocity* is assumed to be incompressible everywhere, including the interfacial region. In the latter approach, on the other hand, the *mass averaged velocity* is assumed to satisfy the mass conservation instead of incompressibility, leading to a slightly compressible mixture inside the interfacial region. In [31], the authors derived a quasi-incompressible phase model which allows the mixture to be slightly compressible inside the interface, see also [1]; a similar quasi-incompressible model, which admits an energy law, was proposed recently in [47]. On the other hand, incompressible phase-field models were derived in [9] and [14], however, these models do not seem to admit an dissipative energy law; In [44] and [43], the authors derived incompressible phase-field models, which admit an dissipative energy law, with Allen–Cahn [44] and Cahn–Hilliard [43] dynamics for the cases of variable density and viscosity, but the models were derived with an ad-hoc adjustment, which is mathematically consistent but not frame invariant, on the convection term. In [2], the authors derived a thermodynamically consistent, which admits an energy law but not frame invariant, diffuse interface models for incompressible two-phase flows with different densities. Then, they derived in [3] another diffuse interface model which is thermodynamically consistent, frame invariant and admits an energy law. We want to point out, although all these models are modeling similar problems

of mixtures of two different incompressible fluids, each one of them, including the current model, does have its range of validation and limitations. In particular, all of them can be considered as an approximation to the sharp interface model.

The first objective of this paper is to rederive the thermodynamically consistent phase-field model in [2] from an energetic variational point of view.[1] The second objective is to design some efficient and accurate numerical schemes for the model which decouple the solution of velocity, pressure, and phase functions. It is particularly challenging to design effective, energy stable numerical schemes for this system due to the numerous nonlinear couplings. We shall combine several approaches which have proved efficient for the phase equations and for the Navier–Stokes equations, namely, the convex splitting (cf. [13,17,51]) for the phase equations and projection-type approaches [21,23,36,50] for the Navier–Stokes equations. We shall construct two *decoupled* time discretization schemes which satisfy a discrete energy law and which lead to, at each time step, a nonlinear elliptic system for the phase function, and a linear elliptic equation for the velocity and pressure respectively. We would like to point out that they appear to be the first schemes which decouple the computations of phase function, velocity and pressure, while still preserving the discrete energy law. In a subsequent paper [45], the technique developed here was used to derive efficient numerical schemes for the model in [3].

The third objective is to validate this model and the proposed numerical schemes through careful numerical simulations, including the dynamics of an air bubble rising in water, a particularly challenging situation where the density ratio is close to 1,000 and the viscosity ratio is close to 70.

The rest of the paper is organized as follows. In the next section, we describe the phase-field model. In Sect. 3, we provide a detailed energetic derivation for the new model. Then, in Sect. 4, we construct several efficient numerical schemes and prove their stability. In Sect. 5, we provide some numerical evidences to validate the new model and the proposed numerical schemes, and summarize our contributions.

2 A Cahn–Hilliard Phase-Field Model with Variable Density and Viscosity

We consider a mixture of two immiscible, incompressible fluids in a confined domain Ω with densities ρ_1, ρ_2 and viscosities μ_1, μ_2, respectively. As usual, we introduce a phase function (macroscopic labeling function) ϕ such that

$$\phi(x,t) = \begin{cases} 1 & \text{fluid 1,} \\ -1 & \text{fluid 2,} \end{cases} \tag{2.1}$$

with a thin, smooth transition region of width $O(\eta)$. The (equilibrium) configurations and patterns of this mixing layer, in the neighborhood of the level set $\Gamma_t = \{x : \phi(x,t) = 0\}$, is determined by the microscopic interactions between fluid molecules. For the isotropic interactions, the classical self consistent mean field theory (SCMFT) in statistical physics [11] yields the following Ginzburg–Landau type of Helmholtz free energy functional:

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

[1] After we derived the model independently, we learned that the identical model was already derived in [2].

where the first term contributes to the hydro-philic type (tendency of mixing) of interactions between the materials and the second part, the double well bulk energy $F(\phi) = \frac{1}{4\eta^2}(\phi^2-1)^2$, represents the hydro-phobic type (tendency of separation) of interactions. As the consequence of the competition between the two types of interactions, the equilibrium configuration will include a diffusive interface with thickness proportional to the parameter η (cf., for instance, [54]); and, as η approaches zero, we expect to recover the sharp interface separating the two different materials.

The hydrodynamics of this mixture can be viewed as an isothermal system governed by the energetic variational approaches for general dissipative systems. The combinations of the First Law of Thermodynamics and the Second Law of Thermodynamics gives:

$$\frac{d}{dt}E^{\text{total}} = -\Delta, \tag{2.3}$$

where E^{total} is the sum of kinetic energy and the total Helmholtz free energy, and Δ is the entropy production (energy dissipation rate in this case). All the physical ingredients, assumptions, as well as limitations of the system are included in the expressions of the total energy functional and the dissipation functional, and the kinematic (transport) relation of the variables employed in the system.

The hydrodynamics of the mixtures, by nature, is a multiscale problem. The competition of the macroscopic flow properties and the microstructures due to the molecular interactions gives all the intriguing and complicated behaviors of the systems. In fact, the choices of the variables and also the specific physics, in terms of the energetic functionals, demonstrated the specific physical situations or applications in consideration.

In this paper, we are interested in the overall macroscopic flow properties, which self-consistently take into account the microscopic properties of the mixtures. For this purpose, we consider the system with the following total energy:

$$E(\phi, \nabla\phi) = \int_\Omega \left(\rho(\phi)\frac{1}{2}|u|^2 + \lambda(\frac{1}{2}|\nabla\phi|^2 + F(\phi))\right) dx. \tag{2.4}$$

It is clear that the first term is the macroscopic kinetic energy. The second part, the coarse grained internal energy, includes the competition between the hydro-philic and hydro-phobic interactions between two different ingredients. The constant λ represents the competition between the kinetic energy and the total internal energy, and can be directly related to the commonly known surface tension constant [54].

The dynamics of the phase function include both the macroscopic kinematic transport relation and also the long-time microscopic dissipations: ϕ by the following Cahn–Hilliard gradient flow (cf. [5,10,24,26,30,31]):

$$\begin{aligned} &\phi_t + (u\cdot\nabla)\phi = -M\Delta w, \\ &w := \frac{\delta E}{\delta \phi} = \lambda\left(\Delta\phi - f(\phi)\right) - \rho'(\phi)\frac{|u|^2}{2}, \end{aligned} \tag{2.5}$$

where w is the so called chemical potential and M is a mobility constant related to the relaxation time scale, and $f(\phi) = F'(\phi)$. The right-hand side of the equation for ϕ is the coarse grained form of the microscopic dissipation (general diffusion) relation.

The momentum equation (macroscopic force balance) for the whole system takes the usual form:

$$\rho\left(u_t + (u\cdot\nabla)u\right) = \nabla\cdot\tau, \tag{2.6}$$

where the total stress $\tau = \mu D(u) - pI + \tau_e$ with $D(u) = \nabla u + \nabla u^T$ and τ_e is the extra elastic stress induced by the microscopic internal energy. It will be shown in the next section, by a unified energetic variational approach, that the momentum equation becomes:

$$\rho(u_t + (u \cdot \nabla)u) = \nabla \cdot (\mu D(u) - pI - \lambda \nabla\phi \otimes \nabla\phi), \tag{2.7}$$

where p includes both the hydrostatic pressure due to the incompressibility and also the contributions from the induced stress.

In the above, ρ and μ are slave variables of ϕ, which can be defined, for example, as

$$\rho(\phi) = \frac{1+\phi}{2}\rho_1 + \frac{1-\phi}{2}\rho_2, \quad \mu(\phi) = \frac{1+\phi}{2}\mu_1 + \frac{1-\phi}{2}\mu_2. \tag{2.8}$$

Without loss of generalities, we consider the boundary conditions

$$u|_{\partial\Omega} = 0, \quad \frac{\partial\phi}{\partial n}|_{\partial\Omega} = 0, \quad \frac{\partial w}{\partial n}|_{\partial\Omega} = 0. \tag{2.9}$$

The Cahn–Hilliard phase equation (2.5) and the momentum equations (2.7) with the boundary condition (2.9), together with the incompressibility constraint

$$\nabla \cdot u = 0, \tag{2.10}$$

form a closed system for the particular set of variables of our choice for this study, (u, p, ϕ, w), and with the auxiliary variable ρ and μ given by (2.8).

