SIAM J. NUMER. ANAL.
Vol. 53, No. 1, pp. 279–296
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DECOUPLED, ENERGY STABLE SCHEMES FOR PHASE-FIELD MODELS OF TWO-PHASE INCOMPRESSIBLE FLOWS*

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Abstract. In this paper we construct two classes, based on stabilization and convex splitting, of decoupled, unconditionally energy stable schemes for Cahn–Hilliard phase-field models of two-phase incompressible flows. At each time step, these schemes require solving only a sequence of elliptic equations, including a pressure Poisson equation. Furthermore, all of these elliptic equations are linear for the schemes based on stabilization, making them the first, to the best of the authors' knowledge, *totally decoupled, linear, unconditionally energy stable* schemes for phase-field models of two-phase incompressible flows. Thus, the schemes constructed in this paper are very efficient and easy to implement.

Key words. phase-field, two-phase flow, Navier–Stokes, Cahn–Hilliard, energy stable

AMS subject classifications. 65M12, 65M70, 65Z05

DOI. 10.1137/140971154

1. Introduction.

The phase-field approach, whose origin can be traced back to [29] and [38], has been used extensively with much successes and has become one of the major tools to study a variety of interfacial phenomena (cf. [15, 3, 25, 17, 22, 43], the recent review papers [30, 19], and the references therein). A particular advantage of the phase-field approach is that the governing system can be derived from an energy-based variational formalism. This usually leads to thermodynamically consistent energy dissipation laws, which allow us to establish the well posedness (at least local in time) for the coupled nonlinear system.

A main challenge in the numerical approximation of phase-field models is how to construct efficient and easy-to-implement numerical schemes which verify a discrete energy law. It has been observed that 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 [41, 10, 37, 39, 6]. Hence, to accurately simulate the dynamic coarse-graining (macroscopic) processes described by the Allen–Cahn and Cahn–Hilliard equations in typical phase-field models that undergo rapid changes at the interface, it is especially desirable to design numerical schemes that preserve the energy dissipation law at the discrete level. Another main advantage of energy stable schemes is that they can be easily combined with an adaptive time stepping strategy. While it is relatively easy to design energy stable schemes which involve solving coupled nonlinear systems at each time step, it is extremely difficult to construct energy schemes that only involve solving decoupled, and preferably linear, elliptic equations. The main difficulties in constructing such schemes include (i) the coupling between

*Received by the editors June 2, 2014; accepted for publication (in revised form) November 11, 2014; published electronically January 27, 2015.
http://www.siam.org/journals/sinum/53-1/97115.html
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the velocity and phase function through the convection term in the phase equation and nonlinear stress in the momentum equation; (ii) the coupling of the velocity and pressure through the incompressibility constraint; (iii) the stiffness of the phase equation associated with the interfacial width in the phase equation; and (iv) various additional difficulties introduced by the variable density including, but not limited to, how to avoid solving, in the case of large density ratios, an elliptic problem (for the pressure) with density as the (nonconstant) coefficient.

The difficulty (ii) has been well studied during the last forty years (cf. the review [12] and the references therein). The difficulty (iii) is also well studied recently: two classes of methods, one based on stabilization [44, 40, 33, 42] and the other based on convex splitting [8, 9, 39, 6], have proved to be effective. Various approaches have been proposed to deal with variable density in the case of Navier–Stokes equations [13, 28, 24, 14] and in the case of phase-field models [34, 32, 2, 27]. Recently, an interesting approach was proposed in [4, 26] to treat the difficulty (i), where an explicit stabilizing term is added to the convective velocity in the phase equation. This technique was used to construct decoupled energy stable schemes for a phase-field model derived in [23]. However, these schemes require solving complex nonlinear systems at each time step. Hence, the challenge is how to combine all these approaches together to construct a decoupled scheme which preserves all the desirable properties.

The main objective of this paper is to construct two classes, one based on the stabilization and the other based on convex splitting, of efficient and easy-to-implement schemes for the Cahn–Hilliard phase-field models with matched or different densities. More precisely, we shall combine several approaches mentioned above to construct *decoupled* time discretization schemes which satisfy a discrete energy law and which lead to, at each time step, an elliptic system for the phase function, a linear elliptic equation for the velocity, and a Poisson equation for the pressure. Moreover, in the case of stabilization, the elliptic system for the phase function is also linear. To the best of our knowledge, the schemes based on stabilization are the first *totally decoupled, linear, unconditionally energy stable* schemes for phase-field models of two-phase incompressible flows. The techniques developed in this paper can be used to construct efficient numerical schemes in other situations. For example, we have recently extended the approach in this paper to a phase-field model for two-phase complex fluids with matching density [35].

The rest of this paper is organized as follows. In the next section, we describe the Cahn–Hilliard phase-field models that we consider in this paper. In section 3, we construct two classes of decoupled numerical schemes for both the constant and variable density cases, and prove that they are uniquely solvable and unconditionally energy stable. In section 4, we present some numerical simulations to validate our schemes. Some concluding remarks are in section 5.

2. Cahn–Hilliard phase-field models.

We consider phase-field models for a mixture of two immiscible, incompressible fluids in a confined domain $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$ with densities ρ_1, ρ_2 and viscosities μ_1, μ_2, respectively. Without loss of generality, we assume that $\rho_1 < \rho_2$.

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 $O(\eta)$, and consider the following

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Ginzburg–Landau type of Helmholtz free energy functional:

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

where the first term contributes to the hydrophilic 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 hydrophobic 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, [43]).

2.1. Case of matched density. In the case of matched density, i.e., $\rho_1 = \rho_2$, the phase-field model has been well studied; cf., for instance, [15, 3, 17, 22]).

The evolution of the phase function is governed by the Cahn–Hilliard phase equation:

$$\begin{aligned} &\phi_t + \nabla\cdot(u\phi) = M\Delta w, \\ &w := \frac{\delta W}{\delta\phi} = -\lambda(\Delta\phi - f(\phi)), \end{aligned} \tag{2.3}$$

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

$$\rho(u_t + (u\cdot\nabla)u) = \nabla\cdot\tau, \tag{2.4}$$

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. By using an energetic variational approach (cf. [22]), one can derive

$$\rho(u_t + (u\cdot\nabla)u) = \nabla\cdot(\mu D(u) - pI - \lambda\nabla\phi\otimes\nabla\phi), \tag{2.5}$$

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

The Cahn–Hilliard phase equation (2.3), the momentum equations (2.5), and the incompressibility constraint

$$\nabla\cdot u = 0, \tag{2.6}$$

together with a suitable set of boundary conditions, form a closed system for the unknown (u, p, ϕ, w).

