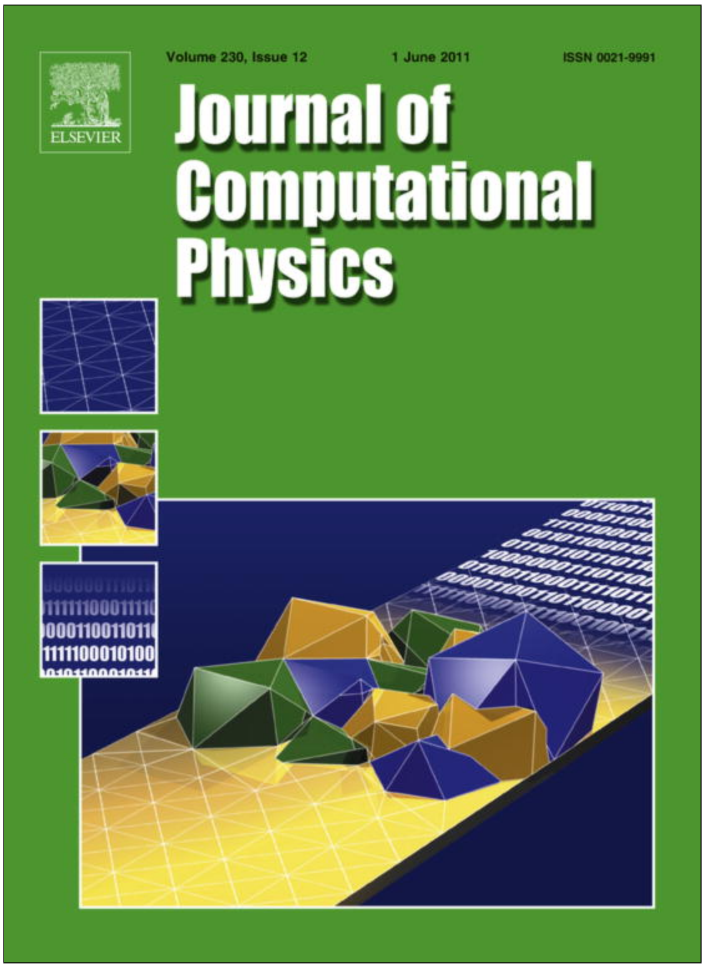
Volume 230, Issue 12
1 June 2011
ISSN 0021-9991
Journal of Computational Physics
ELSEVIER

Journal of Computational Physics 230 (2011) 4991–5009

Contents lists available at ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

A least-squares/finite element method for the numerical solution of the Navier–Stokes-Cahn–Hilliard system modeling the motion of the contact line

Qiaolin He [a,b,*], Roland Glowinski [c,d], Xiao-Ping Wang [e]

[a] Department of Mathematics, Sichuan University, Chengdu 610064, PR China
[b] Department of Mathematics, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong
[c] Department of Mathematics, University of Houston, Houston, TX 77204, USA
[d] Institute of Advanced Study, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong
[e] Department of Mathematics and KAUST-HKUST Micro/Nanofludic Joint Laboratory, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong

ARTICLE INFO

Article history:
Received 29 August 2010
Received in revised form 11 March 2011
Accepted 13 March 2011
Available online 17 March 2011

Keywords:
Navier–Stokes
Cahn–Hilliard
Operator-splitting
Least squares
Conjugate gradient
Contact line

ABSTRACT

In this article we discuss the numerical solution of the Navier–Stokes-Cahn–Hilliard system modeling the motion of the contact line separating two immiscible incompressible viscous fluids near a solid wall. The method we employ combines a finite element space approximation with a time discretization by operator-splitting. To solve the Cahn–Hilliard part of the problem, we use a least-squares/conjugate gradient method. We also show that the scheme has the total energy decaying in time property under certain conditions. Our numerical experiments indicate that the method discussed here is accurate, stable and efficient.

1. Introduction

Describing accurately an immiscible two-phase flow in the vicinity of the contact line, where the fluid–fluid interface intersects the solid wall, is a classical and challenging problem in hydrodynamics. In the past two decades, it has been shown through Molecular Dynamics (MD) simulations that, indeed, a near complete slip does occur at the moving contact line (MCL) [16,17,27,26]. Through the analysis of extensive MD data, it was recently discovered that there is indeed a differential boundary condition, denoted the generalized Navier boundary condition (GNBC), which resolves the MCL problem [19]. In [19], one gives a continuum formulation of the immiscible flow hydrodynamics, including the GNBC, the Navier–Stokes equations, and the Cahn–Hilliard interfacial free energy. It is shown that the numerical results based on the GNBC can reproduce quantitatively the results from the MD simulation. This indicates that the new model can accurately describe the behavior near the contact line. The model has also been used to study several problems involving moving contact line [4,20,28].

A numerical method for the solution of the above coupled system is discussed in [19]; it relies on a standard explicit finite difference scheme whose stability requires a quite demanding limitation of the time step because of the high (fourth) order

* Corresponding author at: Department of Mathematics, Sichuan University, Chengdu 610064, PR China.
E-mail addresses: qlhejenny@gmail.com (Q. He), roland@math.uh.edu (R. Glowinski), mawang@ust.hk (X.-P. Wang).

0021-9991/$ - see front matter © 2011 Elsevier Inc. All rights reserved.
doi:10.1016/j.jcp.2011.03.022

derivatives and strong nonlinearity in the Cahn–Hilliard equation. There have been a lot of work on the numerical methods for the Cahn–Hilliard equation and its non-conservative, lower order version, the Allen–Cahn equation [25,18,8,9]. In particular, attention has been paid to how to construct stable, energy decreasing scheme. An innovative idea, proposed by Eyre [7,6], leads to an unconditionally gradient stable, uniquely solvable one-step scheme based on a convex splitting of total free energy functional into contractive and expansive parts. The idea has also been extended to solve other systems [30,24,5,1,15]. This type of schemes is also analyzed by He et al. [14] in [14] and the stability and convergence properties are investigated using an energy approach. A second-order accurate time-discretization scheme is also discussed in Dean et al. [3] which is shown to be unconditionally stable when combined with a mixed finite element method for the space discretization of the Cahn–Hilliard equation.

The numerical solution of systems coupling the conservative Allen–Cahn and Navier–Stokes equations has also been considered by several authors. Let us mention among others [29,23] and for a thorough discussion of solution methods for the Allen–Cahn–Navier–Stokes type system modeling the flow of two non-miscible incompressible viscous fluids with different densities and viscosities. However, the boundary conditions in [29,23] are much simpler than those considered in the present article.

In this article, we combine an operator-splitting scheme for the time-discretization with a finite element space approximation for the system coupling the Navier–Stokes and Cahn–Hilliard equations; the combination that we consider allows large time discretization steps. To treat the Cahn–Hilliard part of the problem, we introduce a least-squares method to overcome the difficulties associated with the nonlinearity and the boundary conditions. The least-squares problem is solved by a conjugate gradient algorithm operating in a well-chosen functional space. Using an energy method, we show that the scheme has good stability properties.

The article is organized as follows: In Section 2, we give a brief formulation of the problem. In Section 3, we discuss the time-discretization of the coupled Navier–Stokes–Cahn–Hilliard problem by an operator-splitting scheme. In Section 4 we describe a least-squares approach for the solution of the Cahn–Hilliard component of the approximate problem. In Section 5, we discuss some properties of the scheme used to time-discretize the Cahn–Hilliard component of the problem. In Section 6, we address the conjugate gradient solution of the least-squares problem introduced in Section 4. In Section 7 we prove some stability properties of the full operator-splitting scheme. In Section 8 we describe the finite element implementation and provide numerical results in Section 9.

2. Formulation of the problem

Following Qian et al. [19,21], we consider the following Navier–Stokes–Cahn–Hilliard problem:

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right] - \eta\nabla^2\mathbf{u} + \nabla p - \mu\nabla\phi = \mathbf{f}_{ext} \quad \text{in} \quad \Omega\times(0,T), \tag{2.1}$$

$$\nabla\cdot\mathbf{u} = 0 \quad \text{in} \quad \Omega\times(0,T), \tag{2.2}$$

$$\mathbf{u}\cdot\mathbf{n} = 0 \quad \text{on} \quad \partial\Omega\times(0,T), \tag{2.3}$$

$$[\boldsymbol{\sigma}\mathbf{n} + \beta(\phi)\mathbf{u}^{slip} - L(\phi)\nabla\phi]\times\mathbf{n} = \mathbf{0} \quad \text{on} \quad \partial\Omega\times(0,T), \tag{2.4}$$

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi - M\nabla^2\mu = 0 \quad \text{in} \quad \Omega\times(0,T), \tag{2.5}$$

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi + \Gamma L(\phi) = 0 \quad \text{on} \quad \partial\Omega\times(0,T), \tag{2.6}$$

$$\mu = -K\nabla^2\phi + f'(\phi) \quad \text{in} \quad \Omega\times(0,T), \tag{2.7}$$

$$\frac{\partial\mu}{\partial n} = 0 \quad \text{on} \quad \partial\Omega\times(0,T), \tag{2.8}$$

where

$$L(\phi) = K\frac{\partial\phi}{\partial n} + \gamma'_{wf}(\phi), \tag{2.9}$$

and $\mathbf{n}$ is the outward unit normal vector at $\partial\Omega$. A typical function f is given by $f(\phi) = -\frac{a}{2}\phi^2 + \frac{b}{4}\phi^4$ with a and $b > 0$ (Ginzburg–Landau potential). Here $\boldsymbol{\sigma}$ denotes the stress tensor $\boldsymbol{\sigma} = 2\eta\mathbf{D}(\mathbf{u}) - p\mathbf{I}$, where $\mathbf{D}(\mathbf{u}) = \frac{1}{2}[\nabla\mathbf{u} + (\nabla\mathbf{u})^t]$, ρ is the fluid mass density, M is the phenomenological mobility coefficient, K, a and b are material parameters, η is the viscosity, μ is the chemical potential, $\mu\nabla\phi$ is the capillary force density and $\mathbf{f}_{ext}$ is the external body force; Γ is a positive phenomenological parameter, γ_{wf} is the fluid–solid interfacial free energy per unit area, $\beta(\phi)$ is the slip coefficient, which may depend locally on the surface composition ϕ; actually, $\gamma_{wf}(\phi) = -\frac{1}{2}\gamma\cos\theta_s^{surf}\sin\left(\frac{\pi}{2}\phi\right)$, with $\gamma = \frac{2\sqrt{2}a^2\xi}{3b}$ the surface tension and θ_s^{surf} a static contact angle.

To obtain a set of dimensionless equations suitable for numerical computations, as in [19], we scale ϕ by $\sqrt{a/b}$(= 1 in our case), the length by $\xi = \sqrt{K/a}$, the velocity by the wall speed u_w, the time by ξ/u_w, and the pressure/stress by $\eta u_w/\xi$. In dimensionless form, the above system of equations reads as:

$$R\left[\frac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right]=-\nabla p+\nabla^2\mathbf{u}+B\mu\nabla\phi \quad \text{in} \quad \Omega\times(0,T), \tag{2.10}$$

$$\nabla\cdot\mathbf{u}=0 \quad \text{in} \quad \Omega\times(0,T), \tag{2.11}$$

$$\mathbf{u}\cdot\mathbf{n}=0 \quad \text{on} \quad \partial\Omega\times(0,T), \tag{2.12}$$

$$\left[\boldsymbol{\sigma}\mathbf{n}+[\mathcal{L}_s(\phi)]^{-1}\mathbf{u}^{slip}-BL(\phi)\nabla\phi\right]\times\mathbf{n}=\mathbf{0} \quad \text{on} \quad \partial\Omega\times(0,T), \tag{2.13}$$

$$\frac{\partial\phi}{\partial t}+\mathbf{u}\cdot\nabla\phi=\mathcal{L}_d\nabla^2\mu \quad \text{in} \quad \Omega\times(0,T), \tag{2.14}$$

$$\frac{\partial\phi}{\partial t}+\mathbf{u}\cdot\nabla\phi=-\mathcal{V}_sL(\phi) \quad \text{on} \quad \partial\Omega\times(0,T), \tag{2.15}$$

$$L(\phi)=\frac{\partial\phi}{\partial n}+\gamma'_{wf}(\phi)=\frac{\partial\phi}{\partial n}-\frac{\sqrt{2}}{3}\cos\theta_s^{surf}s_\gamma(\phi), \tag{2.16}$$

$$\mu=-\nabla^2\phi+f'(\phi)=-\nabla^2\phi-\phi+\phi^3, \tag{2.17}$$

$$\frac{\partial\mu}{\partial n}=0. \tag{2.18}$$

Here $s_\gamma=\frac{\pi}{2}\cos(\frac{\pi\phi}{2})$. Five dimensionless parameters appear in the above equations. They are (1) $\mathcal{L}_d=\frac{Ma}{u_w\xi}$, which is the ratio of a diffusion length $\frac{Ma}{u_w}$ to ξ, (2) $R=\frac{\rho u_w\xi}{\eta}$, (3) $B=\frac{a^2\xi}{b\eta u_w}=\frac{3\gamma}{2\sqrt{2}\eta u_w}$, (4) $\mathcal{V}_s=\frac{K\Gamma}{u_w}$, which is the ratio of $K\Gamma$ (of velocity dimension) to u_w, and (5) $\mathcal{L}_s(\phi)=\frac{\eta}{\beta(\phi)\xi}$, which is the ratio of the slip length $l_s(\phi)=\frac{\eta}{\beta(\phi)}$ to ξ. Here $\beta(\phi)=(1-\phi)\beta_1/2+(1+\phi)\beta_2/2$.