Direct computation shows that, even in cases of $\rho_1 \neq \rho_2$, the Cahn–Hilliard phase-field system (2.5)–(2.7)–(2.10) still admits the following energy law:

$$\frac{d}{dt}\int_\Omega \left(\frac{1}{2}\rho(\phi)|u|^2 + \frac{\lambda}{2}|\nabla\phi|^2 + \lambda F(\phi)\right) dx = -\int_\Omega \left(\frac{\mu}{2}|D(u)|^2 + M|\nabla w|^2\right) dx. \tag{2.11}$$

While the left-hand side includes all the physics we want to discuss in this system, the macroscopic hydrodynamics and the microscopic mixing, the right-hand side represents dissipation mechanisms from both scales. The viscosity term, the first term on the right-hand side, represents the macroscopic dissipation, and the second term stands for the microscopic internal damping during the mixing.

3 The Energetic Variational Derivation of the System

The complicated mechanical and rheological properties of the coupled system derived in the last section can be attributed to the competitions and couplings between different parts of the total energy functionals (in this case, the kinetic energy and the free energy) and different parts of the dissipation (the viscosity and the internal dissipation of the microstructure). One issue we want to point out is the kinematic assumptions involved in the system.

The energy dissipation law (2.11) is consistent with the second law of thermodynamics. Since we only consider the isothermal situation here, the total dissipation in the right hand side of (2.11) is equal to the total entropy production. The left-hand side is the total energy, which is the sum of kinetic energy plus the (Helmholtz) free energy.

In order to obtain the force balance equations from the general dissipation law (2.3), we employ the Least Action Principle (LAP) for the Hamiltonian part of the system and the

Maximum Dissipation Principle (MDP) for the dissipative part. Formally, LAP just states the fact that force multiplies distance is equal to the work, i.e.,

$$\delta E = \text{force} \times \delta x, \tag{3.1}$$

where x is the position, δ is the variation (derivative) in general senses. This procedure will give the Hamiltonian part of the system and the conservative forces [4,6]. On the other hand, MDP, by Onsager and Rayleigh [33,34,38], yields the dissipative forces of the system:

$$\delta \frac{1}{2}\Delta = \text{force} \times \delta \dot{x}. \tag{3.2}$$

Here the factor $\frac{1}{2}$ is consistent with the choice of quadratic form of the "rates", which in turn describes the linear response theory for long-time near equilibrium dynamics [28].

As we discussed before, the system (2.5)–(2.7)–(2.10) is a multi-scale/multi-physics system. The hydrodynamic equation (2.7) describes the macroscopic (continuum) force balance, while the dynamic equation (2.5) for the phase field ϕ describes the evolution of microstructures due to the mixing of two materials.

Let us start with the Eq. (2.5). Here we introduce the free energy functional, which is the consequences of various coarse graining process, such as the self-consistent mean field theory (SCMFT):

$$\int_{\Omega} \lambda \left(\frac{1}{2}|\nabla \phi|^2 + F(\phi) \right) dx. \tag{3.3}$$

Energetically, this "mixing" energy determines the equilibrium configuration of the mixing. The presence of the gradient term gives rise the spatial microstructures.

In order to describe the effect of the macroscopic flow field $u(x,t)$ to the microstructure, we introduce the kinematic transport relation:

$$\frac{D}{Dt}\phi(x,t) = \phi_t + u \cdot \nabla \phi = 0. \tag{3.4}$$

This relation can also be interpreted as the immiscibility of the mixing, which is independent to the energetic descriptions of the system. This kinematic assumption on ϕ demonstrates the nature of ϕ being a *label* function, satisfying

$$\phi(x(X,t),t) = \phi_0(X), \tag{3.5}$$

where, as usual, X and x represent the Lagrangian and Eulerian coordinates, respectively, and $x(X,t)$ is the flow map such that $x_t(X,t) = u(x(X,t),t)$, $x(X,0) = X$. Hereafter, the spatial derivation without sub-index represents derivative with respect to Eulerian coordinates x, while the derivatives with respect to the Lagrangian coordinates X will be marked out specifically.

We want to point out that, in order to describe the deformation or evolution of configurations or patterns, one needs to introduce the deformation tensor $F = \frac{\partial x}{\partial X}$. The usual (macroscopic) incompressible condition

$$\nabla \cdot u = 0, \tag{3.6}$$

is the direct consequence of the constraint $\det(F) = 1$ and the algebraic identity $\delta \det(F) = \det(F)\,\mathrm{tr}(F^{-1}\delta f)$.

For constant mobility M, the Cahn–Hilliard dynamics (2.5) can be viewed as a relaxation approximation to (3.4), formally by letting M approaches zero. On the other hand, from

the energy dissipation law (2.11), the second term in the right hand side represents the microscopic internal dissipation. From there, one can derive the Cahn–Hilliard dynamics, as a general diffusion mechanism, represents the long-time, near equilibrium behavior for the microscopic time scale. It can also be regarded as the microscopic relaxation (in time) of the microstructures, hence the microscopic force balance.

Now, we want to derive the macroscopic force balance equation (2.7). To this end, we start with the reversible part of the system. From the total energy of the left-hand side of (2.11), we can define the action function, after the Legendre transformation [7], in terms of the volume preserved flow map $x(X,t)$:

$$\begin{aligned} A(x) &= \int\int \left(\frac{1}{2}\rho(\phi)|u|^2 - \frac{\lambda}{2}|\nabla\phi|^2 - \lambda F(\phi)\right) dxdt \\ &= \int\int \left(\frac{1}{2}\rho(\phi_0)|x_t|^2 - \frac{\lambda}{2}|F^{-1}\nabla_X\phi_0(X)|^2 - \lambda F(\phi_0)\right) dXdt. \end{aligned} \tag{3.7}$$

The first equality is obtained by taking the Legendre transform of the total energy functional with respect to u, which gives the negative sign between the kinetic energy and the free energy. The second equality is derived from the volume preserving constraint (incompressibility, i.e., $\det(F) = 1$) of the flow map and the kinematic assumption of ϕ in (3.4) [the transport part of (2.5)].

Suppose there is a one-parameter family of these flow map $x^\epsilon(X,t)$, with $x^0(X,t) = x$, and $\frac{d}{d\epsilon}x^\epsilon(X,t)|_{\epsilon=0} = y(X,t)$. From the volume preserving constraint $\det\frac{\partial x^\epsilon}{\partial X} = 1$, it is easy to show that, if $\tilde{y}(x(X,t),t) = y(X,t)$, one can derive from the algebraic identity of the derivatives of the determinants that:

$$\nabla\cdot\tilde{y} = 0.$$

Taking the variation of $A(x)$ with respect to these volume preserving flow map for arbitrary given divergence free $\tilde{y}$, we arrive at the variational (weak) form:

$$\begin{aligned} &\int\int \left(\rho(\phi_0(X))(x_t,y_t) - \lambda\left(F^{-1}\nabla_X\phi_0(X), -F^{-1}\nabla_X y F^{-1}\nabla_X\phi_0(X)\right)\right) dXdt \\ &= \int\int (-\rho(\phi_0(X))(x_{tt},y) - \lambda(F^{-1}\nabla_X\phi_0(X), -F^{-1}\nabla_X y F^{-1}\nabla_X\phi_0(X)))\, dXdt \\ &= \int\int -(\rho(\phi)(u_t + u\cdot\nabla u,\tilde{y}) + \lambda\,(\nabla\phi, \nabla\tilde{y}\nabla\phi))\, dxdt. \end{aligned} \tag{3.8}$$

Integrating by part and using the fact that $\tilde{y}$ is divergence free, we obtain the macroscopic reversible part of (2.7):

$$\rho(\phi)(u_t + (u\cdot\nabla)u) = -p_1 I - \lambda\nabla\phi\otimes\nabla\phi, \tag{3.9}$$

where p_1 is the Lagrangian multiplier for the constraint on the volume preserving flow map $x(X,t)$, i.e., $\nabla\cdot\tilde{y} = 0$.

We want to point out that, while for the case of equal density, we have

$$\rho(\phi)\,(u_t + u\cdot\nabla u) = (\rho(\phi)u)_t + u\cdot\nabla\,(\rho(\phi)u)\,,$$

but this is no longer true when the densities are not the same, as in our situation. Hence we will need to take the weak form as in (3.8).

Since the macroscopic dissipation in the system is attributed to the viscosity term:

$$\int_\Omega \frac{\mu}{2}|D(u)|^2\,dx,$$

by taking the derivative of the corresponding term in the dissipation with respect to u (Onsager's Maximum Dissipation Principle), we obtain the dissipative part of the (2.7):

$$0 = \nabla \cdot (\mu D(u) - p_2 I)\,, \tag{3.10}$$

where p_2 is the Lagrangian multiplier for the incompressibility constraint $\nabla \cdot u = 0$.

The final Eq. (2.7), the total force balance equation, is just the sum of the two parts. Hence, the total pressure is $p = p_1 + p_2$, both represent the Lagrangian multiplier of the incompressibility, one is from the Lagrangian description and the other from the Eulerian formulation.