By using the identity

$$\begin{aligned} \nabla\cdot(\nabla\phi\otimes\nabla\phi) &= (\Delta\phi - f(\phi))\nabla\phi + \frac{1}{2}\nabla(|\nabla\phi|^2 + F(\phi)) \\ &= -w\nabla\phi + \frac{1}{2}\nabla(|\nabla\phi|^2 + F(\phi)) = \phi\nabla w + \frac{1}{2}\nabla(|\nabla\phi|^2 + F(\phi) - \phi w) \end{aligned}$$

and denoting the modified pressure as $\tilde{p} = p + \frac{1}{2}\lambda|\nabla\phi|^2 + \lambda F(\phi) + \phi w$ (still denoting it by p for simplicity), the system (2.3)–(2.5) can be rewritten as follows:

$$\phi_t + \nabla\cdot(u\phi) - M\Delta w = 0, \tag{2.7a}$$

$$w + \lambda(\Delta\phi - f(\phi)) = 0, \tag{2.7b}$$

$$u_t + (u\cdot\nabla)u - \nabla\mu\cdot D(u) + \nabla p - \phi\nabla w = 0, \tag{2.7c}$$

$$\nabla\cdot u = 0. \tag{2.7d}$$

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Without lose of generality, we have set in the above $\rho \equiv 1$. The above system should be supplemented with a set of suitable boundary conditions, for instance, a periodic boundary condition for all variables or

$$u|_{\partial\Omega} = 0, \quad \frac{\partial \phi}{\partial n}|_{\partial\Omega} = 0, \quad \frac{\partial w}{\partial n}|_{\partial\Omega} = 0. \tag{2.8}$$

By taking the inner product of (2.7a) with $-w$, (2.7b) with ϕ_t, of (2.7c) with u, and adding the three relations, we find that the system (2.7) satisfies the following energy law:

$$\frac{d}{dt}\int_\Omega \left(\frac{1}{2}|u|^2 + \frac{\lambda}{2}|\nabla\phi|^2 + \lambda F(\phi)\right)dx = -\int_\Omega \left(\frac{\mu}{2}|D(u)|^2 + M|\nabla w|^2\right)dx. \tag{2.9}$$

2.2. Case of nonmatching density. We now consider the case where $\rho_1 \neq \rho_2$. First of all, if the density ratio is small ($\sim O(1)$), one could use the well-known Boussinesq approximation to model the effect of density difference by a gravitational force (cf. for instance [22]). When the density ratio is large such that the Boussinesq approximation is no longer valid, the situation becomes more complicated, and there exist several phase-field models derived from various considerations (see [25, 34, 1, 2, 36, 23]). In this paper, we consider the following Cahn–Hilliard phase-field model which is equivalent to the one recently proposed in [2]. The governing equations are as follows:

$$\phi_t + \nabla\cdot(u\phi) - M\Delta w = 0, \tag{2.10a}$$

$$w + \lambda(\Delta\phi - f(\phi)) = 0, \tag{2.10b}$$

$$\rho(u_t + (u\cdot\nabla)u) + J\cdot\nabla u - \nabla\cdot\mu D(u) + \nabla p + \phi\nabla w = 0, \tag{2.10c}$$

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

and

$$J = \frac{\rho_2-\rho_1}{2}M\nabla w, \quad \rho = \frac{\rho_1-\rho_2}{2}\phi + \frac{\rho_1+\rho_2}{2}, \quad \mu = \frac{\mu_1-\mu_2}{2}\phi + \frac{\mu_1+\mu_2}{2}, \tag{2.11}$$

where u, p, ρ, and μ are the velocity, pressure, density, and viscosity of the mixture.

We can derive the following conservation property from (2.10a), (2.11), and (2.10d):

$$\rho_t + \nabla\cdot(\rho u) + \nabla\cdot J = 0. \tag{2.12}$$

By using the above identity, we have

$$\begin{aligned} \partial_t\left(\rho, \frac{|u|^2}{2}\right) &= (\rho u_t, u) + \left(\rho_t, \frac{|u|^2}{2}\right) \\ &= (\rho u_t, u) - \left(\nabla\cdot(\rho u) + \nabla\cdot J, \frac{|u|^2}{2}\right) \\ &= (\rho u_t + \rho u\cdot\nabla u + J\cdot\nabla u, u), \end{aligned} \tag{2.13}$$

where $(\cdot,\cdot)$ is the inner product in $L^2(\Omega)$.

The system (2.10) is thermodynamically consistent and satisfies an energy dissipation law. Indeed, taking the inner product of (2.10a) with w, (2.10b) with ϕ_t, (2.10c) with u, and using (2.13), we can obtain the following energy dissipation law:

$$\frac{d}{dt}\int_\Omega \left(\frac{1}{2}\rho|u|^2 + \frac{\lambda}{2}|\nabla\phi|^2 + \lambda F(\phi)\right)dx = -\int_\Omega \left(\frac{\mu}{2}|D(u)|^2 + M|\nabla w|^2\right)dx. \tag{2.14}$$

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3. Decoupled, energy stable numerical schemes. We recall that in a recent paper [11], the author established rigorous convergence results for a fully discretized, but nonlinearly coupled, scheme. The aim of this section is to construct decoupled, energy stable schemes to solve the systems (2.7) and (2.10). It has been shown that spurious solutions may occur if a numerical scheme does not satisfy the discrete energy dissipation law when the spatial grid and time step sizes are not carefully chosen (cf. [20, 16, 21]). Thus the compliance of discrete energy dissipation laws usually serve as the justification of numerical schemes and results, when no benchmark solutions are available. In addition, with unconditionally energy stable schemes, one can use relatively large time steps, the size of which is dictated only by accuracy considerations, or a suitable adaptive time stepping.

The systems (2.7) and (2.10) are both nonlinearly coupled models. While it is relatively easy to design some fully implicit schemes with energy stability, it is very difficult to design energy stable numerical schemes which are decoupled. Some of the main difficulties that one faces include the following:

- the coupling of the velocity and pressure through the incompressible condition;
- the stiffness in the phase equation associated with the interfacial width;
- the nonlinear coupling between the fluid equation and the phase equation; and
- additional difficulties introduced by the variable density in (2.10).

In [23], we constructed decoupled energy stable, but *nonlinear*, schemes for a thermodynamically consistent Cahn–Hilliard phase-field model developed in [1] (and independently in [23] using a variational derivation). However, the chemical potential in this model includes a velocity term, which prevents us from constructing *linear* decoupled energy stable systems in [23].

We shall construct two sets of numerical schemes (2.7) and (2.10). One is based on a stabilized approach (see [33, 32]), the other is based on a convex splitting approach (see [8, 9]).