The above system has to be completed by initial condition such as:

$$\mathbf{u}(0)=\mathbf{u}_0, \quad \phi(0)=\phi_0. \tag{2.19}$$

For the numerical solution of the above system, by finite element methods, in particular, we should take advantage of a time-discretization by operator-splitting.

3. An operator-splitting scheme for the time-discretization of problem (2.10)–(2.19)

The scheme reads as follows (with $t^n=n\Delta t$):

$$\{\mathbf{u}^0,\ \phi^0\}=\{\mathbf{u}_0,\phi_0\}. \tag{3.1}$$

For $n\geqslant 0$, $\{\mathbf{u}^n,\phi^n\}$ known, we compute $\{\phi^{n+1/2},\mu^{n+1/2}\}$ then $\{\mathbf{u}^{n+1/2},p^{n+1/2}\}$, and finally $\{\mathbf{u}^{n+1},\phi^{n+1}\}$ as follows:

Compute $\{\phi^{n+1/2},\mu^{n+1/2}\}$ so that

$$\frac{\phi^{n+1/2}-\phi^n}{\Delta t}-\mathcal{L}_d\nabla^2\mu^{n+1/2}=0 \quad \text{in} \quad \Omega, \tag{3.2}$$

$$\frac{\phi^{n+1/2}-\phi^n}{\Delta t}+\mathcal{V}_sL(\phi^{n+1/2})=0 \quad \text{on} \quad \partial\Omega, \tag{3.3}$$

$$\mu^{n+1/2}=-\nabla^2\phi^{n+1/2}+f'(\phi^{n+1/2}), \tag{3.4}$$

$$L\left(\phi^{n+1/2}\right)=\frac{\partial\phi^{n+1/2}}{\partial n}+\gamma'_{wf}\left(\phi^{n+1/2}\right), \tag{3.5}$$

$$\frac{\partial\mu^{n+1/2}}{\partial n}=0 \quad \text{on} \quad \partial\Omega, \tag{3.6}$$

then $\{\mathbf{u}^{n+1/2},p^{n+1}\}$, so that

$$R\frac{\mathbf{u}^{n+1/2}-\mathbf{u}^n}{\Delta t}-\nabla^2\mathbf{u}^{n+1/2}+\nabla p^{n+1}-B\mu^{n+1/2}\nabla\phi^{n+1/2}=0 \quad \text{in} \quad \Omega, \tag{3.7}$$

$$\nabla\cdot\mathbf{u}^{n+1/2}=0 \quad \text{in} \quad \Omega, \tag{3.8}$$

$$\mathbf{u}^{n+1/2}\cdot\mathbf{n}=0 \quad \text{on} \quad \partial\Omega, \tag{3.9}$$

$$\left[\boldsymbol{\sigma}^{n+1/2}\mathbf{n}+\left[\mathcal{L}_s(\phi^{n+1/2})\right]^{-1}(\mathbf{u}^{n+1/2}-\mathbf{u_w})-BL\left(\phi^{n+1/2}\right)\nabla\phi^{n+1/2}\right]\times\mathbf{n}=\mathbf{0} \quad \text{on} \quad \partial\Omega. \tag{3.10}$$

Finally, solve the following two (decoupled) pure advection problems:

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}^{n+1/2} \cdot \nabla)\mathbf{u} = \mathbf{0} \quad \text{in} \quad \Omega \times (t^n, t^{n+1}), \tag{3.11}$$

$$\mathbf{u}(t^n) = \mathbf{u}^{n+1/2}, \tag{3.12}$$

$$\frac{\partial \phi}{\partial t} + \mathbf{u}^{n+1/2} \cdot \nabla\phi = 0 \quad \text{in} \quad \Omega \times (t^n, t^{n+1}), \tag{3.13}$$

$$\phi(t^n) = \phi^{n+1/2}, \tag{3.14}$$

and set

$$\mathbf{u}^{n+1} = \mathbf{u}(t^{n+1}), \quad \phi^{n+1} = \phi(t^{n+1}). \tag{3.15}$$

Solving problems (3.11)–(3.14) is easy since $\mathbf{u}^{n+1/2} \cdot \mathbf{n} = 0$ on $\Gamma \times (t^n, t^{n+1})$ implies that no boundary condition is required. The solution of problems such as (3.11)–(3.14) by a wave-like equation approach is discussed in the Chapter 6 of Glowinski [11] (see also [2,12], Appendix A]). This approach is well-suited to finite element implementations; actually, since a detailed description of the wave-like equation methodology can be found in the above references ([2,11] in particular), it was decided to skip it in this article, in order to make room for more novel material. Problem (3.7)–(3.10) is a generalized Stokes problem whose iterative solution and finite element approximation will be discussed in Section 6. The real nontrivial part of our solution process is the solution of the semi-discrete (kind of) Cahn–Hilliard system (3.2)–(3.6). However, solving (3.2)–(3.6) is simpler than what it looks like since we can take advantage of the remarkable structure of this problem, as we shall see in Section 4.

Remark 3.1. As can be expected, the operator-splitting scheme (3.1)–(3.15) is not the only one that can be applied to the solution of problem (2.10)–(2.19). We can, for example, evaluate γ'_{wf} and f', in (3.3)–(3.5), at ϕ^n instead of $\phi^{n+1/2}$, obtaining thus a linear variant of system (3.2)–(3.6).

4. On the solution of problem (3.2)–(3.6)

4.1. Formulation of (3.2)–(3.6) as a nonlinear elliptic problem

Problem (3.2)–(3.6) is a particular case of

$$\frac{\phi - \phi_*}{\Delta t} - \mathcal{L}_d \nabla^2 \mu = 0 \quad \text{in} \quad \Omega, \tag{4.1}$$

$$\frac{\phi - \phi_*}{\Delta t} + \mathcal{V}_s L(\phi) = 0 \quad \text{on} \quad \partial\Omega, \tag{4.2}$$

$$\mu = -\nabla^2\phi + \alpha\phi + h(\phi), \tag{4.3}$$

$$L(\phi) = \frac{\partial \phi}{\partial n} + \gamma'_{wf}(\phi), \tag{4.4}$$

$$\frac{\partial \mu}{\partial n} = 0 \quad \text{on} \quad \partial\Omega, \tag{4.5}$$

where $h(\phi) = -(\alpha + 1)\phi + \phi^3$. Let us introduce

$$\omega = -\mathcal{L}_d \nabla^2 \mu; \tag{4.6}$$

it follows from 4.5 that

$$\int_\Omega \omega dx = -\mathcal{L}_d \int_\Omega \nabla^2 \mu dx = -\mathcal{L}_d \int_{\partial\Omega} \frac{\partial \mu}{\partial n} d(\partial\Omega) = 0. \tag{4.7}$$

As we shall see momentarily, ω may be seen as the main unknown of the problem. Indeed, we have

$$\frac{\phi - \phi_*}{\Delta t} + \omega = 0 \quad \text{in} \quad \Omega, \tag{4.8}$$

$$-\mathcal{L}_d \nabla^2 \mu = \omega \quad \text{in} \quad \Omega, \tag{4.9}$$

$$\frac{\partial \mu}{\partial n} = 0 \quad \text{on} \quad \partial\Omega, \tag{4.10}$$

$$-\nabla^2\phi + \alpha\phi + h(\phi) = \mu \quad \text{in} \quad \Omega, \tag{4.11}$$

$$\frac{1}{\mathcal{V}_s}\left(\frac{\phi - \phi_*}{\Delta t}\right) + \frac{\partial \phi}{\partial n} + \gamma'_{wf}(\phi) = 0 \quad \text{on} \quad \partial\Omega. \tag{4.12}$$

We observe that since $\omega \in L_0^2(\Omega) = \{v | v \in L^2(\Omega), \int_\Omega v dx = 0\}$, the Neumann problem (4.9), (4.10) has infinitely many solutions in $H^1(\Omega)$ (in fact, in $H^2(\Omega)$ if Ω is convex and/or $\partial\Omega$ is smooth enough) but only one in $H^1(\Omega) \cap L_0^2(\Omega)$. We observe also that

$$\int_\Omega \phi dx = \int_\Omega \phi_* dx. \tag{4.13}$$

From these observations, there is equivalence between the Cahn–Hilliard system (4.8)–(4.12) and:

Find $\{\omega, C\} \in (H^1(\Omega) \cap L_0^2(\Omega)) \times \mathbf{R}$ such that

$$\frac{\phi_1 - \phi_*}{\Delta t} + \omega = 0 \quad \text{in} \quad \Omega, \tag{4.14}$$

$$-\mathcal{L}_d \nabla^2 \hat{\mu} = \omega \quad \text{in} \quad \Omega, \tag{4.15}$$

$$\frac{\partial \hat{\mu}}{\partial n} = 0 \quad \text{on} \quad \partial\Omega, \quad \int_\Omega \hat{\mu} dx = 0, \tag{4.16}$$

$$-\nabla^2 \phi_2 + \alpha \phi_2 = \hat{\mu} + C - h(\phi_1) \quad \text{in} \quad \Omega, \tag{4.17}$$

$$\frac{1}{\mathcal{V}_s}\left(\frac{\phi_2 - \phi_*}{\Delta t}\right) + \frac{\partial \phi_2}{\partial n} = -\gamma'_{wf}(\phi_1) \quad \text{on} \quad \partial\Omega, \tag{4.18}$$

$$\phi_2 = \phi_1. \tag{4.19}$$

If one is considering the solution of system (4.8)–(4.12) via (4.20)–(4.23), one can take advantage of the following variational formulation of (4.14)–(4.19):

$$\int_\Omega (\phi_1 - \phi_*)\theta dx = -\Delta t \int_\Omega \omega\theta dx, \quad \forall \theta \in H^1(\Omega), \tag{4.20}$$

$$\hat{\mu} \in H^1(\Omega) \cap L_0^2(\Omega),$$

$$\int_\Omega \nabla\hat{\mu} \cdot \nabla\theta dx = \frac{1}{\mathcal{L}_d} \int_\Omega \omega\theta dx, \quad \forall \theta \in H^1(\Omega), \tag{4.21}$$

$$\phi_2 \in H^1(\Omega),$$

$$\int_\Omega \nabla\phi_2 \cdot \nabla\varphi dx + \alpha \int_\Omega \phi_2 \varphi dx + \frac{1}{\mathcal{V}_s \Delta t} \int_{\partial\Omega} \phi_2 \varphi d(\partial\Omega) = \int_\Omega (\hat{\mu} + C)\varphi dx - \int_\Omega h(\phi_1)\varphi dx + \frac{1}{\mathcal{V}_s \Delta t} \int_{\partial\Omega} \phi_* \varphi d(\partial\Omega) - \int_{\partial\Omega} \gamma'_{wf}(\phi_1)\varphi d(\partial\Omega), \quad \forall \varphi \in H^1(\Omega), \tag{4.22}$$

$$\phi_2 - \phi_1 = 0. \tag{4.23}$$

4.2. A least-squares method for the solution of problem (4.20)–(4.23)

In order to solve problem (3.2)–(3.6), via (4.20)–(4.23), we advocate the following least-squares formulation of this last problem:

Find $\{\omega_S, C_S\} \in (H^1(\Omega) \cap L_0^2(\Omega)) \times \mathbf{R}$ such that

$$J(\omega_S, C_S) \leqslant J(\omega, C), \quad \forall \{\omega, C\} \in \left(H^1(\Omega) \cap L_0^2(\Omega)\right) \times \mathbf{R}, \tag{4.24}$$

with (the notation being obvious):

$$J(\omega, C) = \frac{1}{2\mathcal{V}_s \Delta t} \int_{\partial\Omega} |\phi_2 - \phi_1|^2 d(\partial\Omega) + \frac{1}{2} \int_\Omega |\nabla(\phi_2 - \phi_1)|^2 dx + \frac{\alpha}{2} \int_\Omega |\phi_2 - \phi_1|^2 dx, \tag{4.25}$$

ϕ_1 and ϕ_2 being functions of $\{\omega, C\}$ via the solution of the following well-posed problems (assuming $\phi_* \in H^1(\Omega)$):

$$\phi_1 \in H^1(\Omega),$$

$$\int_\Omega (\phi_1 - \phi_*)\theta dx = -\Delta t \int_\Omega \omega\theta dx, \quad \forall \theta \in H^1(\Omega), \tag{4.26}$$

$$\hat{\mu} \in H^1(\Omega) \cap L_0^2(\Omega),$$

$$\int_\Omega \nabla\hat{\mu} \cdot \nabla\theta dx = \frac{1}{\mathcal{L}_d} \int_\Omega \omega\theta dx, \quad \forall \theta \in H^1(\Omega), \tag{4.27}$$

$$\phi_2 \in H^1(\Omega),$$

$$\int_\Omega \nabla\phi_2 \cdot \nabla\varphi dx + \alpha \int_\Omega \phi_2 \varphi dx + \frac{1}{\mathcal{V}_s \Delta t} \int_{\partial\Omega} \phi_2 \varphi d(\partial\Omega) = \int_\Omega (\hat{\mu} + C)\varphi dx - \int_\Omega h(\phi_1)\varphi dx + \frac{1}{\mathcal{V}_s \Delta t} \int_{\partial\Omega} \phi_* \varphi d(\partial\Omega) - \int_{\partial\Omega} \gamma'_{wf}(\phi_1)\varphi d(\partial\Omega), \quad \forall \varphi \in H^1(\Omega). \tag{4.28}$$

If $\{\omega_S, C_S\}$ is solution of the least-squares problem (4.24), it verifies

$$\frac{\partial J}{\partial C}(\omega_S, C_S) = 0, \quad < \frac{\partial J}{\partial \omega}(\omega_S, C_S), \theta >= 0, \quad \forall \theta \in H^1(\Omega) \cap L_0^2(\Omega), \tag{4.29}$$

where $\langle \cdot, \cdot \rangle$ denotes the duality-pairing between the dual-space of $H^1(\Omega) \cap L_0^2(\Omega)$ and $H^1(\Omega) \cap L_0^2(\Omega)$.

We are going to discuss now the computation of $\frac{\partial J}{\partial C}(\omega, C)$ and $< \frac{\partial J}{\partial \omega}(\omega, C), \theta >$ since knowing these differentials may prove very useful for the solution of problem (4.24) (or close variants of it, such as (4.54) hereafter) by iterative methods operating in the space $(H^1(\Omega) \cap L_0^2(\Omega)) \times \mathbf{R}$.

4.3. On the computation of the partial differentials of functional J

In order to compute the partial differentials of functional J, we are going to employ a rather classical perturbation method. The perturbation of $\{\omega, C\} \in (H^1(\Omega) \cap L_0^2(\Omega)) \times \mathbf{R}$ by $\{\delta\omega, \delta C\} \in (H^1(\Omega) \cap L_0^2(\Omega)) \times \mathbf{R}$ yields

$$\begin{aligned}\delta J = \frac{\partial J}{\partial C}(\omega, C)\delta C + \left\langle \frac{\partial J}{\partial \omega}(\omega, C), \delta\omega \right\rangle = \frac{1}{\Delta t \mathcal{V}_s}\int_{\partial\Omega}(\phi_2 - \phi_1)\delta\phi_2 d(\partial\Omega) + \int_\Omega \nabla(\phi_2 - \phi_1)\cdot\nabla\delta\phi_2 dx \\ + \alpha\int_\Omega(\phi_2 - \phi_1)\delta\phi_2 dx - \frac{1}{\Delta t \mathcal{V}_s}\int_{\partial\Omega}(\phi_2 - \phi_1)\delta\phi_1 d(\partial\Omega) - \int_\Omega \nabla(\phi_2 - \phi_1)\cdot\nabla\delta\phi_1 dx - \alpha\int_\Omega(\phi_2 - \phi_1)\delta\phi_1 dx.\end{aligned} \tag{4.30}$$

Since

$$\delta\phi_1 = -\Delta t\delta\omega, \tag{4.31}$$

relation 4.30 becomes

$$\begin{aligned}\delta J = \frac{\partial J}{\partial C}(\omega, C)\delta C + \left\langle \frac{\partial J}{\partial \omega}(\omega, C), \delta\omega \right\rangle = \frac{1}{\Delta t \mathcal{V}_s}\int_{\partial\Omega}(\phi_2 - \phi_1)\delta\phi_2 d(\partial\Omega) + \int_\Omega \nabla(\phi_2 - \phi_1)\cdot\nabla\delta\phi_2 dx \\ + \alpha\int_\Omega(\phi_2 - \phi_1)\delta\phi_2 dx + \frac{1}{\mathcal{V}_s}\int_{\partial\Omega}(\phi_2 - \phi_1)\delta\omega d(\partial\Omega) + \Delta t\int_\Omega \nabla(\phi_2 - \phi_1)\cdot\nabla\delta\omega dx + \alpha\Delta t\int_\Omega(\phi_2 - \phi_1)\delta\omega dx.\end{aligned} \tag{4.32}$$

We still have to express the integrals in the right-hand side of (4.32) as functions of $\delta\omega$ and δC. To achieve such a goal we observe that, from (4.28) and (4.31), we have

$$\begin{aligned}\delta\phi_2 \in H^1(\omega), \int_\Omega \nabla\delta\phi_2\cdot\nabla\varphi dx + \alpha\int_\Omega \delta\phi_2\varphi dx + \frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}\delta\phi_2\varphi d(\partial\Omega) = \int_\Omega(\delta\hat{\mu} + \delta C)\varphi dx - \int_\Omega h'(\phi_1)\delta\phi_1\varphi dx \\ - \int_{\partial\Omega}\gamma''_{wf}(\phi_1)\delta\phi_1 d(\partial\Omega), = \int_\Omega(\delta\hat{\mu} + \delta C)\varphi dx + \Delta t\int_\Omega h'(\phi_1)\delta\omega\varphi dx + \Delta t\int_{\partial\Omega}\gamma''_{wf}(\phi_1)\delta\omega\varphi d(\partial\Omega), \quad \forall\varphi \in H^1(\Omega).\end{aligned} \tag{4.33}$$

Taking $\varphi = \phi_2 - \phi_1$ in (4.33), we obtain

$$\begin{aligned}\int_\Omega \nabla(\phi_2 - \phi_1)\cdot\nabla\delta\phi_2 dx + \alpha\int_\Omega(\phi_2 - \phi_1)\delta\phi_2 dx + \frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}(\phi_2 - \phi_1)\delta\phi_2 d(\partial\Omega) \\ = \int_\Omega(\phi_2 - \phi_1)(\delta\hat{\mu} + \delta C)dx + \Delta t\int_\Omega h'(\phi_1)(\phi_2 - \phi_1)\delta\omega dx + \Delta t\int_{\partial\Omega}\gamma''_{wf}(\phi_1)(\phi_2 - \phi_1)\delta\omega dx.\end{aligned} \tag{4.34}$$

Combining (4.34) with (4.32), we obtain

$$\begin{aligned}\delta J &= \frac{\partial J}{\partial C}(\omega, C)\delta C + \left\langle \frac{\partial J}{\partial \omega}(\omega, C), \delta\omega \right\rangle \\ &= \int_\Omega(\phi_2 - \phi_1)(\delta\hat{\mu} + \delta C)dx + \Delta t\int_\Omega h'(\phi_1)(\phi_2 - \phi_1)\delta\omega dx + \Delta t\int_{\partial\Omega}\gamma''_{wf}(\phi_1)(\phi_2 - \phi_1)\delta\omega dx \\ &+ \frac{1}{\mathcal{V}_s}\int_{\partial\Omega}(\phi_2 - \phi_1)\delta\omega d(\partial\Omega) + \Delta t\int_\Omega \nabla(\phi_2 - \phi_1)\cdot\nabla\delta\omega dx + \alpha\Delta t\int_\Omega(\phi_2 - \phi_1)\delta\omega dx.\end{aligned} \tag{4.35}$$

We are almost done, since what's left is to express $\int_\Omega \delta\hat{\mu} dx$ as a function of $\delta\omega$; to do so let us consider the following well-posed variational problem (of the Neumann's type):

$$\begin{aligned}&\hat{\pi} \in H^1(\Omega) \cap L_0^2(\Omega), \\ &\int_\Omega \nabla\hat{\pi}\cdot\nabla\varphi dx = \int_\Omega(\phi_2 - \phi_1)\varphi dx, \quad \forall\varphi \in H^1(\Omega) \cap L_0^2(\Omega).\end{aligned} \tag{4.36}$$

On the other hand, it follows from (4.27) that

$$\delta\hat{\mu} \in H^1(\Omega) \cap L_0^2(\Omega),$$
$$\int_\Omega \nabla\delta\hat{\mu} \cdot \nabla\theta dx = \frac{1}{\mathcal{L}_d}\int_\Omega \delta\omega\theta dx, \quad \forall\theta \in H^1(\theta). \tag{4.37}$$

Take $\varphi = \delta\hat{\mu}$ in (4.36) and $\theta = \hat{\pi}$ in (4.37); by comparison, we obtain

$$\int_\Omega (\phi_2 - \phi_1)\delta\hat{\mu} dx = \frac{1}{\mathcal{L}_d}\int_\Omega \hat{\pi}\delta\omega dx. \tag{4.38}$$

Combining (4.38) with (4.35), we obtain:

$$\begin{aligned}\delta J &= \frac{\partial J}{\partial C}(\omega, C)\delta C + \left\langle \frac{\partial J}{\partial \omega}(\omega, C), \delta\omega \right\rangle \\ &= \frac{1}{\mathcal{L}_d}\int_\Omega \hat{\pi}\delta\omega dx + \int_\Omega (\phi_2 - \phi_1)\delta C dx + \Delta t\int_\Omega h'(\phi_1)(\phi_2 - \phi_1)\delta\omega dx + \Delta t\int_{\partial\Omega} \gamma''_{wf}(\phi_1)(\phi_2 - \phi_1)\delta\omega dx \\ &\quad + \frac{1}{\mathcal{V}_s}\int_{\partial\Omega} (\phi_2 - \phi_1)\delta\omega d(\partial\Omega) + \Delta t\int_\Omega \nabla(\phi_2 - \phi_1) \cdot \nabla\delta\omega dx + \alpha\Delta t\int_\Omega (\phi_2 - \phi_1)\delta\omega dx,\end{aligned} \tag{4.39}$$

that is:

$$\frac{\partial J}{\partial C}(\omega, C) = \int_\Omega (\phi_2 - \phi_1) dx, \tag{4.40}$$

$$\begin{aligned}\left\langle \frac{\partial J}{\partial \omega}(\omega, C), \theta \right\rangle &= \frac{1}{\mathcal{L}_d}\int_\Omega \hat{\pi}\theta dx + \Delta t\int_\Omega h'(\phi_1)(\phi_2 - \phi_1)\theta dx \\ &\quad + \Delta t\int_{\partial\Omega} \gamma''_{wf}(\phi_1)(\phi_2 - \phi_1)\theta d(\partial\Omega) + \frac{1}{\mathcal{V}_s}\int_{\partial\Omega} (\phi_2 - \phi_1)\theta d(\partial\Omega) \\ &\quad + \Delta t\int_\Omega \nabla(\phi_2 - \phi_1) \cdot \nabla\theta dx + \alpha\Delta t\int_\Omega (\phi_2 - \phi_1)\theta dx, \quad \forall\theta \in H^1(\Omega) \cap L_0^2(\Omega).\end{aligned} \tag{4.41}$$

Remark 4.1. One can easily show that $\hat{\pi}$ is the unique solution in $H^1(\Omega) \cap L_0^2(\Omega)$ of the Poisson–Neumann problem

$$-\nabla^2\hat{\pi} = \phi_2 - \phi_1 - \frac{\int_\Omega (\phi_2 - \phi_1) dx}{|\Omega|} \quad \text{in} \quad \Omega, \tag{4.42}$$
$$\frac{\partial\hat{\pi}}{\partial n} = 0$$

with $|\Omega|$ = meas. (Ω); one can take advantage of $\int_\Omega (\phi_1 - \phi_*) dx = 0$ to simplify (4.42).

