Numerical Approximations for Allen-Cahn Type Phase Field Model of Two-Phase Incompressible Fluids with Moving Contact Lines

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Abstract. In this paper, we present some efficient numerical schemes to solve a two-phase hydrodynamics coupled phase field model with moving contact line boundary conditions. The model is a nonlinear coupling system, which consists the Navier-Stokes equations with the general Navier Boundary conditions or degenerated Navier Boundary conditions, and the Allen-Cahn type phase field equations with dynamical contact line boundary condition or static contact line boundary condition. The proposed schemes are linear and unconditionally energy stable, where the energy stabilities are proved rigorously. Various numerical tests are performed to show the accuracy and efficiency thereafter.

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1 Introduction

Phase field (or diffuse interface) methods have been used widely and successfully to simulate a variety of interfacial phenomena, and have become one of the major tools to study the interfacial dynamics in many science and engineering fields (cf.\textsuperscript{[4–6, 8, 9, 12, 13, 15, 16,}}

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and the references therein). The starting point of the phase-field approach is that the interface between multiple material components is viewed as a transition layer, where the two components are assumed to mix to a certain degree. Hence, the dynamics of the interface can be determined by the competition between the kinetic energy and the “elastic” mixing energy. Based on the variational formalism, the derived phase field model usually follows the thermodynamically consistent (or called energy stable) energy dissipation law, making it possible to carry out mathematical analysis, to develop efficient numerical schemes, and further to perform reliable numerical simulations.

In typical phase field models, there are mainly two categories of system equations: the Allen-Cahn equation (Bray [2]) and the Cahn-Hilliard equation (Cahn and Hilliard [3]), based on choices of diffusion rates. From the numerical point of view, the Allen-Cahn equation is a second-order equation, which is easier to solve numerically but does not conserve the volume fraction, while the Cahn-Hilliard equation is a fourth-order equation which conserves the volume fraction but is relatively harder to solve numerically. Since the PDE of either system usually follows the energy law, people are particularly interested in developing efficient numerical schemes that can satisfy a thermo-consistent energy law in the discrete level. Moreover, it is specifically desirable to develop some “easy-to-implement” (linear or decoupled) schemes in order to avoid expensive computational cost spent on the iterations needed by the nonlinear schemes.

In [18–21], the authors developed an efficient phase field model to simulate the so-called “moving contact line” (MCL) problem, where the fluid-fluid interface may touch the solid wall. For such situation, the simple no-slip boundary conditions implying that the position of the contact line does not move, are not applicable since there may exist quite a few molecules near the surface that they “bounce along” down the surface. Thus the phase field model derived in [18–21] consists of Navier-Stokes equations with the general Navier boundary condition (GNBC), and the equations for the phase field variable with the so-called dynamical contact line boundary condition (DCLBC). Due to the considerations of volume conservation, the dynamics of the phase field variable is governed by the fourth order Cahn-Hilliard equation. We recall that a nonlinear, energy stable numerical scheme was proposed in [10], where the convective term was treated semi-implicitly, and the double well potential was handled by the convex splitting approach. Such a scheme requires solving a coupled nonlinear system that usually is not convenient for the computations.

Therefore, in this paper, we aim to develop some efficient numerical schemes to solve the phase field model with MCLs. To avoid the difficulties to solve the fourth order Cahn-Hilliard equation, we adopt the second order Allen-Cahn equation by assuming that the relaxation of the phase variable is governed by the $L^2$ gradient flow. To overcome non-conservation of the volume fraction, an extra term is added in the free energy to penalize the volume, which is one of the common practices in the framework of phase field models [8, 26]. We develop two numerical schemes, one for the static contact line boundary condition (SCLBC) and the other for the DCLBC. Both schemes are linear and unconditionally energy stable. Moreover, the computations of the phase variable are
completely decoupled from that of the velocity in the scheme for the SCLBC. Ample
numerical examples are implemented to show the accuracy and efficiency thereafter.

The rest of the paper is organized as follows. In Section 2, we present the phase-
field model of moving contact line condition and show the energy dissipation law for
the system. In Section 3, we propose two energy stable schemes and prove their energy
stabilities. In Section 4, we present some numerical simulations to illustrate the efficiency
and accuracy of the proposed numerical schemes. Some concluding remarks are given in
Section 5.

2 The PDE system and its energy law

In [18–21], the flow-coupled phase field model consists the Navier-Stokes (NS) equations
with the GNBC (2.4) for the momentum equation, and the Cahn-Hilliard equations (CH)
with the DCLBC (2.8) for the phase field variable. The non-dimensional version of the
system reads as follows:

Incompressible Navier-Stokes equations for hydrodynamics:

\[
\begin{align*}
\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u} &= \nu \Delta \mathbf{u} - \nabla p + \lambda \mu \nabla \phi, \\
\nabla \cdot \mathbf{u} &= 0, \\
\mathbf{u} \cdot \mathbf{n} &= 0, \quad \text{on } \partial \Omega, \\
l(\phi)(\mathbf{u}_\tau - \mathbf{u}_w) + \nu \partial_n \mathbf{u}_\tau - \lambda L(\phi) \nabla \tau \phi &= 0, \quad \text{on } \partial \Omega.
\end{align*}
\]

The Cahn-Hilliard type phase field equations:

\[
\begin{align*}
\phi_t + \nabla \cdot (\mathbf{u} \phi) &= M \Delta \mu, \\
\mu &= -\varepsilon \Delta \phi + f(\phi), \\
\partial_n \mu &= 0, \quad \text{on } \partial \Omega, \\
\phi_t + \mathbf{u}_\tau \cdot \nabla \phi &= -\gamma L(\phi), \quad \text{on } \partial \Omega.
\end{align*}
\]

Now we list detailed descriptions for all the variables. \( \mathbf{u} \) is the fluid velocity, \( p \) is the
pressure, \( \phi \) is the phase field variable, \( \mu \) is the chemical potential, and the function \( L(\phi) \)
is given by

\[
L(\phi) = \varepsilon \partial_n \phi + g'(\phi),
\]

where \( g(\phi) \) is the boundary interfacial energy, \( l(\phi) \geq 0 \) is a given coefficient function
meaning the ratio of the thickness of interface and characteristic length. The function
\( f(\phi) = F'(\phi) \) with \( F(\phi) \) being the Ginzburg-Landau double well potential. More precisely,
\( F(\phi) \) and \( g(\phi) \) are defined as

\[
F(\phi) = \frac{1}{4\varepsilon}(\phi^2 - 1)^2, \quad g(\phi) = -\frac{\sqrt{2}}{3} \cos \theta_s \sin \left( \frac{\pi}{2} \phi \right),
\]

where \( \theta_s \) is the contact angle.
where $\theta_s$ is the static contact angle, $\nu$ is the viscosity coefficient, $\lambda$ denotes the strength of the capillary force comparing to the Newtonian fluid stress, $M$ is the mobility coefficient, $\gamma$ is a boundary relaxation coefficient, and $\varepsilon$ denotes the interface thickness. $\nabla$ denotes the gradient operator, $n$ is the outward normal direction on boundary $\partial \Omega$, $\tau$ is the boundary tangential direction, and vector operator $\nabla_\tau = \nabla - (n \cdot \nabla) n$ is the gradient along tangential direction, $u_w$ is the boundary wall velocity, $u_\tau$ is the boundary fluid velocity in tangential direction. From (2.3), we have $u = u_\tau$ on boundary $\partial \Omega$.