- For the stabilized approach, we assume that the potential function $F(\phi)$ satisfies the following condition: there exists a constant L such that

$$\max_{|\phi|\in\mathbb{R}} |F''(\phi)| \le L. \tag{3.1}$$

One immediately notes that this condition is not satisfied by the standard Ginzburg–Landau double-well potential $F(\phi) = \frac{1}{4\eta^2}(\phi^2-1)^2$. However, since it is well known that the Allen–Cahn equation satisfies the maximum principle (for Cahn–Hilliard equation, a similar result is established in [5]), we can truncate $F(\phi)$ to quadratic growth outside of an interval $[-H, H]$ without affecting the solution if the maximum norm of the initial condition ϕ_0 is bounded by M. Therefore, it has been a common practice (cf. [18, 7, 33]) to consider the Allen–Cahn and Cahn–Hilliard equations with a truncated double-well potential $\tilde{F}(\phi)$. It is then obvious that there exists L such that (3.1) is satisfied with F replaced by $\tilde{F}$.

- For the convex spitting approach, we assume that the nonlinear potential $F(\phi)$ can be split-up as the difference of two convex functionals. For example, for the original double-well potential $F(\phi)$, we can set $F(\phi) = F_c(\phi) - F_e(\phi)$ where $F_c(\phi) = \frac{\phi^4}{4\eta^2}$ and $F_e(\phi) = (\frac{\phi^2}{2} - 1)/\eta^2$ are convex, and

$$f_c(\phi) := F_c'(\phi) = \phi^3/\eta^2, \quad f_e(\phi) := F_e'(\phi) = \phi/\eta^2. \tag{3.2}$$

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3.1. Case of matched density. To simplify the presentation, we will assume that $\mu_1 = \mu_2 = \mu$, although this is no essential additional difficulty to treat the case $\mu_1 \neq \mu_2$ (see the next subsection for its treatment). In [32], we constructed the following numerical scheme for the system (2.7):

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

$$\begin{cases} \dfrac{1}{\delta t}(\phi^{n+1} - \phi^n) + (\tilde{u}^{n+1} \cdot \nabla)\phi^n - M\Delta w^{n+1} = 0, \\ w^{n+1} - \dfrac{\lambda}{\eta^2}(\phi^{n+1} - \phi^n) + \lambda(\Delta\phi^{n+1} - f(\phi^n)) = 0, \\ \partial_n \phi^{n+1}|_{\partial\Omega} = 0, \partial_n w^{n+1}|_{\partial\Omega} = 0; \end{cases} \tag{3.3a}$$

$$\begin{cases} \dfrac{\tilde{u}^{n+1} - u^n}{\delta t} - \mu\Delta\tilde{u}^{n+1} + \nabla p^n + (u^n \cdot \nabla)\tilde{u}^{n+1} - w^{n+1}\nabla\phi^n = 0, \\ \tilde{u}^{n+1}|_{\partial\Omega} = 0; \end{cases} \tag{3.3b}$$

$$\begin{cases} \dfrac{u^{n+1} - \tilde{u}^{n+1}}{\delta t} + \nabla(p^{n+1} - p^n) = 0, \\ \nabla \cdot u^{n+1} = 0, \\ n \cdot u^{n+1}|_{\partial\Omega} = 0. \end{cases} \tag{3.3c}$$

In (3.3a), the term $-\frac{\lambda}{\eta^2}(\phi^{n+1} - \phi^n)$ is added artificially to balance the explicit nonlinear term $f(\phi^n)$ so that the time step will not be severely constrained by the interface thickness η. We have already showed in [32] that the above scheme satisfies a discrete energy law and is unconditionally stable. However, (ϕ^{n+1}, w^{n+1}) and $\tilde{u}^{n+1}$ in the above scheme is weakly coupled by the convection term $(u \cdot \nabla)\phi$ in the phase equation. Hence, it is desirable to construct a scheme which decouples the computation of (ϕ^{n+1}, w^{n+1}) and $\tilde{u}^{n+1}$. Following an idea in [4], we introduce a stabilizing term in the convective velocity and modify the above scheme as follows:

$$\begin{cases} \dfrac{1}{\delta t}(\phi^{n+1} - \phi^n) + \nabla \cdot (u^n_\star \phi^n) - M\Delta w^{n+1} = 0, \\ w^{n+1} - \dfrac{\lambda}{\eta^2}(\phi^{n+1} - \phi^n) + \lambda(\Delta\phi^{n+1} - f(\phi^n)) = 0, \\ \partial_n \phi^{n+1}|_{\partial\Omega} = 0, \partial_n w^{n+1}|_{\partial\Omega} = 0, \end{cases} \tag{3.4a}$$

with

$$u^n_\star = u^n - \delta t \phi^n \nabla w^{n+1}; \tag{3.4b}$$

$$\begin{cases} \dfrac{\tilde{u}^{n+1} - u^n}{\delta t} - \nu\Delta\tilde{u}^{n+1} + \nabla p^n + (u^n \cdot \nabla)\tilde{u}^{n+1} + \phi^n\nabla w^{n+1} = 0, \\ \tilde{u}^{n+1}|_{\partial\Omega} = 0; \end{cases} \tag{3.4c}$$

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$$\begin{cases} \dfrac{u^{n+1}-\tilde{u}^{n+1}}{\delta t} + \nabla(p^{n+1}-p^n) = 0, \\ \nabla\cdot u^{n+1} = 0, \\ n\cdot u^{n+1}|_{\partial\Omega} = 0. \end{cases} \tag{3.4d}$$

Remark 3.1.

- Following an idea in [4], a first-order stabilizing term is introduced in the explicit convective velocity u_*^n. This term is crucial for establishing the unconditional stability.
- Since $u_\star^n \cdot n|_{\partial\Omega} = 0$, we derive from (3.4a) that the scheme still satisfies the desired conservation property $\int_\Omega \phi^{n+1} = \int_\Omega \phi^n$.
- The last step can be rewritten as

$$\begin{cases} -\Delta(p^{n+1}-p^n) = -\dfrac{1}{\delta t}\nabla\cdot\tilde{u}^{n+1}, \\ \partial_n(p^{n+1}-p^n)|_{\partial\Omega} = 0, \end{cases} \quad u^{n+1} = \tilde{u}^{n+1} - \delta t\nabla(p^{n+1}-p^n). \tag{3.5}$$

- In the above scheme, computations of (ϕ^{n+1}, w^{n+1}), $\tilde{u}^{n+1}$, u^{n+1}, and p^{n+1} are totally decoupled! Furthermore, each of the steps consists of solving a *linear* elliptic equation.

For the above scheme, we can establish the following theorem.

THEOREM 3.1. *Assuming that the condition* (3.1) *is satisfied with* $L = 2/\eta^2$, *then the scheme* (3.4) *is uniquely solvable (with the pressure* p *determined up to a constant), unconditionally stable, and satisfies the following discrete energy law:*

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

where $\|\cdot\|$ *denotes the* L^2*-norm in* Ω.