4 Energy Stable Time Discretizations and their Stability Analysis

In this section, we design some time discretizations of the new phase-field model (2.5)–(2.7)–(2.10) introduced in the last section. The goal is to construct time discretization schemes which satisfy a discrete energy dissipation law that is similar to the continuous energy law of (2.11), and are easy to implement in practice.

Let us first reformulate (2.5) and (2.7) into some equivalent forms which are more convenient for numerical approximation. By using the following identities

$$\nabla \cdot (\nabla\phi \otimes \nabla\phi) = \Delta\phi\nabla\phi + \frac{1}{2}\nabla|\nabla\phi|^2, \tag{4.1}$$

$$\nabla p + \lambda\nabla \cdot (\nabla\phi \otimes \nabla\phi) = \nabla(p + \frac{1}{2}\lambda|\nabla\phi|^2 + \lambda F(\phi) + \phi w) - \phi\nabla w + \frac{1}{2}\rho'(\phi)|u|^2\nabla\phi. \tag{4.2}$$

and denoting the modified pressure as $\tilde{p} = p + \frac{1}{2}\lambda|\nabla\phi|^2 + \lambda F(\phi + \phi w)$ (still denote it by p for simplicity), the system (2.5)–(2.7)–(2.10) can be rewritten as follows:

$$\phi_t + \nabla \cdot (u\phi) + M\Delta w = 0, \tag{4.3a}$$

$$w + \frac{1}{2}\rho'(\phi)|u|^2 - \lambda\,(\Delta\phi - f(\phi)) = 0, \tag{4.3b}$$

$$\rho(\phi)\,(u_t + (u \cdot \nabla)u) - \nabla \cdot \mu(\phi)D(u) + \nabla p - \phi\nabla w + \frac{1}{2}\rho'(\phi)|u|^2\nabla\phi = 0, \tag{4.3c}$$

$$\nabla \cdot u = 0, \tag{4.3d}$$

where $\rho(\phi)$ and $\mu(\phi)$ are given by (2.8), and the boundary conditions for (ϕ, w, u) are given in (2.9).

The above coupled nonlinear system presents formidable challenges for algorithm design, analysis and implementation that we will address in this paper. In this section, we will design numerical algorithms which admit a discrete energy dissipation law and overcome three main difficulties associated with this coupled nonlinear system that are described as follows.

- *The coupling between the phase function, chemical potential and the velocity*. It appears very difficult to decouple the computation of ϕ and w from the velocity u while the simple explicit treatment in the convection term of (4.3a) will not lead to any energy dissipation law.
- *The pressure solver with large density ratio*. A common strategy to decouple the computation of the pressure from velocity is to use a projection type scheme as in the case for Navier–Stokes equations (cf., for instance, a recent review in [23]). However, In the usual projection type schemes, the subsystem to determine a pressure approximation if often an

elliptic equation with $\frac{1}{\rho}$ as variable coefficient, making it difficult to solve when the density ratio is large. The additional difficulty is that it is not easy to construct a second-order scheme based on a pressure-correction formulation (cf. [22]). Thus, we will consider a pressure stabilized formulation to avoid solving a pressure elliptic equation with density as a variable coefficient.

- *The stiffness associated with the interfacial width* η. To alleviate the difficulty associated with the stiffness caused by the thin interfacial width, we can introduce a stabilizing term in the phase equation as in [42–44,53]. An alternative way adopted in this paper is to use the idea of convex splitting that was first introduced by Eyre [17]. Recently, the idea has been applied to various gradient flow [13,51], which serves as inspirations for the numerical schemes we present below.

We will first construct numerical schemes based on a gauge-Uzawa formulation [15,32,36,43]. These schemes require solving an elliptic equation for pressure with the variable coefficient $\frac{1}{\rho}$. Then, we will construct numerical schemes based on a pressure-stabilized formulation [21,23,37,41] which only require solving a Poisson equation for pressure.

We assume that we can split $F(\phi)$ as $F_c(\phi) - F_e(\phi)$ with both F_c and F_e being convex, i.e., $F_c''(\phi), F_e''(\phi) \geq 0$. For example, we can take $F_c(\phi) = \phi^4$ and $F_e(\phi) = 2\phi^2 - 1$. In what follows, we denote

$$f(\phi) = F'(\phi), \;\; f_c(\phi) = F_c'(\phi), \;\; f_e(\phi) = F_e'(\phi).$$

Without loss of generality, we assume $0 < \rho_1 \leq \rho_2$ and $0 < \mu_1 \leq \mu_2$.

4.1 Schemes Based on a Gauge-Uzawa Formulation

We construct a first-order gauge-Uzawa scheme for the phase-field model (4.3) as follows.

Given initial conditions ϕ^0, w^0, $s^0 = 0$, u^0, we compute $(\phi^{n+1}, w^{n+1}, \tilde{u}^{n+1}, u^{n+1}, s^{n+1})$ for $n \geq 0$ by

$$\begin{cases} \frac{1}{\delta t}(\phi^{n+1} - \phi^n) + \nabla \cdot \left(\left(u^n + \delta t \frac{\phi^n \nabla w^{n+1}}{\rho(\phi^{n+1})} \right) \phi^n \right) + M \Delta w^{n+1} = 0, \\ w^{n+1} + \frac{1}{2}\rho'(\phi^{n+1})|u^n|^2 - \lambda \left(\Delta \phi^{n+1} - f_c(\phi^{n+1}) + f_e(\phi^n) \right) = 0, \\ \partial_n \phi^{n+1}|_{\partial\Omega} = 0, \quad \partial_n w^{n+1}|_{\partial\Omega} = 0; \end{cases} \tag{4.4a}$$

$$\begin{cases} \rho(\phi^{n+1}) \frac{\tilde{u}^{n+1} - u^n}{\delta t} + \rho(\phi^{n+1})(\tilde{u}^{n+1} \cdot \nabla)\tilde{u}^{n+1} + \frac{1}{2}\rho(\phi^{n+1}) \left(\nabla \cdot \tilde{u}^{n+1} \right) \tilde{u}^{n+1} \\ \quad - \nabla \cdot \mu(\phi^n) D(\tilde{u}^{n+1}) + \mu_{min} \nabla s^n - \phi^n \nabla w^{n+1} \\ \quad + \frac{1}{2}\rho'(\phi^{n+1})|\tilde{u}^{n+1}|^2 \nabla \phi^{n+1} = 0, \\ \tilde{u}^{n+1}|_{\partial\Omega} = 0; \end{cases} \tag{4.4b}$$

$$\begin{cases} -\nabla \cdot \left(\frac{1}{\rho(\phi^{n+1})} \nabla \psi^{n+1} \right) = \nabla \cdot \tilde{u}^{n+1}, \\ \partial_n \psi^{n+1}|_{\partial\Omega} = 0; \end{cases} \tag{4.4c}$$

$$\begin{cases} u^{n+1} = \tilde{u}^{n+1} + \frac{1}{\rho(\phi^{n+1})} \nabla \psi^{n+1}, \\ s^{n+1} = s^n - \nabla \cdot \tilde{u}^{n+1}; \end{cases} \tag{4.4d}$$

with

$$\rho(\phi) = (\phi + 1)^2 \rho_1/4 + (\phi - 1)^2 \rho_2/4, \quad \mu(\phi) = (\phi + 1)^2 \mu_1/4 + (\phi - 1)^2 \mu_2/4, \tag{4.4e}$$

and $\mu_{min} = \min \mu(\phi) > 0$.

Several remarks are in order.

Remark 4.1 An additional stabilizing term, $\rho(\phi^{n+1})\frac{u^n}{2}\nabla\cdot\tilde{u}^{n+1}$, is added in (4.4b). This term does not bring any inconsistency to the governing PDE system (4.3c) because the term $\rho\frac{u}{2}\nabla\cdot u$ vanishes in the PDE level from the incompressibility.

Remark 4.2 The computations of (ϕ^{n+1}, w^{n+1}), $\tilde{u}^{n+1}$, ψ^{n+1} and (u^{n+1}, s^{n+1}) are totally decoupled! We believe, to the best of our knowledge, that this is the first scheme for two-phase flows which is both totally decoupled and unconditionally stable (see below).

Remark 4.3 Note that a first order term, $\delta t\frac{\phi^n\nabla w^{n+1}}{\rho(\phi^{n+1})}$, is added to the convective velocity u^n in (4.4a). Hence, the above scheme is formally a first-order approximation to the system (4.3).