When $\gamma \to +\infty$, the DCLBC (2.8) reduces to the (SCLBC),

$$L(\phi) = 0, \quad \text{on } \partial \Omega,$$

and the GNBC (2.4) reduces to the NBC,

$$l(\phi)(u_\tau - u_w) + \nu \partial_\nu u_\tau = 0, \quad \text{on } \partial \Omega.$$  

There are quite a few challenges to develop numerical algorithms for the above system. In order to design a numerical scheme that naturally satisfies the discrete energy dissipation law, one must overcome the following difficulties: (i) the fourth order Cahn-Hilliard equation with complicated boundary conditions; (ii) the coupling of the velocity and pressure through the incompressible condition; (iii) the stiffness in the phase equation associated with the interfacial width; (iv) the nonlinear couplings between the velocity and the phase variable in the stresses and convectons; and (v) the nonlinear couplings between the velocity and the phase variable on the boundary conditions.

In this paper, to avoid the difficulty to solve the fourth order Cahn-Hilliard equation with complicated boundary conditions, we assume the relaxation of the interface follows the $L^2$ gradient flow. Therefore the fourth order Cahn-Hilliard equation is replaced by the second order Allen-Cahn equation. Thus the phase field equation is given as follows.

$$\phi_t + \mathbf{u} \cdot \nabla \phi = -M \mu, \quad (2.13)$$
$$\mu = -\varepsilon \Delta \phi + f(\phi), \quad (2.14)$$
$$\phi_t + u_\tau \cdot \nabla_\tau \phi = -\gamma L(\phi), \quad \text{on } \partial \Omega. \quad (2.15)$$

It is well known that the Allen-Cahn equation does not conserve the volume. Inspired by the Allen-Cahn type phase field vesicle model in [8,26], we add a penalty term in the phase field equation, to enforce this conservation property. Then the modified Allen-Cahn (AC) equations are as follows,

$$\phi_t + \mathbf{u} \cdot \nabla \phi = -M \mu, \quad (2.16)$$
$$\mu = -\varepsilon \Delta \phi + f(\phi) + \Lambda \left( \int_\Omega \phi dx - \alpha \right), \quad (2.17)$$
$$\phi_t + u_\tau \cdot \nabla_\tau \phi = -\gamma L(\phi), \quad \text{on } \partial \Omega, \quad (2.18)$$

where $\alpha = \int_\Omega \phi |_{t=0} dx$ is the initial volume and $\Lambda$ is the positive penalty parameter. We shall show the effectiveness of volume conservation later in the numerical experiment.
We now derive the energy dissipation law for PDEs system (2.1)-(2.4) and (2.16)-(2.18). Note for any function \(f, g \in L^2(\Omega)\), we use \((f, g)\) to denote \(\int_{\Omega} f g dx\), \((f, g)_{\partial \Omega}\) to denote \(\int_{\partial \Omega} f g ds\), and \(\|f\| = (f, f)\) and \(\|f\|_{\partial \Omega}^2 = (f, f)_{\partial \Omega}\).

**Theorem 2.1.** The NS-AC-GNBC-DCLBC system ((2.1)-(2.4), (2.16)-(2.18)) is a dissipative system satisfying the following energy dissipation law,

\[
\frac{d}{dt} E = -\nu \|\nabla u\|^2 - \lambda M \|\mu\|^2 - \lambda \gamma \|L(\phi)\|^2_{\partial \Omega} - \|I(\phi)\|_{\partial \Omega}^2 - (l(\phi) u_s, u_w)_{\partial \Omega},
\]

where \(u_s = u_o - u_w\) is the velocity slip on boundary \(\partial \Omega\), and

\[
E = \frac{\|u\|^2}{2} + \lambda \left( \frac{\|\nabla \phi\|^2}{2} + (F(\phi), 1) + \frac{\lambda}{2} \left( \int_{\Omega} \phi dx - \alpha \right)^2 \right) + \lambda (g(\phi), 1)_{\partial \Omega}.
\]

**Proof.** By taking the inner product of (2.1) with \(u\), using the incompressible condition (2.2) and the zero flux boundary condition (2.3), we have

\[
\frac{1}{2} \frac{d}{dt} \|u\|^2 = \nu (\partial_n u, u)_{\partial \Omega} - \nu \|\nabla u\|^2 + \lambda (\mu \nabla \phi, u).
\]

By taking the inner product of (2.16) with \(\lambda \mu\), we get

\[
\lambda (\phi_t, \mu) + \lambda (u \cdot \nabla \phi, \mu) = -\lambda M \|\mu\|^2.
\]

By taking the inner product of (2.17) with \(\lambda \phi_t\), we have

\[
\lambda (\mu, \phi_t) = -\lambda \varepsilon (\partial_n \mathbf{E}, \phi_t)_{\partial \Omega} + \frac{1}{2} \lambda \varepsilon \frac{d}{dt} \|\nabla \phi\|^2 + \frac{\lambda}{2} \frac{d}{dt} (F(\phi), 1) + \frac{1}{2} \lambda \Lambda \frac{d}{dt} \left( \int_{\Omega} \phi dx - \alpha \right)^2.
\]

Summing up Eqs. (2.20)-(2.22), we obtain

\[
\frac{1}{2} \frac{d}{dt} \|u\|^2 + \frac{1}{2} \lambda \varepsilon \frac{d}{dt} \|\nabla \phi\|^2 + \frac{\lambda}{2} \frac{d}{dt} (F(\phi), 1) + \frac{1}{2} \lambda \Lambda \frac{d}{dt} \left( \int_{\Omega} \phi dx - \alpha \right)^2 = -\nu \|\nabla u\|^2 - \lambda M \|\mu\|^2 + \nu (\partial_n u, u)_{\partial \Omega} + \lambda \varepsilon (\partial_n \phi, \phi_t)_{\partial \Omega}.
\]

Then, by using (2.8), (2.9) and boundary condition (2.4), we have

\[
\nu (\partial_n u, u)_{\Omega} = \nu (\partial_n u_{\tau}, u_{\tau})_{\partial \Omega} = (\lambda L(\phi) \nabla \tau \phi \cdot \nabla \tau \phi - \gamma L(\phi), u_{\tau})_{\partial \Omega} = (\lambda (L(\phi) \nabla \tau \phi, u_{\tau})_{\partial \Omega} - (l(\phi) u_s, u_s + u_w)_{\partial \Omega},
\]

and

\[
\lambda \varepsilon (\partial_n \phi, \phi_t)_{\partial \Omega} = \lambda (L(\phi) - g'(\phi), \phi_t)_{\partial \Omega} = (\lambda (L(\phi), \phi_t)_{\partial \Omega} - \lambda (l(\phi), 1)_{\partial \Omega} = (\lambda (L(\phi), -u_{\tau} \cdot \nabla \tau \phi - \gamma L(\phi))_{\partial \Omega} - \lambda \frac{d}{dt} (g(\phi), 1)_{\partial \Omega} = -\lambda (L(\phi) \nabla \tau \phi, u_{\tau})_{\partial \Omega} - \lambda \gamma \|L(\phi)\|^2_{\partial \Omega} - \lambda \frac{d}{dt} (g(\phi), 1)_{\partial \Omega}.
\]
Summing up (2.23), (2.24) and (2.25), we obtain the energy desired energy estimate (2.19).