Proof. Since each of the steps in the scheme (3.4) consists of a linear elliptic equation, it is easy to see that the scheme is uniquely solvable for $(\phi, w) \in H^1(\Omega)\times H^1(\Omega)$, $\tilde{u}^{n+1} \in (H_0^1(\Omega))^d$, $p^{n+1}\in H^1(\Omega)\backslash\mathbb{R}$, and $u^{n+1}\in (L^2(\Omega))^d$.

Notice the following:

$$\frac{\tilde{u}^{n+1}-u^n}{\delta t} + \phi^n\nabla w^{n+1} = \frac{\tilde{u}^{n+1}-u_*^n}{\delta t}. \tag{3.6}$$

Taking the inner product of (3.4c) with $2\delta t\tilde{u}^{n+1}$, using the above relation and the well-known property

$$(u\cdot\nabla v, v) = 0 \;\forall u\in H,\; v\in (H_0^1(\Omega))^d, \tag{3.7}$$

where $H = \{u \in (L^2(\Omega))^d : \nabla\cdot u = 0,\; u\cdot n|_{\partial\Omega} = 0\}$, we derive

$$\|\tilde{u}^{n+1}\|^2 - \|u_\star^n\|^2 + \|\tilde{u}^{n+1}-u_*^n\|^2 + 2\mu\delta t\|\nabla\tilde{u}^{n+1}\|^2 + 2\delta t(\nabla p^n, \tilde{u}^{n+1}) = 0. \tag{3.8}$$

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To deal with the last term in the above, we first take the inner product of (3.4d) with $2\delta t\nabla p^n$ to obtain

$$\delta t^2(\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2 - \|\nabla p^{n+1} - \nabla p^n\|^2) = 2\delta t(\tilde{u}^{n+1}, \nabla p^n); \tag{3.9}$$

we also derive from (3.4d) that

$$\delta t^2\|\nabla p^{n+1} - \nabla p^n\|^2 = \|\tilde{u}^{n+1} - u^{n+1}\|^2; \tag{3.10}$$

we then take the inner product of (3.4d) with u^{n+1} to get

$$\|u^{n+1}\|^2 + \|u^{n+1} - \tilde{u}^{n+1}\|^2 = \|\tilde{u}^{n+1}\|^2. \tag{3.11}$$

Combining the above four equalities, we find

$$\begin{aligned}\|u^{n+1}\|^2 - \|u^n_\star\|^2 + \|\tilde{u}^{n+1} - u^n_\star\|^2 + 2\mu\delta t\|\nabla\tilde{u}^{n+1}\|^2 \\ + \delta t^2(\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2) = 0.\end{aligned} \tag{3.12}$$

Next, we use the relation (3.4b) to deal with $\|u^n_\star\|^2$ in the above. Taking the inner product of (3.4b) with $2u^n_\star$, we obtain

$$\|u^n_\star\|^2 - \|u^n\|^2 + \|u^n_\star - u^n\|^2 = -2\delta t(\phi^n\nabla w^{n+1}, u^n_\star). \tag{3.13}$$

Adding the two relations above, we obtain

$$\begin{aligned}\|u^{n+1}\|^2 - \|u^n\|^2 + \|u^n_\star - u^n\|^2 + \|\tilde{u}^{n+1} - u^n_\star\|^2 + 2\mu\delta t\|\nabla\tilde{u}^{n+1}\|^2 \\ + \delta t^2(\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2) = -2\delta t(\phi^n\nabla w^{n+1}, u^n_\star).\end{aligned} \tag{3.14}$$

It now remains to deal with the last term in the above.

Taking the inner product of the first equation of (3.4a) with $2\delta t w^{n+1}$, we get

$$2(\phi^{n+1} - \phi^n, w^{n+1}) + 2\delta t(\nabla\cdot(\phi^n u^n_\star), w^{n+1}) + 2M\delta t\|\nabla w^{n+1}\|^2 = 0; \tag{3.15}$$

and taking the inner product of the second equation of (3.4a) with $-2(\phi^{n+1} - \phi^n)$, we obtain

$$\begin{aligned}&-2(w^{n+1}, \phi^{n+1} - \phi^n) + \frac{2\lambda}{\eta^2}\|\phi^{n+1} - \phi^n\|^2 \\ &+ \lambda(\|\nabla\phi^{n+1}\|^2 - \|\nabla\phi^n\|^2 + \|\nabla\phi^{n+1} - \nabla\phi^n\|^2) + 2\lambda(f(\phi^n), \phi^{n+1} - \phi^n) = 0.\end{aligned} \tag{3.16}$$

For the last term in (3.16), we use the Taylor expansion

$$F(\phi^{n+1}) - F(\phi^n) = f(\phi^n)(\phi^{n+1} - \phi^n) + \frac{f'(\xi^n)}{2}(\phi^{n+1} - \phi^n)^2. \tag{3.17}$$

Finally, combining (3.14), (3.15), (3.16), and (3.17), and using the assumption (3.1) with $L = 2/\eta^2$, we obtain

$$\begin{aligned}\|u^{n+1}\|^2 - \|u^n\|^2 + \|\tilde{u}^n_\star - u^n\|^2 + \|\tilde{u}^{n+1} - u^n\|^2 + 2\mu\delta t\|\nabla\tilde{u}^{n+1}\|^2 \\ &+ \delta t^2(\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2) \\ &+ 2M\delta t\|\nabla w^{n+1}\|^2 + \frac{2\lambda}{\eta^2}\|\phi^{n+1} - \phi^n\|^2 \\ &+ \lambda(\|\nabla\phi^{n+1}\|^2 - \|\nabla\phi^n\|^2 + \|\nabla\phi^{n+1} - \nabla\phi^n\|^2) \\ &+ 2\lambda(F(\phi^{n+1}) - F(\phi^n), 1) \\ &\le \lambda(f'(\xi^n)(\phi^{n+1} - \phi^n), \phi^{n+1} - \phi^n) \le \frac{2\lambda}{\eta^2}\|\phi^{n+1} - \phi^n\|^2.\end{aligned}$$

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The desired result is then a direct consequence of the above inequality. ∎

Instead of introducing a stabilizing term in the scheme (3.4) to deal with the explicit treatment of $f(\phi)$, we can also use the so-called convex splitting approach. To this end, we replace (3.4a) by

$$\begin{cases} \frac{1}{\delta t}(\phi^{n+1}-\phi^n)+\nabla\cdot(u_*^n\phi^n)-M\Delta w^{n+1}=0, \\ w^{n+1}+\lambda(\Delta\phi^{n+1}-f_c(\phi^{n+1})+f_e(\phi^n))=0, \\ \partial_n\phi^{n+1}|_{\partial\Omega}=0, \partial_n w^{n+1}|_{\partial\Omega}=0, \end{cases} \tag{3.18}$$

where u_*^n is still given by (3.4b).

For this convex splitting scheme, we have the following result.