4.4. A linear variant of the formulation (4.1)–(4.6)

Suppose that, following Remark 3.1, we evaluate in system (3.3)–(3.5), γ'_{wf} and f' at ϕ^n instead of $\phi^{n+1/2}$, then system (4.1)–(4.6) has to be replaced by

$$\frac{\phi - \phi_*}{\Delta t} - \mathcal{L}_d\nabla^2\mu = 0 \quad \text{in} \quad \Omega, \tag{4.43}$$
$$\frac{\phi - \phi_*}{\Delta t} + \mathcal{V}_s L(\phi) = 0 \quad \text{on} \quad \partial\Omega, \tag{4.44}$$
$$\mu = -\nabla^2\phi + \alpha\phi + h(\phi_*), \tag{4.45}$$
$$L(\phi) = \frac{\partial\phi}{\partial n} + \gamma'_{wf}(\phi_*), \tag{4.46}$$
$$\frac{\partial\mu}{\partial n} = 0 \quad \text{on} \quad \partial\Omega. \tag{4.47}$$

Similarly, system (4.14)–(4.19) has to be replaced by
Find $\{\omega, C\} \in (H^1(\Omega) \cap L_0^2(\Omega)) \times \mathbf{R}$ such that

$$\frac{\phi_1 - \phi_*}{\Delta t} + \omega = 0 \quad \text{in} \quad \Omega, \tag{4.48}$$
$$-\mathcal{L}_d\nabla^2\hat{\mu} = \omega \quad \text{in} \quad \Omega, \tag{4.49}$$
$$\frac{\partial\hat{\mu}}{\partial n} = 0 \quad \text{on} \quad \partial\Omega, \quad \int_\Omega \hat{\mu} dx = 0, \tag{4.50}$$
$$-\nabla^2\phi_2 + \alpha\phi_2 = \hat{\mu} + C - h(\phi_*) \quad \text{in} \quad \Omega, \tag{4.51}$$

$$\frac{1}{\mathcal{V}_s}\left(\frac{\phi_2-\phi_*}{\Delta t}\right)+\frac{\partial\phi_2}{\partial n}=-\gamma'_{wf}(\phi_*)\quad\text{on}\quad\partial\Omega,\tag{4.52}$$

$$\phi_2=\phi_1.\tag{4.53}$$

A least-squares formulation of the above problem is clearly the following variant of problem (4.24):

Find $\{\omega_S,C_S\}\in(H^1(\Omega)\cap L_0^2(\Omega))\times\mathbf{R}$ such that

$$J(\omega_S,C_S)\leqslant J(\omega,C),\quad\forall\{\omega,C\}\in\left(H^1(\Omega)\cap L_0^2(\Omega)\right)\times\mathbf{R},\tag{4.54}$$

with:

$$J(\omega,C)=\frac{1}{2\mathcal{V}_s\Delta t}\int_{\partial\Omega}|\phi_2-\phi_1|^2d(\partial\Omega)+\frac{1}{2}\int_\Omega|\nabla(\phi_2-\phi_1)|^2dx+\frac{\alpha}{2}\int_\Omega|\phi_2-\phi_1|^2dx,\tag{4.55}$$

ϕ_1 and ϕ_2 being functions from $\{\omega,C\}$ via the solution of the following well-posed problems (assuming $\phi_*\in H^1(\Omega)$):

$$\int_\Omega(\phi_1-\phi_*)\theta dx=-\Delta t\int_\Omega\omega\theta dx,\quad\forall\theta\in H^1(\Omega),\tag{4.56}$$

$$\begin{aligned}&\hat{\mu}\in H^1(\Omega)\cap L_0^2(\Omega),\\&\int_\Omega\nabla\hat{\mu}\cdot\nabla\theta dx=\frac{1}{\mathcal{L}_d}\int_\Omega\omega\theta dx,\quad\forall\theta\in H^1(\Omega),\end{aligned}\tag{4.57}$$

$$\begin{aligned}&\phi_2\in H^1(\Omega),\\&\int_\Omega\nabla\phi_2\cdot\nabla\varphi dx+\alpha\int_\Omega\phi_2\varphi dx+\frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}\phi_2\varphi d(\partial\Omega)=\int_\Omega(\hat{\mu}+C)\varphi dx-\int_\Omega h(\phi_*)\varphi dx+\frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}\phi_*\varphi d(\partial\Omega)\\&\qquad-\int_{\partial\Omega}\gamma'_{wf}(\phi_*)\varphi d(\partial\Omega),\quad\forall\varphi\in H^1(\Omega).\end{aligned}\tag{4.58}$$

We have then

$$\frac{\partial J}{\partial C}(\omega,C)=\int_\Omega(\phi_2-\phi_1)dx,\tag{4.59}$$

$$\begin{aligned}&\left\langle\frac{\partial J}{\partial\omega}(\omega,C),\theta\right\rangle=\frac{1}{\mathcal{L}_d}\int_\Omega\hat{\pi}\theta dx+\frac{1}{\mathcal{V}_s}\int_{\partial\Omega}(\phi_2-\phi_1)\theta d(\partial\Omega)\\&\quad+\Delta t\int_\Omega\nabla(\phi_2-\phi_1)\cdot\nabla\theta dx+\alpha\Delta t\int_\Omega(\phi_2-\phi_1)\theta dx,\quad\forall\theta\in H^1(\Omega)\cap L_0^2(\Omega).\end{aligned}\tag{4.60}$$

with $\hat{\pi}$ the solution of

$$\begin{aligned}&\hat{\pi}\in H^1(\Omega)\cap L_0^2(\Omega),\\&\int_\Omega\nabla\hat{\pi}\cdot\nabla\varphi dx=\int_\Omega(\phi_2-\phi_1)\varphi dx,\quad\forall\varphi\in H^1(\Omega)\cap L_0^2(\Omega).\end{aligned}\tag{4.61}$$

Following, e.g., [10,13,11,22], we can derive, from the above relations, a conjugate gradient algorithm operating in the Hilbert space $(H^1(\Omega)\cap L_0^2(\Omega))\times\mathbf{R}$, for the solution of the least-squares problem (4.54). Assuming that the above space is equipped with the scalar product

$$\{\{v,A\},\{w,B\}\}\to\frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}vwd(\partial\Omega)+\int_\Omega\nabla v\cdot\nabla wdx+\alpha\int_\Omega vwdx+AB$$

(a natural choice here) and the associated norm, such an algorithm reads as follows:

$$\{\omega^0,C^0\}\quad\text{is given in}\quad(H^1(\Omega)\cap L_0^2(\Omega))\times\mathbf{R}.\tag{4.62}$$

Compute

$$\phi_1^0=\phi_*-\Delta t\omega^0.\tag{4.63}$$

Solve first

$$\begin{aligned}&\hat{\mu}^0\in H^1(\Omega)\cap L_0^2(\Omega),\\&\int_\Omega\nabla\hat{\mu}^0\cdot\nabla\theta dx=\frac{1}{\mathcal{L}_d}\int_\Omega\omega^0\theta dx,\quad\forall\theta\in H^1(\theta),\end{aligned}\tag{4.64}$$

then

$$\phi_2^0 \in H^1(\Omega),$$
$$\int_\Omega \nabla\phi_2^0 \cdot \nabla\varphi dx + \alpha\int_\Omega \phi_2^0\varphi dx + \frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}\phi_2^0\varphi d(\partial\Omega) = \int_\Omega(\hat{\mu}^0 + C^0)\varphi dx - \int_\Omega h(\phi_*)\varphi dx + \frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}\phi_*\varphi d(\partial\Omega) - \int_{\partial\Omega}\gamma'_{wf}(\phi_*)\varphi d(\partial\Omega), \quad \forall\varphi \in H^1(\Omega), \tag{4.65}$$

and finally

$$\hat{\pi}^0 \in H^1(\Omega) \cap L_0^2(\Omega),$$
$$\int_\Omega \nabla\hat{\pi}^0 \cdot \nabla\varphi dx = \int_\Omega(\phi_2^0 - \phi_1^0)\varphi dx, \quad \forall\varphi \in H^1(\Omega) \cap L_0^2(\Omega). \tag{4.66}$$

Solve now

$$g_1^0 \in H^1(\Omega)\cap L_0^2(\Omega), \quad \int_\Omega \nabla g_1^0 \cdot \nabla\theta dx + \alpha\int_\Omega g_1^0\theta dx + \frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega} g_1^0\theta d(\partial\Omega)$$
$$= \frac{1}{\mathcal{L}_d}\int_\Omega \hat{\pi}^0\theta dx + \frac{1}{\mathcal{V}_s}\int_{\partial\Omega}(\phi_2^0 - \phi_1^0)\theta d(\partial\Omega) + \Delta t\int_\Omega \nabla(\phi_2^0 - \phi_1^0)\cdot\nabla\theta dx + \alpha\Delta t\int_\Omega(\phi_2^0 - \phi_1^0)\theta dx,$$
$$\forall\theta \in H^1(\Omega)\cap L_0^2(\Omega), \tag{4.67}$$

and compute

$$g_2^0 = \int_\Omega(\phi_2^0 - \phi_*)dx. \tag{4.68}$$

Set

$$\mathbf{g}^0 = \{g_1^0, g_2^0\} \tag{4.69}$$

and

$$\mathbf{w}^0 = \{w_1^0, w_2^0\}. \tag{4.70}$$

Then for $m \geqslant 0$, assuming that $\{\omega^m, C^m\}, \mathbf{g}^m = \{g_1^m, g_2^m\}$ and $\mathbf{w}^m = \{w_1^m, w_2^m\}$ are known, the last two different from $\mathbf{0}$, compute

$$\bar{\phi}_1^m = -\Delta t w_1^m, \tag{4.71}$$

solve

$$\bar{\hat{\mu}}^m \in H^1(\Omega)\cap L_0^2(\Omega),$$
$$\int_\Omega \nabla\bar{\hat{\mu}}^m \cdot \nabla\theta dx = \frac{1}{\mathcal{L}_d}\int_\Omega w^m\theta dx, \quad \forall\theta \in H^1(\Omega), \tag{4.72}$$

then

$$\bar{\phi}_2^m \in H^1(\Omega),$$
$$\int_\Omega \nabla\bar{\phi}_2^m \cdot \nabla\varphi dx + \alpha\int_\Omega \bar{\phi}_2^m\varphi dx + \frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}\bar{\phi}_2^m\varphi d(\partial\Omega) = \int_\Omega(\bar{\hat{\mu}}^m + w_2^m)\varphi dx, \quad \forall\varphi \in H^1(\Omega) \tag{4.73}$$

and finally

$$\bar{\hat{\pi}}^m \in H^1(\Omega)\cap L_0^2(\Omega),$$
$$\int_\Omega \nabla\bar{\hat{\pi}}^m \cdot \nabla\varphi dx = \int_\Omega(\bar{\phi}_2^m - \bar{\phi}_1^m)\varphi dx, \quad \forall\varphi \in H^1(\Omega)\cap L_0^2(\Omega). \tag{4.74}$$