Remark 4.4 Since ϕ should take the values ±1 except at the interfacial region, so if we ignore the mass conservation for the mixture inside the interfacial region, the form of $\rho(\phi)$ and $\mu(\phi)$ can be quite flexible. We choose to define ρ in (4.4e) (resp. μ) as the parabolic average of ρ_1 and ρ_2 (resp. μ_1 and μ_2) which satisfies

$$\rho''(\phi) > 0 \text{ and } \rho_{min} = \min_{\phi\in\mathbb{R}}\rho(\phi) > 0. \tag{4.5}$$

Remark 4.5 In the above scheme, s^n is the so called gauge variable, and a proper pressure approximation is (cf. [36]):

$$p^{n+1} = -\frac{\psi^{n+1}}{\delta t} + \mu_{min}s^{n+1}. \tag{4.6}$$

We also derive from (4.4c)–(4.4d) that $\mathrm{div}u^{n+1} = 0$.

Remark 4.6 Given the data at the n-th level, (4.4a) is an quasilinear elliptic system. Note that the special choice of the "average" for $\rho(\phi)$ in (4.4e) prevents (4.4a) from developing singularity. Thus, the existence of a solution to this system follows from the standard elliptic theories (see for instance the standard references in [16,20]). We will outline the main arguments here for the readers' convenience.

We will use the Hölder spaces here. Similar arguments can also be extended to other functional spaces, such as Hilbert–Soblev spaces.

Assuming $\{\phi^n, w^n\} \in C^{1,\alpha}$ for some $0 < \alpha < 1$, we will apply the Leray–Schauder fixed point theorem to the system (4.4a). Consider the following system with a parameter $\sigma \in [0, 1]$:

$$\begin{cases} \sigma\left\{\frac{1}{\delta t}(\phi-\phi^n) + \nabla\cdot\left(\left(u^n + \delta t\frac{\phi^n\nabla w}{\rho(\phi)}\right)\phi^n\right) - Mw\right\} + M(1+\Delta)w^{n+1} = 0, \\ \sigma\left\{w + \frac{1}{2}\rho'(\phi)|u^n|^2 - \lambda(-f_c(\phi) + f_e(\phi^n)) + \lambda\phi\right\} - \lambda(1+\Delta)\phi^{n+1} = 0, \\ \partial_n\phi^{n+1}|_{\partial\Omega} = 0, \quad \partial_n w^{n+1}|_{\partial\Omega} = 0. \end{cases} \tag{4.7}$$

For any fixed $\sigma \in [0, 1]$, the above system defines an operator $T_\sigma(\phi, w) = (\phi^{n+1}, w^{n+1}) : C^{1,\alpha}\times C^{1,\alpha} \to C^{1,\alpha}\times C^{1,\alpha}$. One can readily check that this operator possess the following properties:

- For $\sigma = 0$, the system only has an unique solution $\phi^{n+1} = w^{n+1} = 0$.
- For any fixed σ, and arbitrary $\phi, w \in C^{1,\alpha}$, from the Schauder estimates of linear elliptic equations (see for instance, Theorem 2.40 in [16] for a more general statement), one can show that the solution of (4.7) $\phi^{n+1}, w^{n+1} \in C^{2,\alpha}$, which is compactly embedded in $C^{1,\alpha}$ [25]. Hence, T_σ is a compact operator.

- Thanks to the a-priori Holder estimates for quasilinear elliptic equations [20], one can show that all fixed points of T_σ are uniformly bounded in $C^{1,\alpha} \times C^{1,\alpha}$.

With these properties, the Leray–Schauder fixed point theorem [20] asserts that the operator T_σ with $\sigma = 1$) possess a fixed point (ϕ^{n+1}, w^{n+1}), which is a solution of the original system (4.4a).

Remark 4.7 The Eq. (4.4b) is also an quasilinear elliptic system. By using a similar argument as above, one can also show that there exists at least one solution for (4.4b).

Theorem 4.1 *Solutions to the scheme* (4.4) *satisfy the following discrete energy law for any* $\delta t > 0$*:*

$$\begin{aligned}
&\frac{1}{2}\|\sigma^{n+1}u^{n+1}\|^2 + \lambda\left(\frac{1}{2}\|\nabla\phi^{n+1}\|^2 + (F(\phi^{n+1}),1)\right)\\
&\quad + \frac{1}{2}\mu_{min}\delta t\|s^{n+1}\|^2 + \delta t\left(M\|\nabla w^{n+1}\|^2 + \frac{1}{2}\mu_{min}\|\nabla\tilde{u}^{n+1}\|^2\right)\\
&\quad + \frac{1}{2}\|\frac{1}{\sigma^{n+1}}\nabla\psi^{n+1}\|^2\\
&\le \frac{1}{2}\|\sigma^n u^n\|^2 + \lambda\left(\frac{1}{2}\|\nabla\phi^n\|^2 + (F(\phi^n),1)\right) + \frac{1}{2}\mu_{min}\delta t\|s^n\|^2,
\end{aligned}$$

where $\sigma^{n+1} = \sqrt{\rho(\phi^{n+1})}$.

Proof Let us denote

$$u_\star^n = u^n + \delta t\frac{\phi^n\nabla w^{n+1}}{\rho(\phi^{n+1})}. \tag{4.8}$$

We first take the inner product of (4.4b) with $2\delta t\tilde{u}^{n+1}$. For the nonlinear terms, we have

$$\begin{aligned}
&\left(\frac{1}{2}\rho'(\phi^{n+1})|\tilde{u}^{n+1}|^2\nabla\phi^{n+1},\tilde{u}^{n+1}\right)\\
&\quad + \left(\rho(\phi^{n+1})\tilde{u}^{n+1}\cdot\nabla\tilde{u}^{n+1} + \frac{1}{2}(\nabla\cdot\tilde{u}^{n+1})\rho(\phi^{n+1})\tilde{u}^{n+1},\tilde{u}^{n+1}\right)\\
&= \left(\tilde{u}^{n+1},\nabla(\rho(\phi^{n+1})\frac{|\tilde{u}^{n+1}|^2}{2})\right) + \frac{1}{2}((\nabla\cdot\tilde{u}^{n+1})\rho(\phi^{n+1})\tilde{u}^{n+1},\tilde{u}^{n+1}) = 0.
\end{aligned}$$

Hence, noticing that

$$\rho(\phi^{n+1})\frac{\tilde{u}^{n+1}-u^n}{\delta t} - \phi^n\nabla w^{n+1} = \rho(\phi^{n+1})\frac{\tilde{u}^{n+1}-u_\star^n}{\delta t},$$

using the identity

$$(a-b,2a) = |a|^2 - |b|^2 + |a-b|^2, \tag{4.9}$$

and (4.9), we obtain

$$\begin{aligned}
&\|\sigma^{n+1}\tilde{u}^{n+1}\|^2 - \|\sigma^{n+1}u_\star^n\|^2 + \|\sigma^{n+1}\left(\tilde{u}^{n+1}-u_\star^n\right)\|^2\\
&\quad + \delta t\|\sqrt{\mu^n}D\left(\tilde{u}^{n+1}\right)\|^2 + 2\mu_{min}\delta t\left(\nabla s^n,\tilde{u}^{n+1}\right) = 0.
\end{aligned} \tag{4.10}$$

Using (4.4d) and the fact that $\mathrm{div} u^{n+1} = 0$, we derive

$$\begin{aligned}
\left(\sigma^{n+1}u^{n+1}, \sigma^{n+1}u^{n+1}\right) &= \left(\rho(\phi^{n+1})u^{n+1}, u^{n+1}\right) \\
&= \left(\rho(\phi^{n+1})\left(\tilde{u}^{n+1} + \frac{1}{\rho(\phi^{n+1})}\nabla\psi^{n+1}\right), u^{n+1}\right) \\
&= \left(\rho(\phi^{n+1})\tilde{u}^{n+1}, u^{n+1}\right) \\
&= \left(\rho(\phi^{n+1})\tilde{u}^{n+1}, \tilde{u}^{n+1} + \frac{1}{\rho(\phi^{n+1})}\nabla\psi^{n+1}\right) \\
&= \|\sigma^{n+1}\tilde{u}^{n+1}\|^2 + \left(u^{n+1} - \frac{1}{\rho(\phi^{n+1})}\nabla\psi^{n+1}, \nabla\psi^{n+1}\right) \\
&= \|\sigma^{n+1}\tilde{u}^{n+1}\|^2 - \|\frac{1}{\sigma^{n+1}}\nabla\psi^{n+1}\|^2, \qquad (4.11)
\end{aligned}$$

and

$$\begin{aligned}
2\mu_{min}\delta t\left(\nabla s^n, \tilde{u}^{n+1}\right) &= 2\mu_{min}\delta t\left(s^n, -\nabla\cdot\tilde{u}^{n+1}\right) = 2\mu_{min}\delta t\left(s^n, s^{n+1} - s^n\right) \\
&= \mu_{min}\delta t\left(\|s^{n+1}\|^2 - \|s^n\|^2 - \|s^{n+1} - s^n\|^2\right) \\
&= \mu_{min}\delta t\left(\|s^{n+1}\|^2 - \|s^n\|^2\right) - \mu_{min}\delta t\|\nabla\cdot\tilde{u}^{n+1}\|^2. \qquad (4.12)
\end{aligned}$$