THEOREM 3.2. *The scheme* (3.18)–(3.4b)–(3.4c)–(3.4d) *is uniquely solvable (with pressure p determined up to a constant), unconditionally stable, and satisfies the following discrete energy law:*

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

Proof. We show first that the solution of (3.18) is unique. We derive from (3.18) that (ϕ^{n+1}, w^{n+1}) is the solution of the following system:

$$\begin{aligned} &\frac{1}{\delta t}\phi-a(x)w+\Delta w=g(x), \quad \partial_n w|_{\partial\Omega}=0; \\ &w+\lambda(\Delta\phi-f_c(\phi))=h(x), \quad \partial_n\phi|_{\partial\Omega}=0, \end{aligned} \tag{3.19}$$

where $a(x)=\delta t|\nabla\phi^n|^2\ge 0$, $g(x)$, and $h(x)$ are known functions depending on the approximate solutions at $t=t^n$. Assuming that (ϕ,w) and $(\tilde{\phi},\tilde{w})$ are two solutions of (3.19), we find

$$\begin{aligned} &\frac{1}{\delta t}(\phi-\tilde{\phi})-a(x)(w-\tilde{w})+\Delta(w-\tilde{w})=0, \quad \partial_n(w-\tilde{w})|_{\partial\Omega}=0; \\ &(w-\tilde{w})+\lambda\Delta(\phi-\tilde{\phi})-\lambda(f_c(\phi)-f_c(\tilde{\phi}))=0, \quad \partial_n(\phi-\tilde{\phi})|_{\partial\Omega}=0. \end{aligned} \tag{3.20}$$

Taking the inner products of the first equation with $-(w-\tilde{w})$, and of the second equation with $-\frac{1}{\delta t}(\phi-\tilde{\phi})$, summing up the two relations, and using the fact that $(f_c(\phi)-f_c(\tilde{\phi}),\phi-\tilde{\phi})\ge 0$, we obtain

$$\|\sqrt{a(x)}(w-\tilde{w})\|^2+\|\nabla(w-\tilde{w})\|^2+\frac{1}{\delta t}\|\nabla(\phi-\tilde{\phi})\|^2\le 0.$$

Hence, we have $w-\tilde{w}=\phi-\tilde{\phi}=0$.

The existence of a solution for (3.18) can be established by a standard argument using the Leray–Schauder fixed point theorem (see, for instance, [23] for details on a similar problem).

The proof of energy stability is essentially the same as that of Theorem 3.1 with the following modifications.

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The last term, $2\lambda(f(\phi^n),\phi^{n+1}-\phi^n)$, in (3.16) becomes $2\lambda(f_c(\phi^{n+1})-f_e(\phi^n),\phi^{n+1}-\phi^n)$. Then, (3.17) should be replaced by

$$\begin{aligned} F_c(\phi^{n+1})-F_c(\phi^n) &= f_c(\phi^{n+1})(\phi^{n+1}-\phi^n)-\frac{f_c'(\xi^{n+1})}{2}(\phi^{n+1}-\phi^n)^2, \\ F_e(\phi^{n+1})-F_e(\phi^n) &= f_e(\phi^n)(\phi^{n+1}-\phi^n)+\frac{f_e'(\eta^n)}{2}(\phi^{n+1}-\phi^n)^2, \end{aligned} \tag{3.21}$$

which implies that

$$(F(\phi^{n+1})-F(\phi^n),1)\le (f_c(\phi^{n+1})-f_e(\phi^n),\phi^{n+1}-\phi^n), \tag{3.22}$$

since $f_c'(\phi)\ge 0$ and $f_e'(\phi)\ge 0$ for any ϕ. ∎

3.2. Case of nonmatching density. We now consider the model (2.10). To deal with the variable density, we define a cut-off function

$$\hat\phi=\begin{cases}\phi, & |\phi|\le 1,\\ \mathrm{sign}(\phi), & |\phi|>1.\end{cases} \tag{3.23}$$

We construct first a scheme based on the stabilization.

Given initial conditions ρ^0, ϕ^0, w^0, u^0, and p^0, we compute $(\rho^{n+1},\phi^{n+1},w^{n+1},\tilde u^{n+1},u^{n+1},p^{n+1})$ for $n\ge 0$ by

$$\begin{cases}\dfrac{1}{\delta t}(\phi^{n+1}-\phi^n)+\nabla\cdot(u_\star^n\phi^n)-M\Delta w^{n+1}=0,\\ w^{n+1}-\dfrac{\lambda}{\eta^2}(\phi^{n+1}-\phi^n)+\lambda(\Delta\phi^{n+1}-f(\phi^n))=0,\\ \partial_n\phi^{n+1}|_{\partial\Omega}=0, \partial_n w^{n+1}|_{\partial\Omega}=0,\end{cases} \tag{3.24a}$$

with

$$u_\star^n=u^n-\delta t\frac{\phi^n\nabla w^{n+1}}{\rho^n}; \tag{3.24b}$$

(3.24c)

$$\begin{cases}\rho^n\dfrac{u^{n+1}-u^n}{\delta t}-\nabla\cdot\mu^n D(u^{n+1})+\nabla(2p^n-p^{n-1})+\rho^n(u^n\cdot\nabla)u^{n+1}+J^n\cdot\nabla u^{n+1}\\ \qquad +\phi^n\nabla w^{n+1}+\dfrac12 u^{n+1}\dfrac{\rho^{n+1}-\rho^n}{\delta t}+\dfrac12\nabla\cdot(\rho^n u^n)u^{n+1}+\dfrac12\nabla\cdot J^n u^{n+1}=0,\\ u^{n+1}|_{\partial\Omega}=0,\end{cases}$$

with

$$J^n=\frac{\rho_2-\rho_1}{2}\nabla w^n; \tag{3.24d}$$

$$\begin{cases}\Delta(p^{n+1}-p^n)=\dfrac{\chi}{\delta t}\nabla\cdot u^{n+1},\\ \partial_n p^{n+1}|_{\partial\Omega}=0;\end{cases} \tag{3.24e}$$

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with $\chi = \frac{1}{2}\min(\rho_1, \rho_2)$ and

$$\rho^{n+1} = \frac{\rho_1 - \rho_2}{2}\hat{\phi}^{n+1} + \frac{\rho_1 + \rho_2}{2}, \qquad \mu^{n+1} = \frac{\mu_1 - \mu_2}{2}\hat{\phi}^{n+1} + \frac{\mu_1 + \mu_2}{2}. \tag{3.24f}$$

Several remarks are in order.