Solve now

$$\bar{g}_1^m \in H^1(\Omega)\cap L_0^2(\Omega), \quad \int_\Omega \nabla\bar{g}_1^m \cdot \nabla\theta dx + \alpha\int_\Omega \bar{g}_1^m\theta dx + \frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}\bar{g}_1^m\theta d(\partial\Omega)$$
$$= \frac{1}{\mathcal{L}_d}\int_\Omega \bar{\hat{\pi}}^m\theta d + \frac{1}{\mathcal{V}_s}\int_{\partial\Omega}(\bar{\phi}_2^m - \bar{\phi}_1^m)\theta d(\partial\Omega) + \Delta t\int_\Omega \nabla\left(\bar{\phi}_2^m - \bar{\phi}_1^m\right)\cdot\nabla\theta dx$$
$$+ \alpha\Delta t\int_\Omega(\bar{\phi}_2^m - \bar{\phi}_1^m)\theta dx, \quad \forall\theta \in H^1(\Omega)\cap L_0^2(\Omega), \tag{4.75}$$

and compute

$$\bar{g}_2^m = \int_\Omega(\bar{\phi}_2^m - \bar{\phi}_1^m)dx, \tag{4.76}$$

$$\rho_m = \frac{\frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}|g_1^m|^2 d(\partial\Omega) + \alpha\int_\Omega |g_1^m|^2 dx + \int_\Omega |\nabla g_1^m|^2 dx + |g_2^m|^2}{\frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}\bar{g}_1^m w_1^m d(\partial\Omega) + \alpha\int_\Omega \bar{g}_1^m w_1^m dx + \int_\Omega \nabla\bar{g}_1^m\cdot\nabla w_1^m dx + \bar{g}_2^m w_2^m}. \tag{4.77}$$

Set

$$\omega^{m+1} = \omega^m - \rho_m w_1^m, \quad C^{m+1} = C^m - \rho_m w_2^m, \tag{4.78}$$

and

$$g_1^{m+1} = g_1^m - \rho_m \bar{g}_1^m, \quad g_2^{m+1} = g_2^m - \rho_m \bar{g}_2^m. \tag{4.79}$$

If $\frac{\frac{1}{\mathcal{V}_s \Delta t}\int_{\partial\Omega}|g_1^{m+1}|^2 d(\partial\Omega)+\int_\Omega |\nabla g_1^{m+1}|^2 dx+\alpha\int_\Omega |g_1^{m+1}|^2 dx+|g_2^{m+1}|^2}{\frac{1}{\mathcal{V}_s \Delta t}\int_{\partial\Omega}|g_1^{0}|^2 d(\partial\Omega)+\int_\Omega |\nabla g_1^{0}|^2 dx+\alpha\int_\Omega |g_1^{0}|^2 dx+|g_2^{0}|^2} \leqslant tol$, take $\{\omega, C\} = \{\omega^{m+1}, C^{m+1}\}, \phi = \phi_2^{m+1}$ and $\mu = \hat{\mu}^{m+1} + C^{m+1}$; else take

$$\gamma_m = \frac{\frac{1}{\mathcal{V}_s \Delta t}\int_{\partial\Omega}|g_1^{m+1}|^2 d(\partial\Omega)+\int_\Omega |\nabla g_1^{m+1}|^2 dx+\alpha\int_\Omega |g_1^{m+1}|^2 dx+|g_2^{m+1}|^2}{\frac{1}{\mathcal{V}_s \Delta t}\int_{\partial\Omega}|g_1^{m}|^2 d(\partial\Omega)+\int_\Omega |\nabla g_1^{m}|^2 dx+\alpha\int_\Omega |g_1^{m}|^2 dx+|g_2^{m}|^2} \tag{4.80}$$

and compute

$$\mathbf{w}^{m+1} = \mathbf{g}^{m+1} + \gamma_m \mathbf{w}^m. \tag{4.81}$$

Do $m = m + 1$ and return to (4.71).

Remark 4.2. Since problem (4.54) is of the least-squares type, a natural stopping criterion is provided by

$$\frac{J(\omega^{m+1}, C^{m+1})}{\frac{1}{\mathcal{V}_s \Delta t}\int_{\partial\Omega}|\phi_2^0|^2 d(\partial\Omega)+\int_\Omega |\nabla \phi_2^0|^2 dx+\alpha\int_\Omega |\phi_2^0|^2 dx} \leqslant tol.$$

Remark 4.3. To obtain ϕ_2^{m+1} and $\hat{\mu}^{m+1}$ in algorithm (4.62)–(4.81), one solves (4.57) and (4.58) with $\{\omega, C\} = \{\omega^{m+1}, C^{m+1}\}$.

Remark 4.4. The numerical results discussed in Section 9 have been obtained using algorithm (4.62)–(4.81) applied to the solution of problems of the (4.43)–(4.47) type (as advocated in Remark 3.1).

5. A stability property of the time-discretization scheme (4.48)–(4.53)

Assuming that (4.48)–(4.53) verifies the stability property given by (5.1), below, we are going to show that the time-discrete analogue of an energy functional naturally associated with the Cahn–Hilliard part of the model is decreasing. Indeed, we have the following:

Theorem 1. *If ϕ_1^{n+1} is the solution of (4.48)–(4.53) and α in (4.51) is sufficiently large, then the energy defined by $F_t(\phi) = \frac{1}{2}\int_\Omega |\nabla\phi|^2 dx + \frac{1}{4}\int_\Omega (\phi^2-1)^2 dx + \int_{\partial\Omega}\gamma_{wf}(\phi)d(\partial\Omega)$ is decreasing in time. More precisely, if the positive constant α satisfies*

$$\alpha \geqslant \frac{3M^2}{2} - \frac{1}{2}, \quad M = \sup_{x\in\Omega}\{|\phi_1^n|, |\phi_1^{n+1}|\}, \tag{5.1}$$

and

$$\Delta t \leqslant \frac{24}{\sqrt{2}\mathcal{V}_s \cos\theta_s^{surf}\pi^2}, \tag{5.2}$$

then for all $n \geqslant 0$,

$$F_t(\phi_1^{n+1}) - F_t(\phi_1^n) \leqslant 0. \tag{5.3}$$

Proof. Following the method in [14], taking $\theta = \hat{\mu}^{n+1} + C$ in (4.56), which is the weak form of 4.48, by (4.57) and (4.58), we have

$$\begin{aligned}
0 &= \int_\Omega (\phi_1^{n+1} - \phi_1^n)(\hat{\mu}^{n+1} + C)dx + \Delta t \mathcal{L}_d \int_\Omega |\nabla(\hat{\mu}^{n+1} + C)|^2 dx \\
&= \int_\Omega \nabla\phi_2^{n+1}\cdot\nabla(\phi_1^{n+1} - \phi_1^n)dx + \alpha\int_\Omega \phi_2^{n+1}(\phi_1^{n+1} - \phi_1^n)dx + \int_\Omega h(\phi_1^n)(\phi_1^{n+1} - \phi_1^n)dx - \int_{\partial\Omega}\frac{\partial\phi_2^{n+1}}{\partial n}(\phi_1^{n+1} - \phi_1^n)d(\partial\Omega) \\
&\quad + \Delta t\mathcal{L}_d\int_\Omega |\nabla(\hat{\mu}^{n+1} + C)|^2 dx \geqslant \int_\Omega \nabla\phi_2^{n+1}\cdot\nabla(\phi_1^{n+1} - \phi_1^n)dx + \alpha\int_\Omega \phi_2^{n+1}(\phi_1^{n+1} - \phi_1^n)dx \\
&\quad + \frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}\phi_2^{n+1}(\phi_1^{n+1} - \phi_1^n)d(\partial\Omega) + \int_\Omega h(\phi_1^n)(\phi_1^{n+1} - \phi_1^n)dx - \frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}\phi_1^n(\phi_1^{n+1} - \phi_1^n)d(\partial\Omega) \\
&\quad + \int_{\partial\Omega}\gamma'_{wf}(\phi_1^n)(\phi_1^{n+1} - \phi_1^n)d(\partial\Omega).
\end{aligned} \tag{5.4}$$

Using (4.53),

$$0 \geqslant \int_\Omega \nabla\phi_1^{n+1}\cdot\nabla(\phi_1^{n+1}-\phi_1^n)dx + \alpha\int_\Omega(\phi_1^{n+1}-\phi_1^n)^2dx + \alpha\int_\Omega \phi_1^n(\phi_1^{n+1}-\phi_1^n)dx\alpha + \int_\Omega h(\phi_1^n)(\phi_1^{n+1}-\phi_1^n)dx + \int_{\partial\Omega}\gamma'_{wf}(\phi_1^n)(\phi_1^{n+1}-\phi_1^n)d(\partial\Omega) + \frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}(\phi_1^{n+1}-\phi_1^n)^2d(\partial\Omega). \tag{5.5}$$

Since $h(\phi) = -(\alpha+1)\phi+\phi^3$,

$$\begin{aligned}0 &\geqslant \int_\Omega \nabla\phi_1^{n+1}\cdot\nabla(\phi_1^{n+1}-\phi_1^n)dx + \alpha\int_\Omega(\phi_1^{n+1}-\phi_1^n)^2dx + \int_\Omega(-\phi_1^n+(\phi_1^n)^3)(\phi_1^{n+1}-\phi_1^n)dx\\
&\quad + \int_{\partial\Omega}\gamma'_{wf}(\phi_1^n)(\phi_1^{n+1}-\phi_1^n)d(\partial\Omega) + \frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}(\phi_1^{n+1}-\phi_1^n)^2d(\partial\Omega)\\
&= \int_\Omega \nabla\phi_1^{n+1}\cdot\nabla(\phi_1^{n+1}-\phi_1^n)dx + \alpha\int_\Omega(\phi_1^{n+1}-\phi_1^n)^2dx + \int_\Omega\left((\phi_1^n)^2-1\right)\phi_1^n(\phi_1^{n+1}-\phi_1^n)dx\\
&\quad + \int_{\partial\Omega}\left(\gamma_{wf}(\phi_1^{n+1})-\gamma_{wf}(\phi_1^n)-\frac{1}{2}\gamma''_{wf}(\xi)(\phi_1^{n+1}-\phi_1^n)^2\right)d(\partial\Omega) + \frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}(\phi_1^{n+1}-\phi_1^n)^2d(\partial\Omega).\end{aligned} \tag{5.6}$$

Using the equalities $ab = \frac{a^2+b^2-(a-b)^2}{2}$ and $2a(a-b) = a^2-b^2+(a-b)^2$,

$$\begin{aligned}0 &\geqslant \frac{1}{2}\int_\Omega|\nabla\phi_1^{n+1}|^2dx - \frac{1}{2}\int_\Omega|\nabla\phi_1^n|^2dx + \frac{1}{2}\int_\Omega\left(1-(\phi_1^n)^2\right)(\phi_1^{n+1}-\phi_1^n)^2dx + \frac{1}{2}\int_\Omega\left((\phi_1^n)^2-1\right)((\phi_1^{n+1})^2-(\phi_1^n)^2)dx\\
&\quad + \alpha\int_\Omega(\phi_1^{n+1}-\phi_1^n)^2dx + \int_{\partial\Omega}\left(\gamma_{wf}(\phi_1^{n+1})-\gamma_{wf}(\phi_1^n)-\frac{1}{2}\gamma''_{wf}(\xi)(\phi_1^{n+1}-\phi_1^n)^2\right)d(\partial\Omega) + \frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}(\phi_1^{n+1}-\phi_1^n)^2d(\partial\Omega)\\
&= \frac{1}{2}\int_\Omega|\nabla\phi_1^{n+1}|^2dx - \frac{1}{2}\int_\Omega|\nabla\phi_1^n|^2dx + \frac{1}{2}\int_\Omega\left(1-(\phi_1^n)^2\right)(\phi_1^{n+1}-\phi_1^n)^2dx\\
&\quad + \int_\Omega\left(-\frac{1}{2}(\phi_1^{n+1})^2+\frac{1}{2}(\phi_1^n)^2+\frac{1}{4}(\phi_1^{n+1})^4-\frac{1}{4}(\phi_1^n)^4-\frac{1}{4}\left[(\phi_1^{n+1})^2-(\phi_1^n)^2\right]^2\right)dx + \alpha\int_\Omega(\phi_1^{n+1}-\phi_1^n)^2dx\\
&\quad + \int_{\partial\Omega}\left(\gamma_{wf}(\phi_1^{n+1})-\gamma_{wf}(\phi_1^n)-\frac{1}{2}\gamma''_{wf}(\xi)(\phi_1^{n+1}-\phi_1^n)^2\right)d(\partial\Omega) + \frac{1}{\mathcal{V}_s\Delta t}\int_{\partial\Omega}(\phi_1^{n+1}-\phi_1^n)^2d(\partial\Omega)\\
&= \frac{1}{2}\int_\Omega|\nabla\phi_1^{n+1}|^2dx - \frac{1}{2}\int_\Omega|\nabla\phi_1^n|^2dx + \frac{1}{4}\int_\Omega\left((\phi_1^{n+1})^2-1\right)^2dx - \frac{1}{4}\int_\Omega\left((\phi_1^n)^2-1\right)^2dx\\
&\quad + \int_\Omega\left(\frac{1}{2}-\frac{1}{2}(\phi_1^n)^2-\frac{1}{4}\left[(\phi_1^{n+1}+\phi_1^n)^2\right]+\alpha\right)(\phi_1^{n+1}-\phi_1^n)^2dx\\
&\quad + \int_{\partial\Omega}\left(\gamma_{wf}(\phi_1^{n+1})-\gamma_{wf}(\phi_1^n)+\left(-\frac{1}{2}\gamma''_{wf}(\xi)+\frac{1}{\mathcal{V}_s\Delta t}\right)(\phi_1^{n+1}-\phi_1^n)^2\right)d(\partial\Omega),\end{aligned} \tag{5.7}$$

where ξ is a value between ϕ_1^n and ϕ_1^{n+1}, by $\gamma_{wf}(\phi) = -\frac{\sqrt{2}}{3}\cos\theta_s^{surf}\sin(\frac{\pi}{2}\phi)$, we have

$$F_t(\phi_1^{n+1}) \leqslant F_t(\phi_1^n), \tag{5.8}$$

when

$$\alpha \geqslant \frac{3M^2}{2}-\frac{1}{2}, \quad M = \sup_{x\in\Omega}\{|\phi_1^n|, |\phi_1^{n+1}|\} \tag{5.9}$$

and

$$\Delta t \leqslant \frac{24}{\sqrt{2}\mathcal{V}_s\cos\theta_s^{surf}\pi^2}. \quad \square \tag{5.10}$$