**Remark 2.1.** We have the similar energy dissipation law for the NS-CH-GNBC-DCLBC ((2.1)-(2.8)), where the total free energy is

\[
E = \frac{1}{2} \| \mathbf{u} \|^2 + \lambda \left( \frac{\| \nabla \phi \|^2}{2} + (F(\phi), 1) \right) + \lambda (g(\phi), 1)_{\partial \Omega}.
\]

Even though the above PDE energy law is straightforward, the nonlinear terms in \( \mu \) involves the second order derivatives. Therefore it is not convenient to use them as test functions in numerical approximations, which makes it difficult for implementations. To overcome this difficulty, we need to reformulate the momentum equation (2.1) to an alternative formulation such that it is convenient for numerical approximation.

Let \( \dot{\phi} = \phi_t + \mathbf{u} \cdot \nabla \phi \), and notice that \( \mu = -\frac{\dot{\phi}}{M} \), then the momentum equation (2.1) can be rewritten as the following equivalent form,

\[
\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u} = \nu \nabla^2 \mathbf{u} - \nabla p - \lambda M \dot{\phi} \nabla \phi. \tag{2.26}
\]

This equivalent form (2.26)-(2.2)-(2.3)-(2.4) and (2.16)-(2.18) still admits the similar energy law. To this end, by taking the \( L^2 \) inner product of (2.26) with \( \mathbf{u} \), of (2.16) with \( \lambda M \phi_t \), and of (2.17) with \( -\lambda \phi_t \), we derive

\[
\frac{1}{2} \frac{d}{dt} \| \mathbf{u} \|^2 + \frac{1}{2} \lambda \varepsilon \frac{d}{dt} \| \nabla \phi \|^2 + \frac{1}{2} \lambda \varepsilon \frac{d}{dt} (F(\phi), 1) = -\nu \| \nabla \mathbf{u} \|^2 - \lambda M \| \dot{\phi} \|^2 + \nu (\partial_n \mathbf{u}, \mathbf{u})_{\partial \Omega} + \lambda \varepsilon (\partial_n \phi_t, \phi_t)_{\partial \Omega}. \tag{2.28}
\]

Taking the summation of the above equalities, we have

\[
\frac{d}{dt} E = -\nu \| \nabla \mathbf{u} \|^2 - \lambda M \| \phi \|^2 - \lambda \gamma \| L(\phi) \|_{\partial \Omega}^2 - \| (\phi) \|^2 \| \mathbf{u}_s \|^2_{\partial \Omega} - (\phi \mathbf{u}_s, \mathbf{u}_w)_{\partial \Omega}.
\]

Using (2.24) and (2.25), we have the energy dissipation law.
3 Energy stable numerical schemes

We aim to develop easy-to-implement energy stable schemes where the word “easy” means linear or decoupled. To this end, we assume that $F(\phi)$ satisfies the conditions as follows:

- There exists a constant $L$ such that
  \[ \max_{|\phi| \in \mathbb{R}} |F''(\phi)| \leq L. \]  
  (3.1)

We note that this condition is not satisfied by the usual Ginzburg-Landau double-well potential $F(\phi) = \frac{1}{4\epsilon}(\phi^2 - 1)^2$. However, since it is well-known that the Allen-Cahn equation satisfies the maximum principle, we can truncate $F(\phi)$ to quadratic growth outside of an interval $[-M_1, M_1]$ without affecting the solution if the maximum norm of the initial condition $\phi_0$ is bounded by $M_1$. Therefore, it has been a common practice $[7, 11, 22]$ to consider the Allen-Cahn equation with a truncated double-well potential $\hat{F}(\phi)$. Without loss of generality, we introduce the following $\hat{F}(\phi)$ to replace $F(\phi)$:

\[
\hat{F}(\phi) = \begin{cases} 
\frac{1}{4\epsilon} (\phi+1)^2, & \text{if } \phi < -1, \\
\frac{1}{4\epsilon} (\phi^2 - 1)^2, & \text{if } -1 \leq \phi \leq 1, \\
2(\phi^2 - 1)^2, & \text{if } \phi > 1.
\end{cases} \]  
(3.2)

We drop the $\cdot$ in symbols for convenience. Correspondingly, we define $f(\phi) = F'(\phi)$ and two Lipschitz constants

\[
L_1 := \max_{\phi \in \mathbb{R}} |f'(\phi)| = \frac{2}{\epsilon}, \quad L_2 := \max_{\phi \in \mathbb{R}} |g''(\phi)| = \frac{\sqrt{2}\pi^2}{12} |\cos \theta_s|. \]  
(3.3)

3.1 Linear and decoupled schemes (LD)

We first focus on the NS-AC-NBC-SCLBC system where the boundary conditions are relatively simple. We emphasize that there is no coupling between the velocity and phase field variable on the boundary, that makes it possible to develop the following decoupled, linear scheme. For convenience, we remind readers with the governing system here.

The hydrodynamics equations:

\[
\begin{align*}
\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u} - \nu \Delta \mathbf{u} + \nabla p + \frac{\lambda}{M} \phi \nabla \phi &= 0, \\
\nabla \cdot \mathbf{u} &= 0, \\
\mathbf{u} \cdot \mathbf{n} &= 0, & \text{on } \partial \Omega, \\
l(\phi)(\mathbf{u}_T - \mathbf{u}_w) + \nu \partial_n \mathbf{u}_T &= 0, & \text{on } \partial \Omega.
\end{align*}
\]  
(3.4)

\( (3.5) \)

\( (3.6) \)

\( (3.7) \)
The Allen-Cahn type phase field equations:
\[
\phi_t + (u \cdot \nabla)\phi = M \left( \varepsilon \Delta \phi - f(\phi) - \Lambda \left( \int_{\Omega} \phi dx - \alpha \right) \right), \quad (3.8)
\]
\[
L(\phi) = 0, \quad \text{on} \quad \partial \Omega. \quad (3.9)
\]

Let \( \delta t > 0 \) be a time discretization step and suppose \( u^n, \phi^n \) and \( p^n \) are given, where the superscript \( n \) on variables denotes approximations of corresponding variables at time \( n\delta t \). Assuming \( S_1, S_2 \) are two positive stabilizing coefficients to be determined, the first-order time discretization scheme to solve NS-AC-NBC-SCLBC system (3.4)-(3.9) reads as follows.