- The last three terms in (3.24c) are a first-order approximation of the term
$$\frac{1}{2}(\rho_t + \nabla \cdot (\rho u) + \nabla \cdot J)u \ \text{ at } t_{n+1}.$$
This term vanishes due to (2.12). Hence, (3.24c) is indeed a consistent first-order approximation to (2.7c).
- We derive from (3.24f) and (3.23) that $\rho^{n+1} \geq \min(\rho_1, \rho_2)$ and $\mu^{n+1} \geq \min(\mu_1, \mu_2)$.
- In order to avoid solving an elliptic equation with $1/\rho$ as a variable coefficient, we adapt a pressure-stabilized form in the above scheme which leads to a pressure Poisson equation.
- As for the scheme (3.4), the systems for (ϕ^{n+1}, w^{n+1}), u^{n+1}, and p^{n+1} are decoupled and *linear*.

THEOREM 3.3. *Assuming that the condition* (3.1) *is satisfied with $L = 2/\eta^2$, then the scheme* (3.24) *is uniquely solvable (with pressure p determined up to a constant), unconditionally stable, and satisfies the following discrete energy law:*

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

where $\sigma^k = \sqrt{\rho^k}$.

Proof. The unique solvability is a direct consequence of the fact that each of the steps in the scheme (3.24) consists of a linear elliptic equation.

Using integration by part, we can show that

$$(u \cdot \nabla v, v) + \frac{1}{2}((\nabla \cdot u)v, v) = 0 \quad \text{ if } u \cdot n|_{\partial\Omega} = 0. \tag{3.25}$$

Thanks to (3.25), we have

$$\begin{aligned}
&\left((\rho^n u^n \cdot \nabla)u^{n+1} + \frac{1}{2}\nabla \cdot (\rho^n u^n)u^{n+1}, u^{n+1}\right) = 0,\\
&\left(J^n \cdot \nabla u^{n+1} + \frac{1}{2}J^n \cdot \nabla u^{n+1}, u^{n+1}\right) = 0.
\end{aligned} \tag{3.26}$$

We also derive from (3.24b) that

$$\rho^n\frac{u^{n+1} - u^n}{\delta t} + \phi^n\nabla w^{n+1} = \rho^n\frac{u^{n+1} - u_*^n}{\delta t}. \tag{3.27}$$

Now, taking the inner product of (3.24c) with $2\delta t u^{n+1}$, and using (3.26) and (3.27), we obtain

$$\begin{aligned}
&\|\sigma^n u^{n+1}\|^2 - \|\sigma^n u_\star^n\|^2 + \|\sigma^n(u^{n+1} - u_\star^n)\|^2\\
&\qquad + \|\sigma^{n+1}u^{n+1}\|^2 - \|\sigma^n u^{n+1}\|^2 + \delta t\|\sqrt{\mu^n}D(u^{n+1})\|^2\\
&\qquad + 2\delta t(p^{n+1} - 2p^n + p^{n-1}, \nabla \cdot u^{n+1}) - 2\delta t(p^{n+1}, \nabla \cdot u^{n+1}) = 0.
\end{aligned} \tag{3.28}$$

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Then, by taking the inner product of (3.24e) with $\frac{2\delta t^2}{\chi}(p^{n+1}-2p^n+p^{n-1})$ and with $-\frac{2\delta t^2}{\chi}p^{n+1}$ separately, we obtain

$$-\frac{\delta t^2}{\chi}(\|\nabla(p^{n+1}-p^n)\|^2-\|\nabla(p^n-p^{n-1})\|^2+\|\nabla(p^{n+1}-2p^n+p^{n-1})\|^2) = 2\delta t(\nabla\cdot u^{n+1}, p^{n+1}-2p^n+p^{n-1}), \tag{3.29}$$

and

$$\frac{\delta t^2}{\chi}(\|\nabla p^{n+1}\|^2-\|\nabla p^n\|^2+\|\nabla(p^{n+1}-p^n\|^2) = -2\delta t(\nabla\cdot u^{n+1}, p^{n+1}). \tag{3.30}$$

Adding the above two equalities together, we get

$$\begin{aligned} &2\delta t(p^{n+1}-2p^n+p^{n-1},\nabla\cdot u^{n+1})-2\delta t(p^{n+1},\nabla\cdot u^{n+1})\\ &\quad=\frac{\delta t^2}{\chi}(\|\nabla p^{n+1}\|^2-\|\nabla p^n\|^2)+\frac{\delta t^2}{\chi}\|\nabla(p^n-p^{n-1})\|^2\\ &\quad-\frac{\delta t^2}{\chi}\|\nabla(p^{n+1}-2p^n+p^{n-1})\|^2. \end{aligned} \tag{3.31}$$

Next, we take the difference of (3.24e) at step t^{n+1} and step t^n to derive

$$\frac{\delta t^2}{\chi}\|\nabla(p^{n+1}-2p^n+p^{n-1})\|^2 \le \chi\|u^{n+1}-u^n\|^2 \le \frac{1}{2}\|\sigma^n(u^{n+1}-u^n)\|^2. \tag{3.32}$$

We then derive from (3.28), (3.31), and (3.32) that

$$\begin{aligned} &\|\sigma^{n+1}u^{n+1}\|^2-\|\sigma^n u_\star^n\|^2+\|\sigma^n(u^{n+1}-u_\star^n)\|^2+\delta t\|\sqrt{\mu^n}D(u^{n+1})\|^2\\ &\quad+\frac{\delta t^2}{\chi}(\|\nabla p^{n+1}\|^2-\|\nabla p^n\|^2)+\frac{\delta t^2}{\chi}\|\nabla(p^{n+1}-p^n)\|^2\\ &\quad\le\frac{1}{2}\|\sigma^n(u^{n+1}-u^n)\|^2. \end{aligned} \tag{3.33}$$

To deal with the last term, we rewrite (3.24b) as

$$\frac{\rho^n(u_\star^n-u^n)}{\delta t} = -\phi^n\nabla w^{n+1}, \tag{3.34}$$

and take the inner product of (3.34) with $2\delta t u_\star^n$ to obtain

$$\|\sigma^n u_\star^n\|^2-\|\sigma^n u^n\|^2+\|\sigma^n(u_\star^n-u^n)\|^2 = -2\delta t(\phi^n\nabla w^{n+1}, u_\star^n). \tag{3.35}$$

On the other hand, we derive from the triangle inequality that

$$\|\sigma^n(u_\star^n-u^n)\|^2+\|\sigma^n(u^{n+1}-u_\star^n)\|^2 \ge \frac{1}{2}\|\sigma^n(u^{n+1}-u^n)\|^2. \tag{3.36}$$

Thus, combining (3.33), (3.36), and (3.35), we obtain

$$\begin{aligned} &\|\sigma^{n+1}u^{n+1}\|^2-\|\sigma^n u^n\|^2+\delta t\|\sqrt{\mu^n}D(u^{n+1})\|^2+\frac{\delta t^2}{\chi}(\|\nabla p^{n+1}\|^2-\|\nabla p^n\|^2)\\ &\quad+\frac{\delta t^2}{\chi}\|\nabla(p^{n+1}-p^n)\|^2 \le -2\delta t(\phi^n\nabla w^{n+1}, u_\star^n). \end{aligned} \tag{3.37}$$

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It remains to deal with the last term on the right-hand side.