It is easy to check by integration by parts that

$$\|D(u)\|^2 = \|\nabla u\|^2 + \|\nabla\cdot u\|^2, \quad \forall u \in H_0^1(\Omega)^d. \qquad (4.13)$$

From $\mu_{min} \le \mu^n$, we obtain

$$\mu_{min}\|\nabla\cdot\tilde{u}^{n+1}\|^2 + \mu_{min}\|\nabla\tilde{u}^{n+1}\|^2 = \|\sqrt{\mu_{min}}D(\tilde{u}^{n+1})\|^2 \le \|\sqrt{\mu^n}D\left(\tilde{u}^{n+1}\right)\|^2. \qquad (4.14)$$

Combining the above inequalities, we arrive at

$$\begin{aligned}
&\|\sigma^{n+1}u^{n+1}\|^2 - \|\sigma^{n+1}u_\star^n\|^2 + \|\frac{1}{\sigma^{n+1}}\nabla\psi^{n+1}\|^2 + \|\sigma^{n+1}(\tilde{u}^{n+1} - u_\star^n)\|^2 \\
&\quad + \mu_{min}\delta t(\|s^{n+1}\|^2 - \|s^n\|^2) + \mu_{min}\delta t\|\nabla\tilde{u}^{n+1}\|^2 \le 0. \qquad (4.15)
\end{aligned}$$

From (4.8), we have

$$\rho(\phi^{n+1})\frac{u_\star^n - u^n}{\delta t} = \phi^n\nabla w^{n+1}. \qquad (4.16)$$

By taking the inner product of (4.16) with $2\delta t u_\star^n$, we obtain

$$\|\sigma^{n+1}u_\star^n\|^2 - \|\sigma^{n+1}u^n\|^2 + \|\sigma^{n+1}(u_\star^n - u^n)\|^2 = 2\delta t\left(\phi^n\nabla w^{n+1}, u_\star^n\right). \qquad (4.17)$$

Next, taking the inner product of the first equation of (4.4a) with $-2\delta t w^{n+1}$, we obtain

$$-2(\phi^{n+1} - \phi^n, w^{n+1}) - 2\delta t((\nabla\cdot(u_\star^n\phi^n), w^{n+1}) + 2M\delta t\|\nabla w^{n+1}\|^2 = 0. \qquad (4.18)$$

By integration by parts, we have

$$-((\nabla\cdot(u_\star^n\phi^n), w^{n+1}) = \left(\phi^n\nabla w^{n+1}, u_\star^n\right). \qquad (4.19)$$

On the other hand, we derive from Taylor expansion that

$$\rho(\phi^{n+1}) - \rho(\phi^n) = \rho'(\phi^{n+1})(\phi^{n+1} - \phi^n) - \frac{1}{2}(\rho''(\xi^n)(\phi^{n+1} - \phi^n), \phi^{n+1} - \phi^n). \qquad (4.20)$$

Next, by taking the inner product of the second equation in (4.4a) with $2(\phi^{n+1}-\phi^n)$, after using the above relation and the fact that $\rho''(\xi^n)>0$ (cf. (4.5)), we obtain

$$\begin{aligned}&2(w^{n+1},\phi^{n+1}-\phi^n)+\|\sigma^{n+1}u^n\|^2-\|\sigma^n u^n\|^2\\&+\lambda\left(\|\nabla\phi^{n+1}\|^2-\|\nabla\phi^n\|^2+\|\nabla\phi^{n+1}-\nabla\phi^n\|^2\right)\\&+2\lambda\left(f_c(\phi^{n+1})-f_e(\phi^n),\phi^{n+1}-\phi^n\right)\le 0.\end{aligned}\tag{4.21}$$

In order to deal with the nonlinear terms, we obtain the following identities by Taylor expansion,

$$\begin{aligned}f_c(\phi^{n+1})(\phi^{n+1}-\phi^n)&=F_c(\phi^{n+1})-F_c(\phi^n)+F_c''(\xi)(\phi^{n+1}-\phi^n)^2,\\f_e(\phi^n)(\phi^{n+1}-\phi^n)&=F_e(\phi^{n+1})-F_e(\phi^n)-F_e''(\zeta)(\phi^{n+1}-\phi^n)^2.\end{aligned}\tag{4.22}$$

Subtracting the second identity from the first one, we find

$$\begin{aligned}&\left(f_c(\phi^{n+1})-f_e(\phi^n),\left(\phi^{n+1}-\phi^n\right)\right)\\&=\left(F(\phi^{n+1})-F(\phi^n),1\right)+\left(F_c''(\xi)+F_e''(\zeta)\right)\|\phi^{n+1}-\phi^n)\|^2\\&\ge\left(F(\phi^{n+1})-F(\phi^n),1\right).\end{aligned}\tag{4.23}$$

Finally, by combining (4.9), (4.15), (4.17),(4.18), (4.21) and (4.23), we arrive at

$$\begin{aligned}&\|\sigma^{n+1}u^{n+1}\|^2-\|\sigma^n u^n\|^2+\|\sigma^{n+1}(\tilde u^{n+1}-u_\star^n)\|^2+\|\sigma^{n+1}(u_\star^n-u^n)\|^2\\&+\mu_{min}\delta t(\|s^{n+1}\|^2-\|s^n\|^2)+\mu_{min}\delta t\|\nabla\tilde u^{n+1}\|^2+\|\frac{1}{\sigma^{n+1}}\nabla\psi^{n+1}\|^2\\&+2M\delta t\|\nabla w^{n+1}\|^2+\lambda(\|\nabla\phi^{n+1}\|^2-\|\nabla\phi^n\|^2+\|\nabla\phi^{n+1}-\nabla\phi^n\|^2)\\&+2\lambda\left(F(\phi^{n+1})-F(\phi^n),1\right)\le 0.\end{aligned}$$

We can then conclude from the above inequality. □

Remark 4.8 As noted before, a first-order stabilizing term, $-\delta t\frac{w^{n+1}\nabla\phi^n}{\rho(\phi^{n+1})}$, is added to the convective velocity u^n in (4.4a). This term can not be replaced by a second-order stabilizing term while maintaining the unconditional stability. However, one may construct efficient decoupled linear schemes at the expense of unconditional stability. For example, a formally second-order, decoupled linear scheme is as follows:

For the sake of simplicity, we shall denote, for any sequence $\{a^k\}$, $a^{*,k+1}=2a^k-a^{k-1}$.

$$\begin{cases}\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\delta t}+\nabla\cdot(u^{*,n+1}\phi^{*,n+1})+M\Delta w^{n+1}=0,\\ w^{n+1}+\frac{1}{2}\rho'(\phi^{*,n+1})|u^{*,n+1}|^2+\frac{1}{\eta^2}(\phi^{n+1}-2\phi^n+\phi^{n-1})\\ +\lambda(-\Delta\phi^{n+1}+2f(\phi^n)-f(\phi^{n-1}))=0,\\ \partial_n\phi^{n+1}|_{\partial\Omega}=0,\quad \partial_n w^{n+1}|_{\partial\Omega}=0;\end{cases}\tag{4.24a}$$

$$\begin{cases}\rho(\phi^{n+1})\frac{3\tilde u^{n+1}-4u^n+u^{n-1}}{2\delta t}+\rho(\phi^{n+1})(u^{*,n+1}\cdot\nabla)u^{*,n+1}\\ -\nabla\cdot\mu(\phi^{n+1})D(\tilde u^{*,n+1})+\nabla p^n+\mu_{min}\nabla s^n\\ -\phi^{*,n+1}\nabla w^{n+1}+\frac{1}{2}\rho'(\phi^{n+1})|u^{*,n+1}|^2\nabla\phi^{*,n+1}=0,\\ \tilde u^{n+1}|_{\partial\Omega}=0;\end{cases}\tag{4.24b}$$

$$\begin{cases}-\nabla\cdot(\frac{1}{\rho(\phi^{n+1})}\nabla\psi^{n+1})=\nabla\cdot\tilde u^{n+1}\\ \partial_n\psi^{n+1}|_{\partial\Omega}=0;\end{cases}\tag{4.24c}$$

$$\begin{cases} u^{n+1} = \tilde{u}^{n+1} + \frac{1}{\rho(\phi^{n+1})}\nabla\psi^{n+1}, \\ s^{n+1} = s^n - \nabla\cdot\tilde{u}^{n+1}, \\ p^{n+1} = p^n - \frac{3}{2\delta t}\psi^{n+1} + \mu_{min}s^{n+1}, \end{cases} \tag{4.24d}$$

with $\rho(\phi)$ and $\mu(\phi)$ defined in (4.4e) and $\mu_{min} = \min\mu(\phi^{n+1}) > 0$.