**Step 1:** We first solve for \( \phi^{n+1} \) from
\[
\frac{\phi^{n+1} - \phi^n}{\delta t} + (u^n \cdot \nabla)\phi^n = M \left( \varepsilon \Delta \phi^{n+1} - f(\phi^n) - S_1(\phi^{n+1} - \phi^n) - \Lambda \left( \int_{\Omega} \phi^{n+1} dx - \alpha \right) \right), \quad (3.10)
\]
\[
\tilde{L}^{n+1} = 0, \quad \text{on} \quad \partial \Omega, \quad (3.11)
\]
where
\[
u \frac{\partial_n \phi^{n+1}}{\delta t} + g'(\phi^n) + S_2(\phi^{n+1} - \phi^n) = 0. \quad (3.12)
\]

**Step 2:** We solve \( \tilde{u}^{n+1} \) from
\[
\frac{\tilde{u}^{n+1} - u^n}{\delta t} + (u^n \cdot \nabla)\tilde{u}^{n+1} - \nu \Delta \tilde{u}^{n+1} + \nabla p^n = 0, \quad (3.13)
\]
\[
\tilde{u}^{n+1} \cdot n = 0, \quad \text{on} \quad \partial \Omega, \quad (3.14)
\]
\[
u \frac{\partial_n \tilde{u}^{n+1}}{\delta t} + l(\phi^n)\tilde{u}^{n+1} = 0, \quad \text{on} \quad \partial \Omega. \quad (3.15)
\]

**Step 3:** We update \( u^{n+1} \) and \( p^{n+1} \) from
\[
\frac{u^{n+1} - \tilde{u}^{n+1}}{\delta t} + \nabla (p^{n+1} - p^n) = 0, \quad (3.16)
\]
\[
\nabla \cdot u^{n+1} = 0, \quad (3.17)
\]
\[
u \frac{\partial_n u^{n+1}}{\delta t} \cdot n = 0, \quad \text{on} \quad \partial \Omega. \quad (3.18)
\]

**Remark 3.1.** We recall that \( f(\phi) \) takes the form \( \frac{1}{\varepsilon} \phi(\phi^2 - 1) \), so the explicit treatment of this term usually leads to a severe restriction on the time step \( \delta t \) when \( \varepsilon \ll 1 \). It is common practice to add a “stabilizing” term to improve the stability [14, 22–24].
Remark 3.2. Inspired by [1, 17, 23, 24], we introduce the explicit convective velocity \( u^u_{n} \) in (3.10) by combining the term \( u^u_{n} \) with surface tension term \( \varphi \nabla \varphi \). This term helps us to decouple the computations of \( \varphi \) from the velocity. From (3.13), we obtain

\[
\mathbf{u}^u_{n} = B^{-1} \left( \mathbf{u}^u_{n} - \frac{\varphi_{n+1} - \varphi^n}{M/\lambda} \nabla \varphi^n \right),
\]

(3.21)

where \( B = (1 + \frac{\delta t}{M/\lambda} \nabla \varphi^n \nabla \varphi^n) \). It is easy to get the \( \det(I + c \nabla \varphi \nabla \varphi) = 1 + c \nabla \varphi \cdot \nabla \varphi \), thus \( B \) is invertible.

We have the energy stability as follows.

Theorem 3.1. Assuming \( \mathbf{u}_{0w} = 0 \), and \( S_1 \geq L_1/2 \) and \( S_2 \geq L_2/2 \), the scheme (3.10)-(3.20) is energy stable in the sense that

\[
E_{tot}^{n+1} + \frac{\delta t^2}{2} \| \nabla p_{n+1} \|^2 + \delta t \left( \nu \| \nabla \mathbf{u}^u_{n+1} \|^2 + \frac{\lambda}{M} \| \varphi_{n+1} \|^2 + \| L^{1/2}(\varphi_{n} \mathbf{u}^u_{n+1}) \|^2 \right)_\Omega \\
\leq E_{tot}^{n} + \frac{\delta t^2}{2} \| \nabla p_{n} \|^2,
\]

(3.22)

where

\[
E_{tot}^{n} = \frac{1}{2} \| \mathbf{u}^u_{n} \|^2 + \lambda \left( \frac{\| \nabla \varphi^n \|^2}{2} + (F(\varphi^n), 1) + \frac{\Lambda}{2} \left( \int_{\Omega} \varphi^n dx - \alpha \right)^2 \right) + \lambda (g(\varphi^n), 1)_{\partial \Omega}.
\]

(3.23)

Proof. By taking inner product of (3.10) with \( \frac{\lambda}{M} \frac{\varphi_{n+1} - \varphi^n}{\delta t} \), and notice the identity

\[
(a - b, 2a) = |a|^2 - |b|^2 + |a - b|^2,
\]

(3.24)

we have

\[
\frac{\lambda}{M} \| \varphi_{n+1} \|^2 - \frac{\lambda}{M} (\mathbf{u}^u_{n}, \nabla \varphi^n, \varphi_{n+1}) - \lambda \varepsilon \left( \Delta \varphi_{n+1}, \frac{\varphi_{n+1} - \varphi^n}{\delta t} \right)
\]

\[
+ \lambda \left( f(\varphi^n), \frac{\varphi_{n+1} - \varphi^n}{\delta t} \right) + \frac{\lambda S_1}{\delta t} \| \varphi_{n+1} - \varphi^n \|^2
\]

\[
+ \frac{\lambda \Lambda}{2\delta t} \left( \left( \int_{\Omega} \varphi^n dx - \alpha \right)^2 - \left( \int_{\Omega} \varphi_{n+1} dx - \alpha \right)^2 + \left( \int_{\Omega} (\varphi_{n+1} - \varphi^n) dx \right)^2 \right) = 0,
\]

(3.25)

and

\[
-\lambda \varepsilon \left( \Delta \varphi_{n+1}, \frac{\varphi_{n+1} - \varphi^n}{\delta t} \right) = \frac{\lambda \varepsilon}{2\delta t} \left( \| \nabla \varphi_{n+1} \|^2 - \| \nabla \varphi^n \|^2 + \| \nabla (\varphi_{n+1} - \varphi^n) \|^2 \right)
\]

\[
- \lambda \varepsilon \left( \frac{\varphi_{n+1} - \varphi^n}{\delta t} \right)_{\partial \Omega}.
\]