Taking the inner product of the first equation in (3.24a) with $2\delta t w^{n+1}$, we obtain

$$2(\phi^{n+1}-\phi^n, w^{n+1}) + 2\delta t((\nabla\cdot(u_\star^n\phi^n), w^{n+1})) + 2M\delta t\|\nabla w^{n+1}\|^2 = 0; \tag{3.38}$$

taking the inner product of the second equation in (3.24a) with $-2(\phi^{n+1}-\phi^n)$, we get

$$\begin{aligned}&-2(w^{n+1},\phi^{n+1}-\phi^n) + \frac{2\lambda}{\eta^2}\|\phi^{n+1}-\phi^n\|^2 + 2\lambda(f(\phi^n),\phi^{n+1}-\phi^n)\\ &\qquad + \lambda(\|\nabla\phi^{n+1}\|^2 - \|\nabla\phi^n\|^2 + \|\nabla\phi^{n+1}-\nabla\phi^n\|^2) = 0.\end{aligned} \tag{3.39}$$

Finally, combining (3.37), (3.38), and (3.39), the Taylor expansion (3.17), and using the assumption (3.1) with $L = 2/\eta^2$, we arrive at

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

which implies the desired result. ∎

As in the case of matched density, we can also construct a convex splitting scheme by replacing (3.24a) in the scheme (3.24) with (3.18) with u_*^n given by (3.24b). For this convex splitting scheme, we have the following result.

THEOREM 3.4. *The convex splitting scheme,* (3.18) *with* (3.24b)–(3.24f)*, is uniquely solvable (with pressure p determined up to a constant), unconditionally stable, and satisfies the following discrete energy law:*

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

where $\sigma^k = \sqrt{\rho^k}$.

The above result can be proved using essentially the same procedure as in the proof of Theorem 3.3 with the modifications outlined in the proof of Theorem 3.1. The details are left to the interested readers.

4. Numerical simulations. We present in this section some numerical experiments using the schemes constructed in the last section. Since it has been well documented that both the convex splitting approach and stabilization approach provide consistent approximations to the phase-field models, we shall only examine the schemes based on stabilization here, as the implementation of the schemes-based convex splitting is more complicated due to its nonlinear nature.

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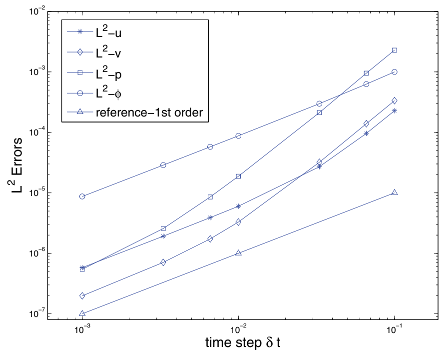
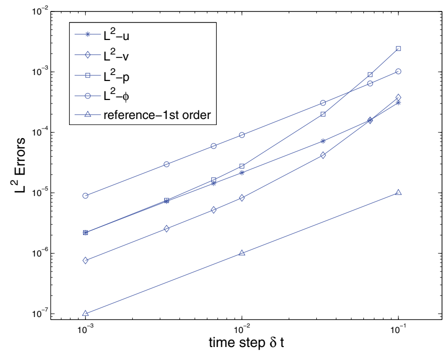


(a) Matched density case.



(b) Nonmatched density case.

FIG. 1. *Temporal convergence rates: L^2 errors of the velocity (x component u, y-component of v), pressure p, and phase field function ϕ as the funciton of time step δt for matched and nonmatched density case.*

Our spatial discretization is based on the Legendre–Galerkin method [31]. We use the inf-sup stable (P_N, P_{N-2}) pair for the velocity and pressure, and P_N for the phase function ϕ and the chemical potential w.

Example 1: Accuray test. We first test the convergence rates of the proposed schemes (3.4) and (3.24). Let $\Omega = [0, 2]^2$, we choose a forcing function such that the exact solution for (2.7) and (2.10) is

$$\begin{cases} \phi(t, x, y) = 2 + \sin(t)\cos(\pi x)\cos(\pi y), \\ u(t, x, y) = \pi \sin(2\pi y)\sin^2(\pi x)\sin(t), \\ v(t, x, y) = -\pi \sin(2\pi x)\sin^2(\pi y)\sin(t), \\ p(t, x, y) = \cos(\pi x)\sin(\pi y)\sin(t). \end{cases} \tag{4.1}$$

We set

$$\rho_1 = 3, \quad \rho_2 = 1 \tag{4.2}$$

for system (2.10) with nonmatching density. We choose $\eta = 0.02, \nu = 1, M = 1, \lambda = 0.001$. We use 129^2 Legendre–Gauss–Lobatto points so the spatial discretization errors are negligible compared with the time discretization error.

For both cases, we plot the L^2 errors of the velocity, pressure, and phase function between the numerical solution and the exact solution at $t = 1$ with different time step sizes in Figure 1. We observe that our numerical schemes (3.4) and (3.24) are asymptotically (at least) first-order accurate in time for all variables.

Example 2: The dynamics of a square shape fluid. We simulate the evolution of a square shaped fluid bubble in the domain of $[-1, 1] \times [-1, 1]$. We assume the fluid bubble and ambient fluid have matched density ($\rho_1 = \rho_2 = 1$) and viscosity ($\mu_1 = \mu_2 = 1$), and use the scheme (3.4). The following parameters are used:

$$\nu = 1, \quad M = 2 \times 10^{-3}, \quad \lambda = 0.01, \quad \eta = 0.02, \quad \delta t = 0.001. \tag{4.3}$$

The initial velocity and pressure are set to zero. A 257×257 grid based on Legendre–Gauss–Lobatto points is used. Figure 2 shows the dynamics evolution of the bubble which turns to a circle under the effect of surface tension. To illustrate that our

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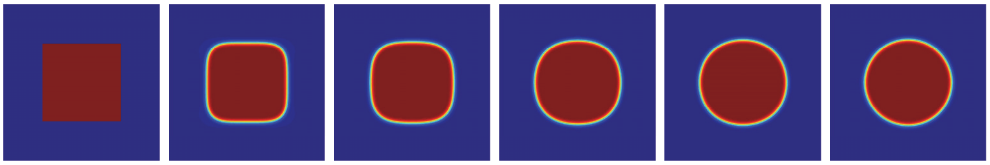

FIG. 2. *The dynamics of a square shape bubble. Snapshots are shown at* $t = 0, 0.5, 1, 2, 3, 10$ *for* $\delta t = 0.001$.