The above scheme is much easier to implement than the scheme (4.4). More precisely, at each time step, it involves a coupled linear system with constant coefficients for (ϕ^{n+1}, w^{n+1}), and an elliptic equation for $\tilde{u}^{n+1}$ and ψ^{n+1}, respectively.

4.2 Schemes Based on a Pressure-Stabilization Formulation

We observe that for problems with large density ratios, the elliptic equation (4.4c) for pressure maybe difficult and time consuming (often consuming more than 90 % of the total cost) to solve compared with a Poisson equation. Therefore, we will design a pressure-stabilized formulation which only requires solving a Poisson equation for the pressure [23,44].

Therefore, we now construct schemes based on the pressure-stabilization formulation (cf., for instance, [21,35,37,41]), namely, the divergence free condition is replaced by

$$\nabla\cdot u - \epsilon\Delta p_t = 0, \tag{4.25}$$

where ϵ is a small parameter.

Inspired by the schemes presented in [23,43], the first order pressure-stabilization scheme is given as follows.

Given initial conditions ϕ^0, $p^0 = 0$, u^0, we update $(\phi^{n+1}, u^{n+1}, p^{n+1})$ for $n \geq 0$ by

$$\begin{cases} \frac{1}{\delta t}(\phi^{n+1} - \phi^n) + \left(u^n + \delta t\frac{\phi^n\nabla w^{n+1}}{\rho(\phi^{n+1})}\right)\cdot\nabla\phi^n + M\Delta w^{n+1} = 0, \\ w^{n+1} + \frac{1}{2}\rho'(\phi^{n+1})|u^n|^2 - \lambda\left(\Delta\phi^{n+1} - f_c(\phi^{n+1}) + f_e(\phi^n)\right) = 0, \\ \partial_n\phi^{n+1}|_{\partial\Omega} = 0, \quad \partial_n w^{n+1}|_{\partial\Omega} = 0; \end{cases} \tag{4.26a}$$

$$\begin{cases} \rho(\phi^{n+1})\frac{u^{n+1}-u^n}{\delta t} + \rho(\phi^{n+1})\left(u^{n+1}\cdot\nabla\right)u^{n+1} + \frac{1}{2}\rho(\phi^{n+1})(\nabla\cdot u^{n+1})u^{n+1} \\ -\nabla\cdot\mu(\phi^n)D(u^{n+1}) + \nabla(2p^n - p^{n-1}) - \phi^n\nabla w^{n+1} + \frac{1}{2}\rho'(\phi^{n+1})|u^{n+1}|^2\nabla\phi^{n+1} = 0, \\ \tilde{u}^{n+1}|_{\partial\Omega} = 0; \end{cases} \tag{4.26b}$$

$$\begin{cases} \Delta(p^{n+1} - p^n) = \frac{\bar{\rho}}{\delta t}\nabla\cdot u^{n+1}, \\ \partial_n p^{n+1}|_{\partial\Omega} = 0; \end{cases} \tag{4.26c}$$

with $\rho(\phi)$, $\mu(\phi)$ as defined in (4.4e) and $\bar{\rho} = \frac{1}{2}\min\rho(\phi^{n+1}) > 0$.

Several remarks are in order.

Remark 4.9 The stabilizing term $\rho(\phi^{n+1})\frac{u^{n+1}}{2}\nabla\cdot u^{n+1}$, formerly with order $O(\delta t^2)$ in the discrete level thanks to (4.26c), that vanishes in the PDE level from the incompressibility, is added in (4.26b).

Remark 4.10 As for the scheme (4.4), the above scheme consists of three decoupled steps for (ϕ^{n+1}, w^{n+1}), u^{n+1} and $p^{n+1} - p^n$, respectively. The main difference between the two schemes is that a Poisson equation for $(p^{n+1} - p^n)$ in the above scheme replaces the elliptic equation (4.4c) in the scheme (4.4). Hence, the above scheme is computationally more

efficient. However, the velocity approximation u^{n+1} is no longer divergence free as in the scheme (4.4).

Remark 4.11 In (4.26), the system (4.26a) and (4.26b) are nonlinear. One can show, as in Remark 4.6, that this system admits at least one solution.

Theorem 4.2 *Solutions to the scheme* (4.26) *satisfy the following discrete energy law:*

$$\begin{aligned}&\frac{1}{2}\|\sigma^{n+1}u^{n+1}\|^2+\lambda\left(\frac{1}{2}\|\nabla\phi^{n+1}\|^2+(F(\phi^{n+1}),1)\right)\\&+\frac{\delta t^2}{2\rho_1}\|\nabla p^{n+1}\|^2+\delta t\left(M\|\nabla w^{n+1}\|^2+\frac{1}{2}\|\sqrt{\mu(\phi^n)}D(u^{n+1})\|^2\right)\\&\le\frac{1}{2}\|\sigma^n u^n\|^2+\lambda\left(\frac{1}{2}\|\nabla\phi^n\|^2+(F(\phi^n),1)\right)+\frac{\delta t^2}{2\rho_1}\|\nabla p^n\|^2.\end{aligned}$$

Proof We still denote

$$u^n_\star=u^n+\delta t\frac{\phi^n\nabla w^{n+1}}{\rho(\phi^{n+1})}. \tag{4.27}$$

By taking the inner product of (4.26b) with $2\delta t u^{n+1}$, we obtain

$$\begin{aligned}&\|\sigma^{n+1}u^{n+1}\|^2-\|\sigma^n u^n_\star\|^2+\|\sigma^{n+1}(u^{n+1}-u^n_\star)\|^2+\delta t\|\sqrt{\mu^n}D(u^{n+1})\|^2\\&+2\delta t\left(p^{n+1}-2p^n+p^{n-1},\nabla\cdot u^{n+1}\right)-2\delta t(p^{n+1},\nabla\cdot u^{n+1})\\&+\left(\rho(\phi^{n+1})(u^{n+1}\cdot\nabla)u^{n+1}+\rho(\phi^{n+1})\frac{u^{n+1}}{2}\nabla\cdot u^{n+1}\right.\\&\left.+\frac{1}{2}\rho'(\phi^{n+1})|u^{n+1}|^2\nabla\phi^{n+1},2\delta t u^{n+1}\right)=0.\end{aligned} \tag{4.28}$$

For the three nonlinear terms in (4.28), we have

$$\begin{aligned}&\left(\rho(\phi^{n+1})(u^{n+1}\cdot\nabla)u^{n+1}+\rho(\phi^{n+1})\frac{u^{n+1}}{2}\nabla\cdot u^{n+1}+\frac{1}{2}\rho'(\phi^{n+1})|u^{n+1}|^2\nabla\phi^{n+1},u^{n+1}\right)\\&=\left(u^{n+1},\nabla(\rho(\phi^{n+1})\frac{|u^{n+1}|^2}{2})\right)+\left(\rho(\phi^{n+1})\frac{|u^{n+1}|^2}{2},\nabla\cdot u^{n+1}\right)=0.\end{aligned} \tag{4.29}$$

By taking the inner product of (4.26c) with $\frac{2\delta t^2}{\bar\rho}(p^{n+1}-2p^n+p^{n-1})$ and with $-\frac{2\delta t^2}{\bar\rho}p^{n+1}$ separately, we derive

$$\begin{aligned}&-\frac{\delta t^2}{\bar\rho}\left(\|\nabla(p^{n+1}-p^n)\|^2-\|\nabla(p^n-p^{n-1})\|^2+\|\nabla\left(p^{n+1}-2p^n+p^{n-1}\right)\|^2\right)\\&=2\delta t\left(\nabla\cdot u^{n+1},p^{n+1}-2p^n+p^{n-1}\right),\end{aligned} \tag{4.30}$$

and

$$\frac{\delta t^2}{\bar\rho}(\|\nabla p^{n+1}\|^2-\|\nabla p^n\|^2+\|\nabla(p^{n+1}-p^n)\|^2)=-2\delta t\left(\nabla\cdot u^{n+1},p^{n+1}\right). \tag{4.31}$$