(3.26)
For the boundary integral terms in (3.26), by using (3.11) and (3.14), we have
\[
-\lambda \epsilon \left( \partial_n \phi^{n+1} + \frac{\phi^{n+1} - \phi^n}{\delta t} \right)_{a \Omega} = \lambda \left( g'(\phi^n) + S_2(\phi^{n+1} - \phi^n), \frac{\phi^{n+1} - \phi^n}{\delta t} \right)_{a \Omega}.
\]  
(3.27)
To handle the nonlinear term associated with \( f \) in (3.25) and the term associated with \( g \) in (3.27), we need the following identities
\[
f(\phi^n) (\phi^{n+1} - \phi^n) = F(\phi^{n+1}) - F(\phi^n) - \frac{f'(\eta)}{2} (\phi^{n+1} - \phi^n)^2,
\]
(3.28)
\[
g'(\phi^n) (\phi^{n+1} - \phi^n) = g(\phi^{n+1}) - g(\phi^n) - \frac{g''(\xi)}{2} (\phi^{n+1} - \phi^n)^2.
\]
(3.29)
Combining Eqs. (3.25), (3.26), (3.27), (3.28) and (3.29), we get
\[
\frac{\lambda \epsilon}{2\delta t} (\| \nabla \phi^{n+1} \|^2 - \| \nabla \phi^n \|^2 + \| \nabla (\phi^{n+1} - \phi^n) \|^2)
+ \frac{\lambda}{\delta t} \left( (F(\phi^{n+1}) - F(\phi^n), 1 + \left(S_1 - \frac{f'(\eta)}{2}, (\phi^{n+1} - \phi^n)^2\right) \right)
+ \frac{\lambda}{\delta t} \left( (g(\phi^{n+1}) - g(\phi^n), 1_{a \Omega} + \left(S_2 - \frac{g''(\xi)}{2}, (\phi^{n+1} - \phi^n)^2\right)_{a \Omega} \right)
+ \frac{\lambda \Lambda}{2\delta t} \left( \left( \int_{\Omega} \phi^{n+1} dx - \alpha \right)^2 - \left( \int_{\Omega} \phi^n dx - \alpha \right)^2 \right) + \left( \int_{\Omega} (\phi^{n+1} - \phi^n) dx \right)^2
- \frac{\lambda}{M} (u^n \cdot \nabla \phi^n, \phi^{n+1})
= -\frac{\lambda}{M} \| \phi^{n+1} \|^2.
\]
(3.30)
By taking the \( L^2 \) inner product of Eq. (3.12) with \( u^n / \delta t \), we obtain
\[
\frac{1}{2\delta t} (\| u^n \|^2 - \| u^n - u^n \|^2 + \| u^n \|^2) = -\frac{\lambda}{M} (\phi^{n+1} \nabla \phi^n, u^n).
\]
(3.31)
By taking the inner product of Eq. (3.15) with \( \hat{u}^{n+1} \), and notice \( \nabla \cdot u^n = 0, u^n \cdot n |_{a \Omega} = 0 \), we have
\[
((u^n \cdot \nabla) \hat{u}^{n+1}, \hat{u}^{n+1}) = 0,
\]
(3.32)
and
\[
\frac{1}{2\delta t} (\| \hat{u}^{n+1} \|^2 - \| u^n \|^2 + \| \hat{u}^{n+1} - u^n \|^2)
= -v \| \nabla \hat{u}^{n+1} \|^2 + v (\partial_n \hat{u}^{n+1}, \hat{u}^{n+1})_{a \Omega} - (\nabla p^n, \hat{u}^{n+1}).
\]
(3.33)
For the boundary term in the above equation, using Eq. (3.17) and noticing that $\tilde{u}^{n+1}_r - \tilde{u}^{n+1}_c = \tilde{u}^{n+1}_c$ and $\tilde{u}^{n+1}_c = 0$, we have

$$\nu(\partial_n \tilde{u}^{n+1}_c, \tilde{u}^{n+1}_c)_{\partial\Omega} = -\|l^{1/2}(\phi^n)\tilde{u}^{n+1}_c\|_{\partial\Omega}^2.$$ (3.34)

By taking inner product of (3.18) with $u^{n+1}$, using (3.19) and (3.20), we have

$$\frac{1}{2\delta t}(\|u^{n+1}\|^2 - \|\tilde{u}^{n+1}\|^2 + \|u^{n+1} - \tilde{u}^{n+1}\|^2) = 0.$$ (3.35)

We can also obtain the following equation directly from Eq. (3.18),

$$\frac{\delta t}{2} \|
abla p^{n+1} - \nabla p^n\|^2 = \frac{1}{2\delta t} \|	ilde{u}^{n+1} - u^{n+1}\|^2.$$ (3.36)

In addition, by taking inner product of (3.18) with $\delta t \nabla p^n$, using incompressible condition (3.19) and boundary condition (3.20), we can get

$$\frac{\delta t}{2}(\|
abla p^{n+1}\|^2 - \|
abla p^n\|^2) = (\tilde{u}^{n+1}, \nabla p^n).$$ (3.37)

By taking the summation of Eqs. (3.30), (3.31), (3.33)-(3.37) and dropping some positive terms, we derive

$$\frac{1}{\delta t}(E_{tot}^{n+1} - E_{tot}^n) + \frac{\delta t}{2}(\|
abla p^{n+1}\|^2 - \|
abla p^n\|^2) + \frac{\lambda \epsilon}{2\delta t} \|\nabla (\phi^{n+1} - \phi^n)\|^2$$

$$= -\left(\nu \|
abla \tilde{u}^{n+1}\|^2 + \frac{\lambda}{M} \|\phi^{n+1}\|^2 + \|l^{1/2}(\phi^n)\tilde{u}^{n+1}_c\|_{\partial\Omega}^2\right)$$

$$- \frac{1}{2\delta t}(\|u^* - u^n\|^2 + \|\tilde{u}^{n+1} - u^n\|^2)$$

$$- \frac{\lambda}{\delta t} \left(\left(S_1 - \frac{f'(\xi)}{2}, (\phi^{n+1} - \phi^n)^2\right) + \left(S_2 - \frac{g''(\zeta)}{2}, (\phi^{n+1} - \phi^n)^2\right)_{\partial\Omega}\right).$$ (3.38)

Thus, assuming $S_1 \geq L_1/2$ and $S_2 \geq L_2/2$ and dropping some unnecessary positive terms, we get the desired energy estimate (3.22).

### 3.2 Linear and coupled scheme (LC)

For the GNBC-DCLBC, the velocity and phase field variable are both coupled together on the boundary conditions. Such couplings make it challenging to construct any decoupled schemes for GNBC-DCLBC. Thus the best scheme we can develop is the following linear coupled scheme, to solve the NS-AC-GNBC-DCLBC system.

Again for readers’ convenience, we recall the governing equations as follows.
The hydrodynamics equations:
\[ \begin{align*}
\mathbf{u}_t + (\mathbf{u} \cdot \nabla) \mathbf{u} - \nu \Delta \mathbf{u} + \nabla p + \frac{\lambda}{M} \phi \nabla \phi &= 0, \\
\nabla \cdot \mathbf{u} &= 0, \\
\mathbf{u} \cdot \mathbf{n} &= 0, \quad \text{on } \partial \Omega, \\
l(\phi)(\mathbf{u}_\tau - \mathbf{u}_w) + \nu \mathbf{u}_\tau - \lambda L(\phi) \nabla \tau \phi &= 0, \quad \text{on } \partial \Omega.
\end{align*} \tag{3.39} \tag{3.40} \tag{3.41} \tag{3.42} \]

The Allen-Cahn type phase field equations:
\[ \begin{align*}
\phi_t + (\mathbf{u} \cdot \nabla) \phi &= M \left( \varepsilon \Delta \phi - f(\phi) - \Lambda \left( \int_{\Omega} \phi \, dx - \alpha \right) \right), \\
\phi_t + (\mathbf{u} \cdot \nabla \tau) \phi &= -\gamma L(\phi), \quad \text{on } \partial \Omega. \tag{3.43} \tag{3.44}
\end{align*} \]

Assuming \( S_1, S_2 \) are two positive stabilizing coefficients to be determined, the first-order time discretization scheme to solve PDE system (3.39)-(3.44) reads as follows.