Remark 5.1. Theorem does not qualify as a stability theorem. Indeed, to prove it we have been assuming that relation (5.1) holds; (5.1) is already a strong stability property in itself.

6. On the solution of the generalized Stokes problem (3.7)–(3.10)

Clearly, problem (3.7)–(3.10) belongs to the following family of generalized Stokes problems

$$R\frac{\mathbf{u}-\mathbf{u}_*}{\Delta t} - \nabla^2\mathbf{u} + \nabla p - B\mu_*\nabla\phi_* = 0 \quad \text{in} \quad \Omega, \tag{6.1}$$

$$\nabla\cdot\mathbf{u} = 0 \quad \text{in} \quad \Omega, \tag{6.2}$$

$$\mathbf{u}\cdot\mathbf{n} = 0 \quad \text{on} \quad \partial\Omega, \tag{6.3}$$

$$\left[\boldsymbol{\sigma}\mathbf{n} + [\mathcal{L}_s(\phi_*)]^{-1}(\mathbf{u}-\mathbf{u_w}) - BL(\phi_*)\nabla\phi_*\right]\times\mathbf{n} = \mathbf{0} \quad \text{on} \quad \partial\Omega, \tag{6.4}$$

where $\mathbf{u}_*$, ϕ_* are known functions, and where $L(\phi_*) = \frac{\partial\phi_*}{\partial n} + \gamma'_{wf}(\phi_*)$.

6.1. Variational formulation of the Stokes problem (3.7)–(3.10)

A classical variational formulation of problem (3.7)–(3.10) is given by:
Find $\{\mathbf{u},p\}\in\mathbf{V}_0\times L^2(\Omega)$ such that

$$\begin{aligned} &R\int_\Omega \frac{\mathbf{u}-\mathbf{u}_*}{\Delta t}\cdot\mathbf{v}dx + 2\int_\Omega \mathbf{D}(\mathbf{u}):\mathbf{D}(\mathbf{v})dx - \int_\Omega p\nabla\cdot\mathbf{v}dx + [\mathcal{L}_s(\phi_*)]^{-1}\int_{\partial\Omega}\mathbf{u}\cdot\mathbf{v}d(\partial\Omega) \\ &\quad = \int_\Omega B\mu_*\nabla\phi_*\cdot\mathbf{v}dx + \int_{\partial\Omega}[\mathcal{L}_s(\phi_*)]^{-1}\mathbf{u_w}\cdot\mathbf{v}d(\partial\Omega) + B\int_{\partial\Omega}L(\phi_*)\nabla\phi_*\cdot\mathbf{v}d(\partial\Omega), \\ &\forall\mathbf{v}\in\mathbf{V}_0, \end{aligned} \tag{6.5}$$

$$\int_\Omega \nabla\cdot\mathbf{u}q dx = 0, \quad \forall q\in L^2(\Omega), \tag{6.6}$$

$$\mathbf{u}\cdot\mathbf{n} = 0, \quad on \quad \partial\Omega, \tag{6.7}$$

where

$$\mathbf{V}_0 = \{\mathbf{v}|\mathbf{v}\in(H^1(\Omega))^d, \quad \mathbf{v}\cdot\mathbf{n} = 0 \quad on \quad \partial\Omega\}.$$

We observe that in the above formulations, p is defined within an additive constant. From now on we will focus on the unique pressure belonging to the space $P_0 = H^1(\Omega)\cap L^2_0(\Omega)$. The solution of problems (6.5)–(6.7) is obtained by a conjugate gradient algorithm which is very close to those discussed in Glowinski [11, Chapter 4].

6.2. Conjugate gradient solution of problem (6.5)–(6.7)

In order to solve problem (6.5)–(6.7), we advocate the following conjugate gradient algorithm:

$$p^0\in P_0 \quad \text{is given in} \quad P_0. \tag{6.8}$$

Find $\mathbf{u}^0\in\mathbf{V}_0$ such that

$$\begin{aligned} &\frac{R}{\Delta t}\int_\Omega \mathbf{u}^0\cdot\mathbf{v}dx + 2\int_\Omega \mathbf{D}(\mathbf{u}^0):\mathbf{D}(\mathbf{v})dx + [\mathcal{L}_s(\phi_*)]^{-1}\int_{\partial\Omega}\mathbf{u}^0\cdot\mathbf{v}d(\partial\Omega) \\ &\quad = \int_\Omega p^0\nabla\cdot\mathbf{v}dx + \int_\Omega B\mu_*\nabla\phi_*\cdot\mathbf{v}dx + \frac{R}{\Delta t}\int_\Omega \mathbf{u}_*\cdot\mathbf{v}dx + [\mathcal{L}_s(\phi_*)]^{-1}\int_{\partial\Omega}\mathbf{u_w}\cdot\mathbf{v}d(\partial\Omega) \\ &\quad\quad + B\int_{\partial\Omega}L(\phi_*)\nabla\phi_*\cdot\mathbf{v}d(\partial\Omega), \quad \forall\mathbf{v}\in\mathbf{V}_0, \end{aligned} \tag{6.9}$$

and set

$$r^0 = \nabla\cdot\mathbf{u}^0. \tag{6.10}$$

Solve now

$$\begin{aligned} &h^0\in P_0, \\ &\int_\Omega \nabla h^0\cdot\nabla q dx = \int_\Omega r^0 q dx, \quad \forall q\in L^2(\Omega). \end{aligned} \tag{6.11}$$

Then set

$$g^0 = r^0 + \frac{R}{\Delta t}h^0, \tag{6.12}$$

$$w^0 = g^0. \tag{6.13}$$

Then, for $n \geqslant 0$, assuming that p^n, r^n, g^n, w^n are known, compute p^{n+1}, r^{n+1}, g^{n+1}, w^{n+1} as follows:
Find $\bar{\mathbf{u}}^k\in\mathbf{V}_0$ such that

$$\frac{R}{\Delta t}\int_\Omega \bar{\mathbf{u}}^k\cdot\mathbf{v}dx + 2\int_\Omega \mathbf{D}(\bar{\mathbf{u}}^k):\mathbf{D}(\mathbf{v})dx + [\mathcal{L}_s(\phi_*)]^{-1}\int_{\partial\Omega}\bar{\mathbf{u}}^k\cdot\mathbf{v}d(\partial\Omega) = \int_\Omega w^k\nabla\cdot\mathbf{v}dx, \quad \forall\mathbf{v}\in\mathbf{V}_0, \tag{6.14}$$

and set

$$\bar{r}^n = \nabla \cdot \bar{\mathbf{u}}^n. \tag{6.15}$$

Compute

$$\rho_n = \frac{\int_\Omega r^n g^n dx}{\int_\Omega \bar{r}^n w^n dx}, \tag{6.16}$$

and then

$$p^{n+1} = p^n - \rho_n w^n, \tag{6.17}$$

$$r^{n+1} = r^n - \rho_n \bar{r}^n. \tag{6.18}$$

Solve, next,

$$\bar{h}^n \in P_0,$$

$$\int_\Omega \nabla \bar{h}^n \cdot \nabla q dx = \int_\Omega \bar{r}^n q dx, \quad \forall q \in L^2(\Omega). \tag{6.19}$$

Then, compute

$$g^{n+1} = g^n - \rho_n \left(\bar{r}^n + \frac{R}{\Delta t} \bar{h}^n \right). \tag{6.20}$$

If $\frac{\int_\Omega r^{n+1} g^{n+1} dx}{\int_\Omega r^0 g^0 dx} \leqslant tol$, take $p = p^{n+1}$ and compute $\mathbf{u}$ from (6.5); else, compute

$$\gamma_n = \frac{\int_\Omega r^{n+1} g^{n+1} dx}{\int_\Omega r^n g^n dx}, \tag{6.21}$$

and update w^{n+1} by

$$w^{n+1} = g^{n+1} + \gamma_n w^n. \tag{6.22}$$

Do $n = n + 1$ and return to 6.14.

7. A stability property of the whole time-discretization scheme (3.11)–(3.14), (4.48)–(4.53), (6.1)–(6.4)

In Section 5 we proved that the time-discrete analogue of the functional $F_t(\phi) = \frac{1}{2}\int_\Omega |\nabla \phi|^2 dx + \frac{1}{4}\int_\Omega (\phi^2 - 1)^2 dx + \int_{\partial\Omega} \gamma_{wf}(\phi) d(\partial\Omega)$ is decreasing when applying scheme (4.48)–(4.53) to the time discretization of the Cahn–Hilliard part of the system under consideration. It is of course natural to ask if a similar property holds for the full Cahn–Hilliard-Navier–Stokes system. Indeed, we are going to prove a generalization of Theorem 1, when applying the time-discretization scheme (3.11)–(3.14), (4.48)–(4.53), (6.1)–(6.4) to the full model. We have thus the following :

Theorem 2. *Suppose that* $\mathbf{u}^{n+1}$, ϕ^{n+1}, $\mathbf{u}^{n+1/2}$, $\phi^{n+1/2}$ *satisfy* (3.11)–(3.14), (4.48)–(4.53), (6.1)–(6.4). *If the positive constant* α *satisfies*

$$\alpha \geqslant \frac{3M^2}{2} - \frac{1}{2}, \quad M = \sup_{x\in\Omega}\{|\phi^n|, |\phi^{n+1/2}|\}, \tag{7.1}$$

and

$$\Delta t \leqslant \frac{24}{\sqrt{2}\mathcal{V}_s \cos\theta_s^{surf} \pi^2}, \tag{7.2}$$

then

$$B\big(F_t(\phi^{n+1}) - F_t(\phi^n)\big) + \frac{1}{2} R\left(\int_\Omega |\mathbf{u}^{n+1}|^2 dx - \int_\Omega |\mathbf{u}^n|^2 dx\right) + \Delta t \int_{\partial\Omega} [\mathcal{L}_s(\phi^{n+1/2})]^{-1} |\mathbf{u}^{n+1} - \mathbf{u_w}|^2 d(\partial\Omega)$$
$$+ \Delta t \int_{\partial\Omega} [\mathcal{L}_s(\phi^{n+1/2})]^{-1} (\mathbf{u}^{n+1} - \mathbf{u_w}) \cdot \mathbf{u_w} d(\partial\Omega) \leqslant 0. \tag{7.3}$$