After adding the above two equalities together, we find

$$\begin{aligned}&2\delta t(p^{n+1}-2p^n+p^{n-1},\nabla\cdot u^{n+1})-2\delta t(p^{n+1},\nabla\cdot u^{n+1})\\&=\frac{\delta t^2}{\bar\rho}(\|\nabla p^{n+1}\|^2-\|\nabla p^n\|^2)+\frac{\delta t^2}{\bar\rho}\|\nabla(p^n-p^{n-1})\|^2-\frac{\delta t^2}{\bar\rho}\|\nabla(p^{n+1}-2p^n+p^{n-1})\|^2.\end{aligned} \tag{4.32}$$

Taking the difference of (4.26c) at step $n+1$ and step n, we can derive

$$\frac{\delta t^2}{\bar{\rho}}\|\nabla(p^{n+1}-2p^n+p^{n-1})\|^2 \le \bar{\rho}\|u^{n+1}-u^n\|^2 \le \frac{1}{2}\|\sigma^{n+1}(u^{n+1}-u^n)\|^2. \quad (4.33)$$

Combining the above inequalities together, we obtain

$$\begin{aligned}&\|\sigma^{n+1}u^{n+1}\|^2-\|\sigma^{n+1}u_\star^n\|^2+\|\sigma^{n+1}(u^{n+1}-u_\star^n)\|^2\\&-\frac{1}{2}\|\sigma^{n+1}(u^{n+1}-u^n)\|^2+\delta t\|\sqrt{\mu^n}D(u^{n+1})\|^2\\&+\frac{\delta t^2}{\bar{\rho}}(\|\nabla p^{n+1}\|^2-\|\nabla p^n\|^2)+\frac{\delta t^2}{\bar{\rho}}\|\nabla(p^{n+1}-p^n)\|^2\le 0.\end{aligned} \quad (4.34)$$

As in the proof of Theorem 4.1, we still have (4.16), then by taking the inner product with $u_\star^n$, the equality (4.17) is still valid.

$$\|\sigma^{n+1}u_\star^n\|^2-\|\sigma^{n+1}u^n\|^2+\|\sigma^{n+1}(u_\star^n-u^n)\|^2=2\delta t\left(\phi^n\nabla w^{n+1},u_\star^n\right) \quad (4.35)$$

The scheme of (4.26a) is exactly same as scheme (4.4a). By taking the inner product of the first equation in (4.26a) with $-2\delta t w^{n+1}$, of the second equation in (4.26a) with $2(\phi^{n+1}-\phi^n)$, we obtain

$$-2\left(\phi^{n+1}-\phi^n,w^{n+1}\right)-2\delta t\left(\nabla\cdot\left(u_\star^n\phi^n\right),w^{n+1}\right)+2M\delta t\|\nabla w^{n+1}\|^2=0. \quad (4.36)$$

and

$$\begin{aligned}&2(w^{n+1},\phi^{n+1}-\phi^n)+\|\sigma^{n+1}u^n\|^2-\|\sigma^n u^n\|^2\\&+\lambda\left(\|\nabla\phi^{n+1}\|^2-\|\nabla\phi^n\|^2+\|\nabla\phi^{n+1}-\nabla\phi^n\|^2\right)+2\lambda\left(F(\phi^{n+1})-F(\phi^n),1\right)\le 0.\end{aligned} \quad (4.37)$$

Using the inequality

$$\|\sigma^{n+1}(u^{n+1}-u_\star^n)\|^2+\|\sigma^{n+1}(u_\star^n-u^n)\|^2\ge\frac{1}{2}\|\sigma^{n+1}(u^{n+1}-u^n)\|^2, \quad (4.38)$$

and combining the (4.34), (4.35), (4.36), (4.37) and (4.38), we finally obtain

$$\begin{aligned}&\|\sigma^{n+1}u^{n+1}\|^2-\|\sigma^n u^n\|^2+\delta t\|\sqrt{\mu^n}D(u^{n+1})\|^2\\&+\frac{\delta t^2}{\bar{\rho}}\left(\|\nabla p^{n+1}\|^2-\|\nabla p^n\|^2+\|\nabla(p^{n+1}-p^n)\|^2\right)\\&+2M\delta t\|\nabla w^{n+1}\|^2+\lambda\left(\|\nabla\phi^{n+1}\|^2-\|\nabla\phi^n\|^2+\|\nabla\phi^{n+1}-\nabla\phi^n\|^2\right)\\&+2\lambda\left(F(\phi^{n+1})-F(\phi^n),1\right)\le 0,\end{aligned} \quad (4.39)$$

which implies the desired result. □

Remark 4.12 As for the gauge-Uzawa schemes, we can also construct decoupled, linear and second-order version of the scheme (4.26), at the expense of unconditional stability. An example of such scheme is given below.

As before, we still denote, for any sequence $\{a^k\}$, $a^{*,k+1}=2a^k-a^{k-1}$. Then, a second-order, semi-implicit version of (4.26) reads:

$$\begin{cases} \frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\delta t} + \nabla\cdot(u^{*,n+1}\phi^{*,n+1}) + M\Delta w^{n+1} = 0, \\ w^{n+1} + \frac{1}{2}\rho'(\phi^{*,n+1})|u^{*,n+1}|^2 + \frac{1}{\eta^2}(\phi^{n+1}-2\phi^n+\phi^{n-1}) \\ \quad +\lambda(-\Delta\phi^{n+1} + 2f(\phi^n) - f(\phi^{n-1})) = 0, \\ \partial_n\phi^{n+1}|_{\partial\Omega} = 0, \quad \partial_n w^{n+1}|_{\partial\Omega} = 0; \end{cases} \tag{4.40a}$$

$$\begin{cases} \frac{\rho(\phi^{n+1})}{2\delta t}(3u^{n+1}-4u^n+u^{n-1}) + \rho(\phi^{n+1})(u^{*,n+1}\cdot\nabla)u^{*,n+1} \\ \quad -\nabla\cdot\mu(\phi^{n+1})D(u^{n+1}) + \nabla(p^n + \frac{4}{3}\psi^n - \frac{1}{3}\psi^{n-1}) \\ \quad -\phi^{*,n+1}\nabla w^{n+1} + \frac{1}{2}\rho'(\phi^{n+1})|u^{*,n+1}|^2\nabla\phi^{*,n+1} = 0, \\ u^{n+1}|_{\partial\Omega} = 0; \end{cases} \tag{4.40b}$$

$$\begin{cases} \Delta\psi^{n+1} = \frac{3\bar{\rho}}{2\delta t}\nabla\cdot u^{n+1}, \\ \partial_n\psi^{n+1}|_{\partial\Omega} = 0, \\ p^{n+1} = p^n + \psi^{n+1} - \mu(\phi^{n+1})\nabla\cdot u^{n+1}, \end{cases} \tag{4.40c}$$

with $\rho(\phi)$, $\mu(\phi)$ as defined in (4.4e) and $\bar{\rho} = \frac{1}{2}\min\rho(\phi^{n+1}) > 0$.

5 Numerical Results and Discussions

We present in this section some numerical experiments using the schemes constructed in the last section.

Let us first describe briefly our spatial discretization which is based on the Legendre–Galerkin method [40]. We use the inf-sup stable (P_N, P_{N-2}) pair for the velocity and pressure (or the gauge or pseudo-pressure), and P_N for the phase function ϕ and the chemical potential w. From the stability proof of last section, the authors believed that there will be straight forward to derive the energy stability for the full discrete scheme, in the spatial discretization in the format of Finite element method or spectral method.

In the scheme (4.4) [resp. (4.26)], we need to solve the nonlinear system (4.4a) [reps. (4.26) which is identical to (4.4a)]. We used the following simple fixed point iteration based on (4.7): Setting $\phi_0^{n+1} = \phi^n$ and $w_0^{n+1} = w^n$, for $k = 0, 1, \ldots$, find ϕ_{k+1}^{n+1} and w_{k+1}^{n+1} by solving

$$\begin{cases} \frac{1}{\delta t}\left(\phi_{k+1}^{n+1} - \phi^n\right) + \left(u^n + \delta t\frac{\phi^n\nabla w_{k+1}^n}{\rho(\phi_k^{n+1})}\right)\cdot\nabla\phi^n + M\Delta w_{k+1}^{n+1} = 0, \\ w_{k+1}^{n+1} + \frac{1}{2}\rho'(\phi_k^{n+1})|u^n|^2 - \lambda\left(-f_c(\phi_k^{n+1}) + f_e(\phi^n)\right) - \lambda\Delta\phi_{k+1}^{n+1} = 0, \\ \partial_n\phi_{k+1}^{n+1}|_{\partial\Omega} = 0, \quad \partial_n w_{k+1}^{n+1}|_{\partial\Omega} = 0. \end{cases} \tag{5.1}$$

This is a coupled second-order system with constant coefficients which can be efficiently solved (cf. [12]). For the examples presented below, the above approach worked reasonably well since the time steps we used were sufficiently small due to the accuracy constraint. In general, a Newton type iterative scheme will be more effective.