**Step 1:** We first solve for \( \tilde{\mathbf{u}}^{n+1}, \phi^{n+1} \) from
\[ \begin{align*}
\frac{\tilde{\mathbf{u}}^{n+1} - \mathbf{u}^n}{\delta t} + (\mathbf{u}^n \cdot \nabla) \tilde{\mathbf{u}}^{n+1} - \nu \Delta \tilde{\mathbf{u}}^{n+1} + \nabla p^n + \frac{\lambda}{M} \phi^{n+1} \nabla \phi^n &= 0, \\
\phi_t^{n+1} - \phi^n &= (\tilde{\mathbf{u}}^{n+1} \cdot \nabla) \phi^n = M \left( \varepsilon \Delta \phi^{n+1} - f(\phi^n) - S_1 (\phi^{n+1} - \phi^n) \right) - \Lambda \left( \int_{\Omega} \phi^{n+1} \, dx - \alpha \right), \tag{3.45} \tag{3.46}
\end{align*} \]
with the boundary conditions
\[ \begin{align*}
\tilde{\mathbf{u}}^{n+1} \cdot \mathbf{n} &= 0, \quad \text{on } \partial \Omega, \\
\nu \mathbf{u}_\tau^{n+1} + l(\phi^n) \mathbf{u}_s^{n+1} - \lambda \tilde{L}^{n+1} \nabla \tau \phi^n &= 0, \quad \text{on } \partial \Omega, \\
\frac{\phi^{n+1} - \phi^n}{\delta t} + (\tilde{\mathbf{u}}^{n+1} \cdot \nabla) \phi^{n+1} &= -\gamma \tilde{L}^{n+1}, \quad \text{on } \partial \Omega, \tag{3.47} \tag{3.48} \tag{3.49}
\end{align*} \]

where
\[ \begin{align*}
\phi^{n+1} &= \phi^{n+1} - \phi^n + (\tilde{\mathbf{u}}^{n+1} \cdot \nabla) \phi^n, \\
\tilde{L}^{n+1} &= \varepsilon \partial_x \phi^{n+1} + g'(\phi^n) + S_2 (\phi^{n+1} - \phi^n). \tag{3.50} \tag{3.51}
\end{align*} \]

**Step 2:** We update \( \mathbf{u}^{n+1} \) and \( p^{n+1} \) from
\[ \begin{align*}
\frac{\mathbf{u}^{n+1} - \tilde{\mathbf{u}}^{n+1}}{\delta t} + \nabla (p^{n+1} - p^n) &= 0, \\
\nabla \cdot \mathbf{u}^{n+1} &= 0, \\
\mathbf{u}^{n+1} \cdot \mathbf{n} &= 0, \quad \text{on } \partial \Omega. \tag{3.52} \tag{3.53} \tag{3.54}
\end{align*} \]

We now present the energy stability proof as follows.
Theorem 3.2. Assuming \( u_0 = 0 \), and \( S_1 \geq L_1/2 \) and \( S_2 \geq L_2/2 \), the scheme (3.45)-(3.54) is energy stable in the sense that

\[
E_{tot}^{n+1} + \frac{\delta t}{2} \| \nabla p^{n+1} \|^2 + \delta t \left( v \| \nabla \mathbf{u}^{n+1} \|^2 + \frac{\lambda}{M} \| \phi^{n+1} \|^2 + \| l^{1/2}(\phi^n) \mathbf{u}_n^{n+1} \|^2_{\partial \Omega} + \gamma \lambda \| \mathbf{L}^{n+1} \|^2_{\partial \Omega} \right)
\]

\[
\leq E_{tot}^n + \frac{\delta t}{2} \| \nabla p^n \|^2,
\]

where \( E_{tot}^n \) is defined in (3.23).

Proof. By taking inner product of (3.46) with \( \frac{\lambda}{M} \phi^{n+1} - \phi^n \), we have

\[
\frac{\lambda}{M} \| \phi^{n+1} \|^2 - \frac{\lambda}{M} (\mathbf{u}_n^{n+1} \cdot \nabla \phi^n, \phi^{n+1}) + \frac{\lambda \epsilon}{2 \delta t} \left( \| \nabla \phi^{n+1} \|^2 - \| \nabla \phi^n \|^2 + \| \nabla (\phi^{n+1} - \phi^n) \|^2 \right)
\]

\[- \lambda \epsilon \left( \partial_n \phi^{n+1}, \frac{\phi^{n+1} - \phi^n}{\delta t} \right)_{\partial \Omega} + \lambda \left( f(\phi^n), \frac{\phi^{n+1} - \phi^n}{\delta t} \right) + \lambda \left( \mathbf{F}_n, \frac{\mathbf{u}_n^{n+1} - \mathbf{u}^n}{\delta t} \right) \| \phi^{n+1} - \phi^n \|^2
\]

\[+ \frac{\lambda \lambda}{2 \delta t} \left( \left( \int_{\Omega} \phi^{n+1} dx - \alpha \right)^2 - \left( \int_{\Omega} \phi^n dx - \alpha \right)^2 + \left( \int_{\Omega} (\phi^{n+1} - \phi^n) dx \right)^2 \right) = 0. \quad (3.56)
\]

For the boundary integral terms above, using (3.51), we have

\[- \lambda \epsilon \left( \partial_n \phi^{n+1}, \frac{\phi^{n+1} - \phi^n}{\delta t} \right)_{\partial \Omega} = \lambda \left( \mathbf{L}^{n+1}, \frac{\phi^{n+1} - \phi^n}{\delta t} \right)_{\partial \Omega} - \lambda (\mathbf{L}^{n+1}, (\mathbf{u}_n^{n+1} \cdot \nabla) \phi^{n+1}). \quad (3.57)
\]