Proof. Taking $\mathbf{v} = \mathbf{u}^{n+1/2}$ in (6.5), we obtain

$$\frac{1}{2} R\left(\int_\Omega |\mathbf{u}^{n+1/2}|^2 dx - \int_\Omega |\mathbf{u}^n|^2 dx + \int_\Omega |\mathbf{u}^{n+1/2} - \mathbf{u}|^2 dx\right) + \Delta t \int_\Omega |\nabla \mathbf{u}^{n+1/2}|^2 dx - \Delta t \int_\Omega p^{n+1} \nabla \cdot \mathbf{u}^{n+1/2} dx$$
$$+ \Delta t \int_{\partial\Omega} [\mathcal{L}_s(\phi^{n+1/2})]^{-1} (\mathbf{u}^{n+1/2} - \mathbf{u_w}) \cdot \mathbf{u}^{n+1/2} d(\partial\Omega)$$
$$= \Delta t B \int_\Omega \mu^{n+1/2} \nabla \phi^{n+1/2} \cdot \mathbf{u}^{n+1/2} dx + \Delta t B \int_{\partial\Omega} L(\phi^{n+1/2}) \nabla \phi^{n+1/2} \cdot \mathbf{u}^{n+1/2} d(\partial\Omega). \tag{7.4}$$

Taking $q = p^{n+1}$ in (6.6) and using $\nabla\cdot\mathbf{u}^{n+1/2} = 0$ in Ω and $\mathbf{u}^{n+1/2}\cdot\mathbf{n} = 0$ on $\partial\Omega$, we have

$$\frac{1}{2}R\left(\int_\Omega |\mathbf{u}^{n+1/2}|^2dx - \int_\Omega |\mathbf{u}^n|^2dx\right) + \Delta t\int_\Omega |\nabla\mathbf{u}^{n+1/2}|^2dx + \Delta t\int_{\partial\Omega}[\mathcal{L}_s(\phi^{n+1/2})]^{-1}(\mathbf{u}^{n+1/2} - \mathbf{u}_\mathbf{w})\cdot\mathbf{u}^{n+1/2}d(\partial\Omega)$$
$$\leqslant \Delta tB\int_{\partial\Omega} L(\phi^{n+1/2})\nabla\phi^{n+1/2}\cdot\mathbf{u}^{n+1/2}d(\partial\Omega). \tag{7.5}$$

From (3.11), we have that

$$\frac{1}{2}\left(\int_\Omega |\mathbf{u}^{n+1}|^2dx - \int_\Omega |\mathbf{u}^{n+1/2}|^2dx + \int_\Omega |\mathbf{u}^{n+1} - \mathbf{u}^{n+1/2}|^2dx\right) = -\Delta t\int_\Omega (\mathbf{u}^{n+1/2}\cdot\nabla\mathbf{u}^{n+1})\cdot\mathbf{u}^{n+1}dx. \tag{7.6}$$

Since $\nabla\cdot\mathbf{u}^{n+1/2} = 0$ in Ω and $\mathbf{u}^{n+1/2}\cdot\mathbf{n} = 0$ on $\partial\Omega$, therefore

$$\int_\Omega |\mathbf{u}^{n+1}|^2dx \leqslant \int_\Omega |\mathbf{u}^{n+1/2}|^2dx. \tag{7.7}$$

By $\nabla\cdot\mathbf{u}^{n+1} = 0$ on $\partial\Omega$, we obtain

$$\frac{1}{2}R\left(\int_\Omega |\mathbf{u}^{n+1}|^2dx - \int_\Omega |\mathbf{u}^n|^2dx\right) + \Delta t\int_{\partial\Omega}[\mathcal{L}_s(\phi^{n+1/2})]^{-1}(\mathbf{u}^{n+1/2} - \mathbf{u}_\mathbf{w})\cdot\mathbf{u}^{n+1/2}d(\partial\Omega)$$
$$\leqslant \Delta tB\int_{\partial\Omega} L(\phi^{n+1/2})\nabla\phi^{n+1/2}\cdot\mathbf{u}^{n+1/2}d(\partial\Omega) = 0. \tag{7.8}$$

Taking $\theta = \mu^{n+1/2}$ in (4.56), we have that

$$\int_\Omega (\phi^{n+1/2} - \phi^n)\mu^{n+1/2}dx + \Delta t\mathcal{L}_d\int_\Omega |\nabla\mu^{n+1/2}|^2dx = 0. \tag{7.9}$$

From the proof of Theorem 1, denoting by $F(\phi)$ the bulk free energy $\frac{1}{2}\int_\Omega|\nabla\phi|^2dx + \frac{1}{4}\int_\Omega(\phi^2 - 1)^2dx$, when conditions (7.1) is satisfied and using (3.13) and (3.14) and relation (4.46), we have the following inequality

$$\begin{aligned}
F(\phi^{n+1/2}) - F(\phi^n) &\leqslant \int_\Omega \mu^{n+1/2}(\phi^{n+1/2} - \phi^n)dx + \int_{\partial\Omega}\frac{\partial\phi^{n+1/2}}{\partial n}(\phi^{n+1/2} - \phi^n)d(\partial\Omega)\\
&= \int_\Omega \mu^{n+1/2}(\phi^{n+1/2} - \phi^n)dx + \int_{\partial\Omega}\frac{\partial\phi^{n+1/2}}{\partial n}(\phi^{n+1} - \phi^n)d(\partial\Omega)\\
&= \int_\Omega \mu^{n+1/2}(\phi^{n+1/2} - \phi^n)dx + \int_{\partial\Omega}(L(\phi^{n+1/2}) - \gamma'_{wf}(\phi^n))(\phi^{n+1} - \phi^n)d(\partial\Omega)\\
&= \int_\Omega \mu^{n+1/2}(\phi^{n+1/2} - \phi^n)dx + \int_{\partial\Omega} L(\phi^{n+1/2})(\phi^{n+1} - \phi^n)d(\partial\Omega)\\
&\quad + \int_{\partial\Omega}\left(-\gamma_{wf}(\phi^{n+1}) + \gamma_{wf}(\phi^n) + \frac{1}{2}\gamma''_{wf}(\xi)(\phi^{n+1} - \phi^n)^2\right)d(\partial\Omega).
\end{aligned} \tag{7.10}$$

Using (3.13) and (3.14), (4.44), (7.9), we obtain

$$\begin{aligned}
F(\phi^{n+1/2}) + \int_{\partial\Omega}\gamma_{wf}(\phi^{n+1})d(\partial\Omega) - F_t(\phi^n) &\leqslant \int_\Omega \mu^{n+1/2}(\phi^{n+1/2} - \phi^n)dx + \int_{\partial\Omega} L(\phi^{n+1/2})(\phi^{n+1} - \phi^n)d(\partial\Omega)\\
&\quad + \int_{\partial\Omega}\frac{1}{2}\gamma''_{wf}(\xi)(\phi^{n+1} - \phi^n)^2d(\partial\Omega)\\
&= -\Delta t\mathcal{L}_d\int_\Omega |\nabla\mu^{n+1/2}|^2dx - \int_{\partial\Omega}\frac{\phi^{n+1/2} - \phi^n}{\Delta t\mathcal{V}_s}(\phi^{n+1} - \phi^n)d(\partial\Omega)\\
&\quad + \int_{\partial\Omega}\frac{1}{2}\gamma''_{wf}(\xi)(\phi^{n+1} - \phi^n)^2d(\partial\Omega)\\
&= -\Delta t\mathcal{L}_d\int_\Omega |\nabla\mu^{n+1/2}|^2dx - \frac{1}{\Delta t\mathcal{V}_s}\int_{\partial\Omega}\left(1 - \frac{1}{2}\gamma''_{wf}(\xi)\Delta t\mathcal{V}_s\right)(\phi^{n+1} - \phi^n)^2dx.
\end{aligned} \tag{7.11}$$

Therefore, when condition (7.2) is satisfied, we obtain that

$$F(\phi^{n+1/2}) + \int_{\partial\Omega}\gamma_{wf}(\phi^{n+1})d(\partial\Omega) - F_t(\phi^n) \leqslant 0. \tag{7.12}$$

Combing (7.8) and (7.12), we have

$$B\left(F(\phi^{n+1/2}) + \int_{\partial\Omega} \gamma_{wf}(\phi^{n+1})d(\partial\Omega) - F_t(\phi^n)\right) + \frac{1}{2}R\left(\int_\Omega |\mathbf{u}^{n+1}|^2 dx - \int_\Omega |\mathbf{u}^n|^2 dx\right)$$
$$+ \Delta t \int_{\partial\Omega} [\mathcal{L}_s(\phi^{n+1/2})]^{-1}(\mathbf{u}^{n+1/2} - \mathbf{u_w}) \cdot \mathbf{u}^{n+1/2} d(\partial\Omega) \leqslant 0. \tag{7.13}$$

From (3.13) and (3.14) and $\nabla \cdot \mathbf{u}^{n+1/2} = 0$ on $\partial\Omega$, we can easily obtain that

$$\int_\Omega |\nabla\phi^{n+1}|^2 dx \leqslant \int_\Omega |\nabla\phi^{n+1/2}|^2 dx,$$

and

$$\int_\Omega \left((\phi^{n+1})^2 - 1\right)^2 dx \leqslant \int_\Omega ((\phi^{n+1/2})^2 - 1)^2 dx.$$

Since (3.11) and (3.12) is also valid on $\partial\Omega$, we obtain (7.3) and conclude the proof. □

Remark 7.1. Remark (5.1) of Section (5) still applies here.

8. Finite element implementation of the operator–splitting/least–squares/conjugate gradient methodology of Sections 3, 4 and 6

We suppose for simplicity that Ω is a bounded polygonal domain of $\mathbf{R}^2$; we introduce then a triangulation $\mathcal{T}_h$ of Ω consisting of a finite number of closed triangles K, all contained in $\overline{\Omega}$, and such that

$$\bigcup_{K\in\mathcal{T}_h} K = \overline{\Omega}; \tag{8.1}$$

as usual, we assume also that:

(i) h is the maximal length of the edges of triangles of $\mathcal{T}_h$;
(ii) if K and K' are two different triangles of $\mathcal{T}_h$, then either $K \cap K' = \emptyset$, or K and K' have only one vertex or a full edge in common.

A triangulation $\mathcal{T}_h$ verifying the above assumptions has been visualized in Fig. 1. Next, from $\mathcal{T}_h$ we define $\mathcal{T}_{h/2}$ by joining the midpoints of the triangles of $\mathcal{T}_h$. We define the finite dimensional spaces P_h and V_h by

$$P_h = \{q | q \in C^0(\overline{\Omega}), q|_K \in P_1, \forall K \in \mathcal{T}_h\} \tag{8.2}$$

and

$$V_h = \{\phi | \phi \in C^0(\overline{\Omega}), \quad \phi|_K \in P_1, \forall K \in \mathcal{T}_{h/2}\}, \tag{8.3}$$

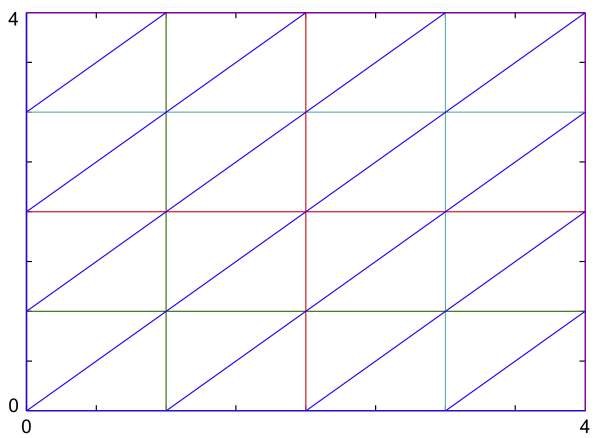

Fig. 1. Triangulation of Ω.

P_1 being the space of the polynomials of two variables of degree $\leqslant 1$. The space P_h will be used to approximate the pressure p, while the spaces $V_h \times V_h$ and V_h will be used to approximate the velocity $\mathbf{u}$ and the phase field ϕ, respectively. Concerning the space $H^1(\Omega) \cap L_0^2(\Omega)$ it will be approximated by

$$V_{0h} = \{\phi | \phi \in V_h, \int_\Omega \phi dx = 0\}. \tag{8.4}$$

The operator-splitting/least-squares/conjugate gradient methodology described in Sections 3–5 is easy to implement from the variational formulation of its various components, given in the above sections. Actually, following Remark 3.1, the numerical results presented below have been obtained using algorithm (4.62)–(4.81) to solve the nonlinear sub-problems of the Cahn–Hilliard's type.