For the elliptic equations for the velocity in both schemes and for the pressure in the scheme (4.4), we used a preconditioned conjugate gradient (PCG) method with a suitable constant-coefficient problem as a preconditioner. These constant coefficient problems were solved by using the fast spectral-Galerkin method [12,40].

5.1 Example 1: A Lighter Bubble Rising in a Heavier Medium

We consider the situation where a lighter bubble (with density ρ_1 and dynamic viscosity μ_{min}) initially inside a heavier medium (with density ρ_2 and dynamic viscosity μ_2) confined in a rectangular domain $\Omega = (0, \mathrm{d}) \times (0, \frac{3}{2}\mathrm{d})$.

The equations are non-dimensionalized using the following scaled variables:

$$\tilde{t} = \frac{t}{t_0}, \tilde{\rho} = \frac{\rho}{\rho_0}, \tilde{x} = \frac{x}{d_0}, \tilde{u} = \frac{u}{u_0}, \tag{5.2}$$

where

$$t_0 = \sqrt{d/g}, d_0 = d; u_0 = \sqrt{dg}, \rho_0 = \min(\rho_1, \rho_2). \tag{5.3}$$

The dimensionless form of (4.3) with an extra gravitational force ρg in the momentum equation, after omitting the $\tilde{}$ from the notation, is:

$$\phi_t + (u \cdot \nabla)\phi + M\Delta w = 0, \tag{5.4a}$$

$$w + \frac{1}{2}\rho'(\phi)|u|^2 - \lambda\left(\Delta\phi - \frac{\phi(\phi^2-1)}{\eta^2}\right) = 0, \tag{5.4b}$$

$$\rho\,(u_t + (u \cdot \nabla)u) - \nabla \cdot (\mu\nabla u) + \nabla p + (w + \frac{1}{2}\rho'(\phi)|u|^2)\nabla\phi = \rho g, \tag{5.4c}$$

$$\nabla \cdot u = 0, \tag{5.4d}$$

with

$$\rho(\phi) = \frac{\tilde{\rho}_1 - \tilde{\rho}_2}{2}\phi + \frac{\tilde{\rho}_1 + \tilde{\rho}_2}{2}, \mu(\phi) = \frac{\tilde{\mu}_{min} - \tilde{\mu}_2}{2}\phi + \frac{\tilde{\mu}_{min} + \tilde{\mu}_2}{2}.$$

In the above, $\tilde{\rho}_1 = \rho_1/\rho_0$, $\tilde{\rho}_2 = \rho_2/\rho_0$, $\tilde{\mu}_{min} = \mu_{min}/(\rho_0 \mathrm{d}^{3/2}\mathrm{g}^{1/2})$, $\tilde{\mu}_2 = \mu_2/(\rho_0 \mathrm{d}^{3/2}\mathrm{g}^{1/2})$.

We set the initial velocity to be zero and initial phase function given by

$$\phi(x, t = 0) = -\tanh\left(\frac{\mathrm{r} - \frac{1}{4}d}{\eta_0}\right), \tag{5.5}$$

where r is the distance from the center of the bubble to the point and η_0 is the diffusive interfacial width.

In the first example, we set $\rho_0 = 1$, $\rho_1 = 10$ and $g = (10, 0)^t$, $\mu = 1$, $\lambda = 0.05$, $\gamma = 2 \times 10^{-6}$ and $\eta_0 = \eta = 0.02\mathrm{d}$. In Fig. 1, we plot the interface contour of $\{\phi : \phi(x) = 0\}$ at several different times obtained by using both the scheme (4.4) and (4.26). We use a grid size of 257^2 and a time step size of $\delta t = 0.001$. No visual difference is observed indicating that (1) the two schemes capture well the dynamics of the bubble evolution, and (2) the new phase-field model is robust as the two very different numerical schemes produce identical results. Furthermore, these results are qualitatively consistent with the results presented in [43] where an ad-hoc but consistent term was added to ensure the stability.

5.2 Example 2: An Air Bubble Rising in Water

The second example we consider is an air bubble rising in water. The physical parameters are $\rho_1 = 1.161$ and $\rho_2 = 995.65$ with $\mu_{min} = 0.0000186, \mu_2 = 0.0007977$. We set $\mathrm{d} = 0.005$, $\mathrm{g} = 9.8$, $\lambda = 0.05$, $\gamma = 2 \times 10^{-8}$ and $\eta_0 = \eta = 0.02\mathrm{d}$. We use a grid size of 257^2 and time step size of $\delta t = 0.0001$. In Fig. 2, we plot a comparison of the level sets $\{\phi : \phi = 0\}$ by the two proposed schemes at different snapshots. We observe that the two

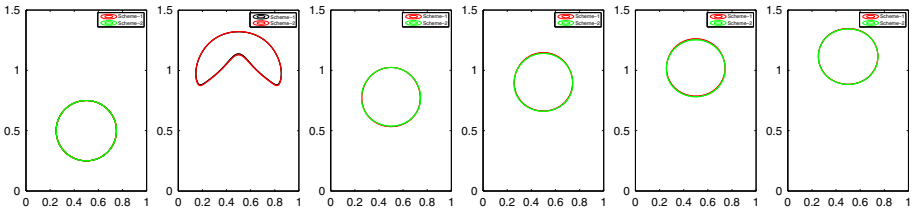
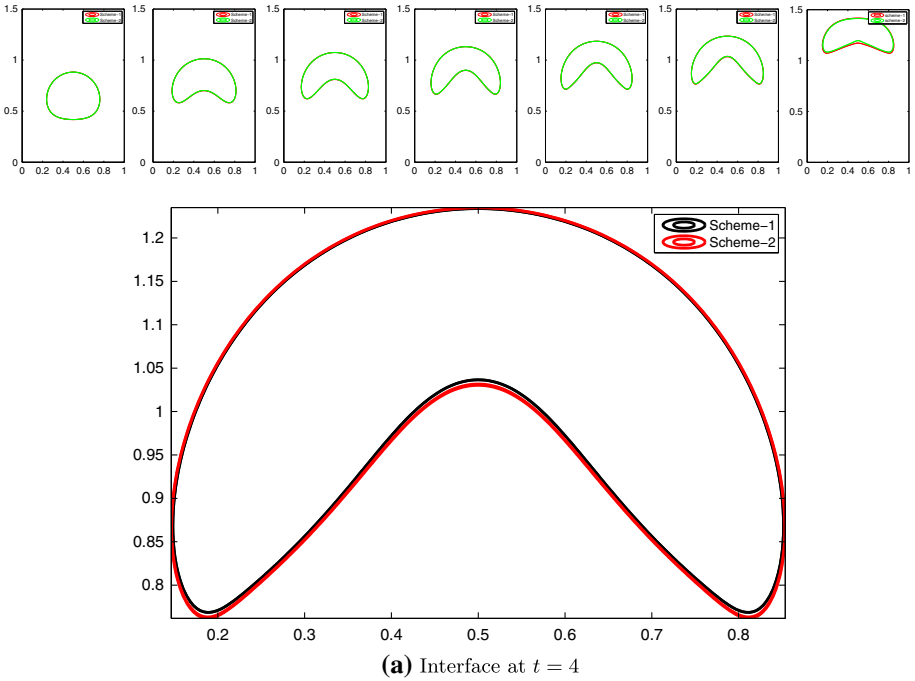


Fig. 1 Example 1: Snapshots of interfaces contours of ϕ at $t = 0, 5, 10, 15, 20, 25$ using (4.4) (Scheme-1) and (4.26) (scheme-2)



(a) Interface at $t = 4$

Fig. 2 Example 2: snapshots at $t = 1, 2, 2.5, 3, 3.5, 4, 7$ using schemes (4.4) (Scheme-1) and (4.26) (Scheme-2).

schemes produce visually identical results. Once again, the results are qualitatively similar to those in [43].

5.3 Summary

We considered the thermodynamically consistent phase-field model, first presented in [2], for incompressible and immiscible two-phase flows with different densities and viscosities. We rederived the model from an energetic variational formulation starting from the first and second thermodynamic laws.

We constructed two classes of decoupled numerical schemes, one based on a gauge-Uzawa formulation and the other based on a pressure-stabilization method. The former leads to a divergence free velocity field but requires solving, at each time step, an elliptic equation for the pressure with $\frac{1}{\rho}$ as coefficients, while the latter leads to a velocity field which is approximately

divergence free, but only requires solving a Poisson equation for the pressure at each time step. Both schemes are unconditionally energy stable. To the authors' best knowledge, these are the first schemes for phase-field models which lead to decoupled computations of phase function, velocity and pressure.

We also presented numerical results to validate the model and the proposed schemes.

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