Combining Eqs. (3.56), (3.57), (3.28) and (3.29), we get

\[
\frac{\lambda \epsilon}{2 \delta t} \left( \| \nabla \phi^{n+1} \|^2 - \| \nabla \phi^n \|^2 + \| \nabla (\phi^{n+1} - \phi^n) \|^2 \right)
\]

\[+ \frac{\lambda}{\delta t} \left( F(\phi^{n+1}) - F(\phi^n), 1 \right) + \frac{\lambda}{\delta t} \left( S_1 - \frac{f'(\eta)}{2}, (\phi^{n+1} - \phi^n)^2 \right)
\]

\[+ \frac{\lambda}{\delta t} \left( g(\phi^{n+1}) - g(\phi^n), 1 \right)_{\partial \Omega} + \frac{\lambda}{\delta t} \left( S_2 - \frac{g''(\xi)}{2}, (\phi^{n+1} - \phi^n)^2 \right)_{\partial \Omega}
\]

\[+ \frac{\lambda \lambda}{2 \delta t} \left( \left( \int_{\Omega} \phi^{n+1} dx - \alpha \right)^2 - \left( \int_{\Omega} \phi^n dx - \alpha \right)^2 + \left( \int_{\Omega} (\phi^{n+1} - \phi^n) dx \right)^2 \right)
\]

\[- \frac{\lambda}{M} \left( \mathbf{u}_n^{n+1} \cdot \nabla \phi^n, \frac{\phi^{n+1} - \phi^n}{\delta t} \right)\]

\[= - \gamma \lambda \| \mathbf{L}^{n+1} \|^2_{\partial \Omega} - \lambda (\mathbf{L}^{n+1}, (\mathbf{u}_n^{n+1} \cdot \nabla) \phi^{n+1}) - \frac{\lambda}{M} \| \phi^{n+1} \|^2. \quad (3.59)
\]
By taking the inner product of Eq. (3.45), we obtain
\[
\frac{1}{2\delta t} (||\tilde{u}^{n+1}||^2 - ||u^n||^2 + ||\tilde{u}^{n+1} - u^n||^2) \\
= -v ||\nabla \tilde{u}^{n+1}||^2 + v(\partial_n \tilde{u}^{n+1}, \tilde{u}^{n+1})_{\partial\Omega} - (\nabla p^n, \tilde{u}^{n+1}).
\] (3.60)

For the boundary term in the above equation, using Eq. (3.48), we have
\[
v(\partial_n \tilde{u}^{n+1}, \tilde{u}^{n+1})_{\partial\Omega} = -\tau^{1/2} (\phi^n)^2 \|\tilde{u}_s^{n+1}\|^2  + \lambda (L^{n+1} \nabla \phi^n, \tilde{u}^{n+1})_{\partial\Omega}.
\] (3.61)

Exactly as Theorem 3.1, for (3.52), we derive
\[
\frac{1}{2\delta t} (||u^{n+1}||^2 - ||\tilde{u}^{n+1}||^2 + ||u^{n+1} - \tilde{u}^{n+1}||^2) = 0,
\] (3.62)
\[
\frac{\delta t}{2} ||\nabla p^{n+1} - \nabla p^n||^2 = \frac{1}{2\delta t} ||\tilde{u}^{n+1} - u^{n+1}||^2,
\] (3.63)
and
\[
\frac{\delta t}{2} (||\nabla p^{n+1}||^2 - ||\nabla p^n||^2 + ||\nabla p^{n+1} - \nabla p^n||^2) = (\tilde{u}^{n+1}, \nabla p^n).
\] (3.64)

By taking the summation of Eqs. (3.59)-(3.64) and dropping some unnecessary positive terms, we derive
\[
\frac{1}{\delta t} (E_{tot}^{n+1} - E_{tot}^n) + \frac{\delta t}{2} (||\nabla p^{n+1}||^2 - ||\nabla p^n||^2) + \frac{\lambda \epsilon}{2\delta t} ||\nabla (\phi^{n+1} - \phi^n)||^2
\]
\[
= -\left( v ||\nabla \tilde{u}^{n+1}||^2 + \frac{\lambda}{M} ||\phi^{n+1}||^2 + \|L^{n+1} \nabla \phi^n\|^2 - \gamma \lambda \|L^{n+1} \nabla \phi^n\|^2 \right)
\]
\[
- \frac{1}{2\delta t} (||\tilde{u}^{n+1} - u^{n+1}||^2 + ||u^{n+1} - \tilde{u}^{n+1}||^2)
\]
\[
- \frac{\lambda}{\delta t} \left( S_1 - \frac{f''(\tilde{z})}{2}, (\phi^{n+1} - \phi^n)^2 \right) + \left( S_2 - \frac{\xi''(\tilde{z})}{2}, (\phi^{n+1} - \phi^n)^2 \right)_{\partial\Omega}.
\] (3.65)

Thus, assuming \(S_1 \geq L_1/2\) and \(S_2 \geq L_2/2\) and dropping some unnecessary positive terms, we get the desired energy estimate (3.55).

4 Numerical simulations

In this section, we present various numerical simulations to validate our proposed schemes. For simplicity, we assume the system in \(x\) direction is periodic, and only the top and bottom boundaries take the GNBC (or NBC) and DCLBC (or SCLBC). For the spatial operators in the scheme, we use second-order central finite difference methods to discretize them over a uniform spatial grid, where the velocity fields are discretized on the center of mesh surface, and pressure \(p\), phase variables \(\phi\) are discretized on cell center.
Except specially specified, the default parameters are given as follows,

\[
\begin{align*}
\lambda &= 1/3, \quad \nu = 1/36, \quad M = 0.0125, \quad \gamma = 100, \\
\epsilon &= 0.01, \quad l(\phi) = 1/1.14, \quad \Lambda = 10/M, \quad S_1 = 1/\epsilon, \quad S_2 = \frac{\sqrt{2\pi^2}}{24} |\cos(\theta_s)|.
\end{align*}
\]  

(4.1)

4.1 Accuracy test

We presume the following functions

\[
\begin{align*}
\phi(x,y,t) &= \sin(2\pi x) \cos\left(2\pi y + \frac{\pi}{2}\right) \cos(t), \\
u(x,y,t) &= (y\sin(t),0), \\
p(x,y,t) &= \sin(2\pi x) \cos(t)
\end{align*}
\]

(4.2)

to be the exact solution, and impose some suitable force fields such that the given solution can satisfy the system. The computational domain is \((x,y) \in [-0.5,0.5] \times [-0.25,0.25]\). We perform the accuracy test for different time steps till \(t = 0.1\), the result of \(L^\infty\) errors of the phase variable \(\phi\) and velocity profile \(u\) is shown in Table 1 and Table 2 for LD scheme and LC scheme, respectively. Both schemes present the first order convergence.

Table 1: Numerical \(L^\infty\) errors for the phase variable \(\phi\) and the velocity \(u\) at \(t = 0.1\) for different time steps using the LD scheme.

<table>
<thead>
<tr>
<th>(\delta t)</th>
<th>(L^\infty) error (\phi)</th>
<th>order</th>
<th>(L^\infty) error (u)</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>1E-2</td>
<td>1E-2</td>
<td></td>
<td>1.2E-3</td>
<td></td>
</tr>
<tr>
<td>5E-3</td>
<td>5E-3</td>
<td>1.00</td>
<td>6.21E-4</td>
<td>0.95</td>
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<tr>
<td>2.5E-3</td>
<td>2.5E-3</td>
<td>1.00</td>
<td>3.14E-4</td>
<td>0.99</td>
</tr>
<tr>
<td>1.25E-3</td>
<td>1.2E-3</td>
<td>1.06</td>
<td>1.58E-4</td>
<td>0.99</td>
</tr>
<tr>
<td>6.25E-4</td>
<td>6.23E-4</td>
<td>0.95</td>
<td>8.03E-5</td>
<td>0.98</td>
</tr>
<tr>
<td>3.125E-4</td>
<td>3.11E-4</td>
<td>1.00</td>
<td>4.13E-5</td>
<td>0.96</td>
</tr>
<tr>
<td>1.5625E-4</td>
<td>1.55E-4</td>
<td>1.00</td>
<td>2.24E-5</td>
<td>0.88</td>
</tr>
</tbody>
</table>

Table 2: Numerical \(L^\infty\) errors for the phase variable \(\phi\) and the velocity \(u\) at \(t = 0.1\) for different time steps using the LC scheme.