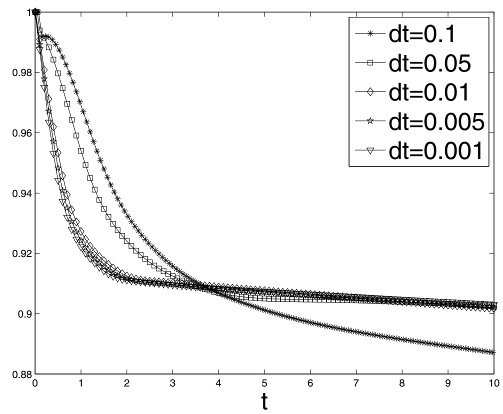

FIG. 3. *Energy plot of Example* 1.

numerical scheme (3.4) indeed obeys the discrete energy law proved in the last section, we plot in Figure 3 the evolution of the discrete total energy for different time steps, $\mathbb{E}^n_{tot}/\mathbb{E}^0_{tot}$ where $\mathbb{E}^n_{tot} = \frac{1}{2}\|u^n\|^2 + \frac{\delta t^2}{2}\|\nabla p^n\|^2 + \lambda(\frac{1}{2}\|\nabla\phi^n\|^2 + (F(\phi^n), 1))$. One observes from these plots that the discrete energy indeed decays with time.

4.1. Example 3: An air bubble rising in water. We simulate in this example an air bubble rising in the water using the scheme (3.24). The computational domain is $\Omega = (0, \mathrm{d}) \times (0, \frac{3}{2}\mathrm{d})$ with initially an air bubble (with density ρ_1 and dynamic viscosity μ_1) in water (with density ρ_2 and dynamic viscosity μ_2). The equations are nondimensionalized using the following scaled variables:

$$\hat{t} = \frac{t}{t_0}, \quad \hat{\rho} = \frac{\rho}{\rho_0}, \quad \hat{x} = \frac{x}{d_0}, \quad \hat{u} = \frac{u}{u_0}, \tag{4.4}$$

where

$$t_0 = \sqrt{d_0/g}, \quad u_0 = \sqrt{d_0 g}, \quad \rho_0 = \min(\rho_1, \rho_2), \quad d_0 = \mathrm{d}. \tag{4.5}$$

The dimensionless form of (2.7) with an extra gravitational force ρg in the momentum equation, after omitting the ˆ from the notation, is as follows:

$$\phi_t + (u \cdot \nabla)\phi - M\Delta w = 0, \tag{4.6a}$$

$$w + \lambda\left(\Delta\phi - \frac{\phi(\phi^2 - 1)}{\eta^2}\right) = 0, \tag{4.6b}$$

$$\rho(u_t + (u \cdot \nabla)u) + J \cdot \nabla u - \nabla \cdot (\mu\nabla u) + \nabla p - w\nabla\phi = \rho g, \tag{4.6c}$$

$$\nabla \cdot u = 0, \tag{4.6d}$$

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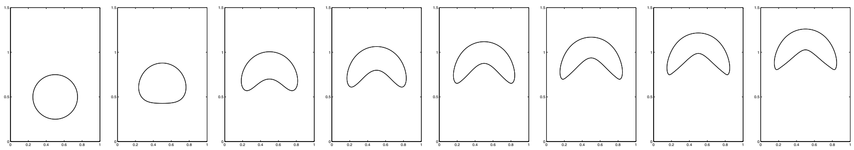

FIG. 4. *Example* 2: *Snapshots of air bubble rising in water at* $t = 0, 1, 2, 2.5, 3, 3.5, 4, 4.5$.

with

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

In the above, $\tilde{\rho}_1 = \rho_1/\rho_0$, $\tilde{\rho}_2 = \rho_2/\rho_0$, $\tilde{\mu}_1 = \mu_1/(\rho_0 \mathrm{d}^{3/2}\mathrm{g}^{1/2})$, and $\tilde{\mu}_2 = \mu_2/(\rho_0 \mathrm{d}^{3/2}\mathrm{g}^{1/2})$.

We set the initial velocity and pressure to be zero, and set the initial phase function as

$$\phi(x, y, t = 0) = \tanh\left(\frac{\sqrt{(x - x_0)^2 + (y - y_0)^2} - \frac{1}{4}\mathrm{d}}{\eta_0}\right), \tag{4.7}$$

where (x_0, y_0) is the center of the bubble, and η_0 is the diffusive interfacial width. The physical parameters are $\rho_0 = \rho_1 = 1.161, \rho_2 = 995.65$ and $\mu_1 = 0.0000186, \mu_2 = 0.0007977$. We set $\mathrm{d} = 0.005$, $\mathrm{g} = 9.8$, $\lambda = 0.05$, $M = 4 \times 10^{-5}$, 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 Figure 4, we plot a comparison of the level sets $\{x : \phi(x) = 0\}$ by scheme (3.24) at different times. The results are qualitatively similar to those given in [32] with a different scheme. Note that due to the gravitational force in the momentum equation, the discrete energy will no longer decay monotonically. However, our numerical tests confirm that the scheme is indeed unconditionally stable, although sufficiently small time steps have to be used to obtain accurate results.

5. Concluding remarks. We considered the time discretization for the Cahn–Hilliard phase-field models of two-phase incompressible flows with constant and variable density. In the case of variable density, we restricted our attention to the model recently proposed in [2].

By combining several approaches which have proved to be effective for dealing with different difficulties of the nonlinear coupled Cahn–Hilliard Navier–Stokes system, we constructed two classes, one based on the stabilization and the other based on convex splitting, of efficient and easy-to-implement schemes for the Cahn–Hilliard phase-field models with constant or variable density. These schemes satisfy a discrete energy law and lead to, at each time step, an elliptic system for the phase function, a linear elliptic equation for the velocity, and a Poisson equation for the pressure. Moreover, in the case of stabilization, the elliptic system for the phase function is also linear. Hence, these schemes are extremely efficient and easy-to-implement. To the best of our knowledge, the schemes based on stabilization are the first *totally decoupled, linear, unconditionally energy stable* schemes for phase-field models of two-phase incompressible flows.

Some of the immediate extensions/projects related to this paper include the following:

- We have only considered time discretization in this paper. While the stability proofs are based on weak formulations with suitable test functions, it is a still a challenge to extend the results to a properly formulated spatial discretization.

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- The dynamics of multiphase flows may exhibit multiple time scales that are expensive to capture accurately with an uniform time stepping scheme. A main advantage of unconditionally energy stable schemes is that they can be combined with an adaptive time-stepping strategy.
- Only first-order accurate schemes are constructed in this paper. As noted in [33], it does not appear possible to construct an unconditionally energy stable scheme using a second-order stabilization term in the Cahn–Hilliard equation. On the other hand, second-order, unconditionally energy stable convex-splitting schemes for the Cahn–Hilliard equation are available. But how to construct second-order, unconditionally energy stable, decoupled schemes for the Cahn–Hilliard Navier–Stokes phase-field models remains to be a challenging task.

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