<table>
<thead>
<tr>
<th>(\delta t)</th>
<th>(L^\infty) error (\phi)</th>
<th>order</th>
<th>(L^\infty) error (u)</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>1E-2</td>
<td>1E-2</td>
<td></td>
<td>1.2E-3</td>
<td></td>
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<tr>
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<td>5E-3</td>
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</tr>
<tr>
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<td>2.5E-3</td>
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<td>3.14E-4</td>
<td>0.99</td>
</tr>
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<td>1.25E-3</td>
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<td>1.58E-4</td>
<td>0.99</td>
</tr>
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<td>0.92</td>
</tr>
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</table>
4.2 Shear flow

We consider the flow between two parallel plates that move in opposite directions at a constant speed. We fix the domain size to be $L_y = 0.4$, $L_x = 2$, and use $201 \times 101$ grid points to discretize the space. The order parameters are specified in (4.1).

The initial velocity field takes the profile of Couette flow, and the initial value of $\phi$ is given as follows,

$$\phi_0(x, y) = \tanh \left( \frac{1}{\sqrt{2} \varepsilon} \left( \frac{L_x}{4} - \left| x - \frac{L_x}{2} \right| \right) \right). \quad (4.3)$$

Fig. 1(a) shows the interface contour $\{ \phi_0 = 0 \}$ of the initial profile $\phi_0$.

We present two numerical results for a classical benchmark numerical simulation from [10, 24]. In simulation I, $u_w = \pm 0.7$, $\theta_s = 64^\circ$, where $u_w$ is the speed of top and bottom

Figure 1: The contours of the interfaces of phase variable $\phi$. (a) The initial configuration of $\phi$ given by (4.3); (b) Contour of $\phi$ at $t = 5$ with contact angle $\theta_s = 64^\circ$ and $u_w = \pm 0.7$; (c) Contour of $\phi$ at $t = 5$ with contact angle $\theta_s = 77.6^\circ$ and $u_w = \pm 0.2$. The results are generated by both of the LD and LC schemes with $200 \times 100$ grid points and $\delta t = 0.001$. 

(c) Simulation II: The steady state of $\phi$ for $\theta_s = 77.6^\circ$. 

(a) The initial profile of the phase field $\phi_0$. 

(b) Simulation I: The steady state of $\phi$ for $\theta_s = 64^\circ$. 

plates, $\theta_s$ is the static contact angle; ± sign means the values on top boundary and bottom boundary have different signs (directions). In simulation II, $u_w = \pm 0.2$ and $\theta_s = \pm 77.6^\circ$. In spite of the fact that our numerical schemes are stable for any time step, we still have to choose some reasonable small time step in order to get the desired accuracy. In the two simulations, the time step is $\delta t = 0.001$.

The interface contours of $\phi$ at the steady state ($t = 5$) are presented in Fig. 1(b)-(c) using both of the LC scheme and LD scheme. We show the plots for the velocity at the top wall $y = 0.2$ when $t = 5$ for both schemes in Fig. 2 as well. These results are consistent to the numerical results obtained using the Cahn-Hilliard model in [10, 24]. We also notice that the LD scheme for NBC-SCLBC actually gives almost identical results as the LC scheme for GNBC-DCLBC for both weak shear flow case with $u_w = \pm 0.2$, and for the strong shear flow case with $u_w = \pm 0.7$.

### 4.3 Dewetting and spreading of a drop

We simulate the dynamics of a drop initially resided on a surface. For various contact angles, the drop will perform different dynamics of dewetting or spreading. We set two contact angles and perform the simulations using both of the LD and LC schemes. We fix the domain size to be $[-1,1] \times [-0.5,0.5]$, and set the other parameters as follows,

$$
\begin{cases}
    \lambda = 1, \quad \nu = 1/12, \quad M = 0.0125, \quad \gamma = 100, \quad \epsilon = 0.01, \quad l(\phi) = 1/0.19, \\
    S_1 = 1/\epsilon, \quad S_2 = \frac{\sqrt{2}\pi^2}{24} |\cos(\theta_s)|, \quad \Lambda = 10/M.
\end{cases}
$$

(4.4)

We take $201 \times 101$ grid points for $x$ and $y$ direction respectively.
In Fig. 3 and Fig. 4, we plot the contour of the drop interface using the LD scheme for NBC-SCLBC system for $\theta_s = 30^\circ$ and $\theta_s = 150^\circ$, respectively. We notice that for the acute contact angle, the drop performs the dewetting process, and for the obtuse contact angle, the drop tends to spread over the solid surface. The detailed results using the LC scheme are omitted because they are essentially the same as the results of the LD scheme. For comparisons, we plot the two contour lines of the steady state ($t = 5$) using LD scheme.
Figure 4: The interface contour of the phase variable $\phi$ using the LD scheme for the system of GNBC-DCLBC. The contact angle is $\theta_s = 150^\circ$.

and LC scheme for these two contact angles in Fig. 5 and Fig. 6, respectively. In Fig. 7, we show the energy plots for both LD and LC scheme for the example of the dewetting case with $\delta t = 0.001$, which shows that our scheme is indeed energy stable. In Fig. 8, we plot the volume change with the time, and it shows the volume of the drop is perfectly preserved. Similar to the weaker shear flow case, both schemes give almost identical results since the velocity involved in these examples are relatively small.
Figure 5: The comparison of the interface contour of the steady state using the LD scheme for NBC-SCLBC, and LC scheme for GNBC-DCLBC with $\theta_s = 30^\circ$.

Figure 6: The comparison of the interface contour of the steady state using the LD scheme for NBC-SCLBC, and LC scheme for GNBC-DCLBC with $\theta_s = 150^\circ$.

Figure 7: Energy plots for dewetting and spreading of a drop with $\theta_s = 30^\circ$. The x-axis is the time, the y-axis is the energy.
5 Concluding remarks

In this paper, for the hydrodynamics coupled with Allen-Cahn type phase-field model that incorporates the moving contact line boundary problems, we construct two efficient, linear numerical schemes. The first scheme is decoupled for the simple version of the boundary conditions (NBC-SCLBC), where one only needs to solve a series of decoupled elliptic equations. The other is linear coupled for the more complicated version of the boundary conditions (GNBC-DCLBC). Both schemes are energy stable and the unconditional energy stability are rigorously proved. Ample numerical simulations are presented to verify the accuracy and efficiency of the proposed model and numerical schemes.

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