9. Numerical results

For numerical experiments whose results are presented below, we have borrowed from [19] the various parameters occurring in the Navier–Stokes-Cahn–Hilliard system discussed here, that is

$$\begin{aligned} &B = 12.0, \quad \mathcal{L}_d = 5.0, \quad \mathcal{V}_s = 5.0, \quad l_s = 3.8, \\ &R = 0.03, \quad \mathbf{u_w} = (0.2, 0.0), \quad \theta_s^{surf} = 77.6^\circ. \end{aligned} \tag{9.1}$$

In our numerical simulation $\alpha = 3$ and $\Omega = (0,100) \times (0,40)$. Concerning the initial conditions we have taken for $\mathbf{u}^0$ the velocity field associated to a uniform shear flow and defined the initial phase field by

$$\phi^0(x_1, x_2) = \tanh\left(\frac{x_1 - 0.5L_{x_1}}{2\sqrt{5}}\right),$$

where L_{x_1} is the length of the computational domain along the Ox_1 axis.

For the stopping criteria of the conjugate gradient algorithms used in our computations we have taken $tol = 10^{-8}$. With this value of tol, for the small values of n, the discrete analogue of algorithm (4.62)–(4.81) requires, typically, 10 iterations to achieve convergence, but as the number of time steps increases the number of iteration falls rapidly at one. Similarly, as n

Table 1
Estimates of the L^2 and L^∞ approximation errors, the solution of reference being the one obtained at $t = 10$ with $I = 1024$, $J = 128$ and $\Delta t = \frac{1}{4}h_1^2$.

	Grids (I,J)	L^2	Order	L^∞	Order
u_1	(128,16)	1.72E−04		4.37E−02	
	(256,32)	4.32E−05	1.99	1.13E−02	1.95
	(512,64)	1.08E−05	2.00	2.79E−03	2.01
u_2	(128,16)	1.70E−04		4.09E−02	
	(256,32)	4.24E−05	2.00	1.05E−02	1.96
	(512,64)	1.05E−05	2.00	2.60E−03	2.01
ϕ	(128,16)	9.91E−05		6.82E−02	
	(256,32)	2.48E−05	2.00	1.73E−02	1.98
	(512,64)	6.19E−06	2.00	4.36E−03	1.99
p	(64,8)	8.87E−05		6.84E−02	
	(128,16)	3.05E−05	1.54	2.99E−02	1.19
	(256,32)	1.02E−05	1.58	1.30E−02	1.20

Table 2
Estimates of the L^2 and L^∞ approximation errors, with a fixed 512×64 grid for the velocity and phrase field and the solution of reference being the one obtained at $t = 50$ with $I = 1024$, $J = 128$.

	Δt	L^2	Order	L^∞	Order
u_1	1.44	4.04E−04		1.04E−01	
	0.72	2.05E−04	0.98	5.30E−02	0.97
	0.36	1.02E−04	1.00	2.65E−02	1.00
u_2	1.44	3.93E−04		9.74E−02	
	0.72	1.98E−04	0.99	4.94E−02	0.98
	0.36	9.92E−05	1.00	2.47E−02	1.00
ϕ	1.44	2.36E−04		1.63E−01	
	0.72	1.18E−04	1.00	8.28E−02	0.98
	0.36	5.88E−05	1.00	4.14E−02	1.00
p	1.44	3.33E−04		4.18E−01	
	0.72	1.85E−04	0.85	2.37E−01	0.82
	0.36	9.79E−05	0.92	1.26E−01	0.91

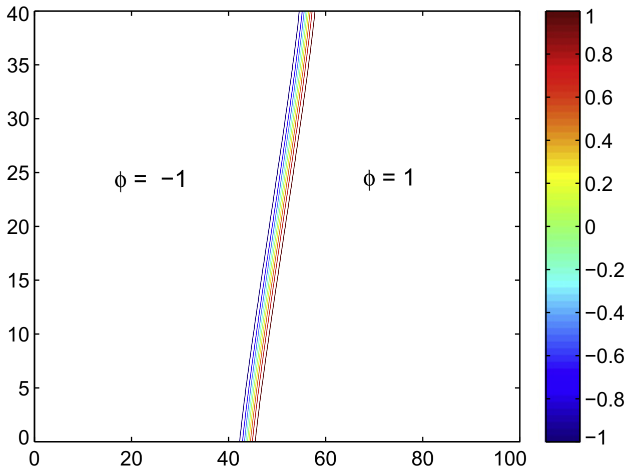

Fig. 2. Contour plot of the phase field ϕ.

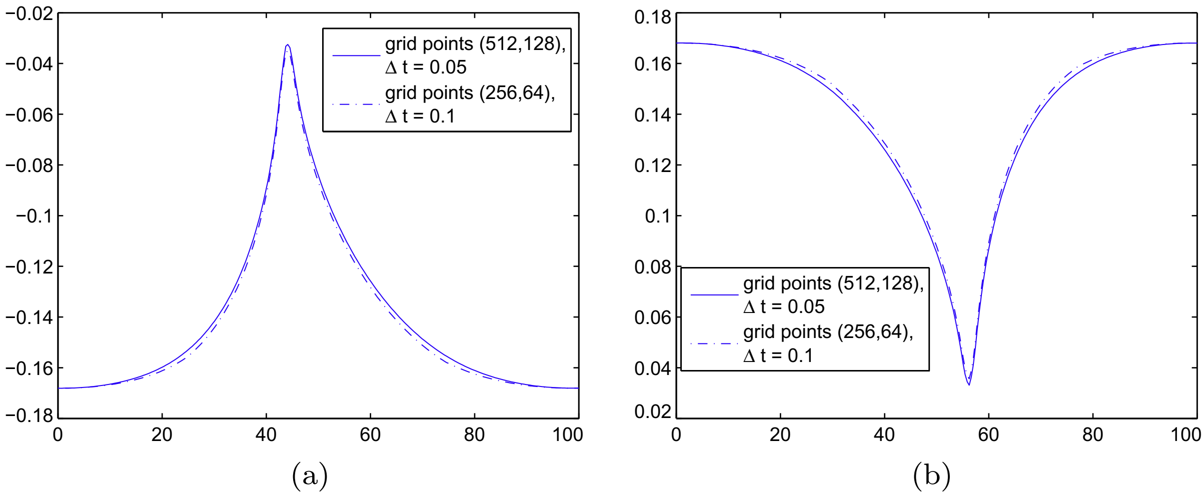

Fig. 3. Velocity u_1 along lower (left) and upper (right) boundaries.

increases, the number of iterations required by the discrete analogue of algorithm (6.8)–(6.22) falls rapidly at 4 as n increases. Of course, both algorithms have been initialized with the corresponding values at the previous time step.

In order to investigate the accuracy with respect to the space variables, that is of the finite element approximation briefly discussed in Section 8, we have compared at $t = 10$ the computed solutions obtained with $\Delta t = \frac{1}{4}h_1^2$ for various values of $h_1 = 100/I$ and $h_2 = 40/J$, the error is mainly due to spatial discretization. Since the exact solution is not known, we have taken as solution of reference the one obtained for $I = 1024$ and $J = 128$. The results have been reported in Table 1. To check the temporal convergence of the scheme, we have compared at $t = 50$ the numerical solutions obtained with a fixed 512×64 grid for various values of Δt. The results have been shown in Table 2.

Table 1 suggests near second order accuracy for the velocity and the phase field; it suggests also order 3/2 (resp., one) for the L^2 (resp., L^∞) norm of the pressure approximation error. Table 2 suggests first order accuracy in time, which is due to the scheme is first order operator-splitting scheme.

On Fig. 2, we have visualized the contours of the phase field, showing the sharp transition between the two phases. Indeed, the results in Fig. 2 are consistent with those visualized in Fig. 3 which show the strong variations of u_1 in the vicinity of the contact region (that is the region where the fluid–fluid interface intersects the solid wall). Clearly, Fig. 3 strongly suggests a large slip near the moving contact line. Actually, the results presented here match those reported in [19], obtained via a quite different computational method. For further validation, we have compared the results obtained at steady state (about $t = 100$), using on the one hand $I = 512$, $J = 128$ and $\Delta t = 0.05$, and on the other hand $I = 256$, $J = 64$ and $\Delta t = 0.1$; the results visualized on Fig. 3 show a very good agreement between these approximate solutions.

Finally, in order to verify that our numerical scheme verifies the stability properties predicted by Theorem 2 (see Section 7), we have reported on Fig. 4 the variations versus n of the energy FW^n defined by

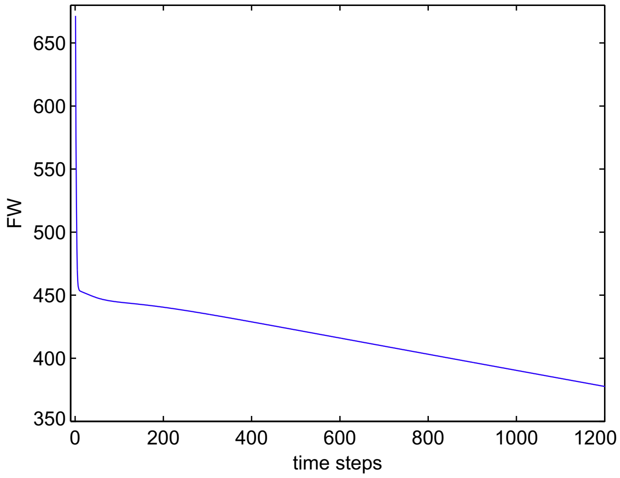

Fig. 4. Variation of the energy FW versus the number of time steps.

$$FW^n = BF_t(\phi^n) + \frac{1}{2}R\int_\Omega |\mathbf{u}^n|^2 dx + \Delta t \sum_{k=0}^{n-1} \int_{\partial\Omega} [\mathcal{L}_s(\phi^{k+1/2})]^{-1}(\mathbf{u}^{k+1} - \mathbf{u}_\mathbf{w}) \cdot \mathbf{u}_\mathbf{w} d(\partial\Omega).$$

If α and Δt verify the stability conditions (7.1) and (7.2), FW^n has to be a decreasing function of n. Those conditions being verified for $\alpha = 3$ and $\Delta t = 0.1$, we expect the decay of FW^n as n increases. Fig. 4 confirms this prediction.

10. Conclusion

In the above sections, we have discussed the numerical solution of the Navier–Stokes-Cahn–Hilliard system modeling the motion of the contact line separating two immiscible incompressible viscous fluids near a solid wall. The time discretization is achieved by a semi-implicit operator-splitting scheme with good stability properties, as shown by a stability analysis and by numerical experiments. These numerical experiments show good accuracy properties even for relatively larger time steps. We strongly believe that the efficiency of the methodology discussed here is largely due to the conjugate gradients algorithms used to treat both the Cahn–Hilliard and the Navier–Stokes components of the problems. Other ingredients contributing to the overall efficiency of the methodology discussed here are the variational formulations of the phase and flow sub-problems, making them well suited to finite element based solution methods.

Acknowledgments

QL He and XP Wang are supported in part by Hong Kong RGC-CERG Grants 603107 and 604209. QL He is supported in part by Youth Foundation of Sichuan University No 2010SCU11072. XPW is also supported in part by Award No SA-C0040/UK-C0016, made by King Abdullah University of Science and Technology (KAUST). R. Glowinski acknowledges the support of the Institute for Advanced Study (IAS) at The Hong Kong University of Science and Technology.

References

[1] B.P. Vollmayr-Lee, Fast and accurate coarsening simulation with an unconditionally stable time step, Phys. Rev. E 68 (8) (2003) 066703.
[2] E. Dean, R. Glowinski, T.-W. Pan, A wave equation approach to the numerical simulation of incompressible viscous fluid flow modeled by the Navier–Stokes equations, in: J.A. de Santo (Ed.), Mathematical and Numerical Aspects of Wave Propagation, SIAM, Philadelphia, 1998, pp. 65–74.
[3] E. Dean, R. Glowinski, D. Trevas, An approximate factorization/least-squares solution method for a mixed finite element approximation of the Cahn–Hilliard equation, Jpn. J. Ind. Appl. Math. 13 (3) (1996) 495–517.
[4] Y. Di, X. Wang, Precursor simulations in spreading using a multi-mesh adaptive finite element method, J. Comput. Phys. 228 (2009) 1380–1390.
[5] E.V.L. Mello, Numerical study of the Cahn–Hilliard equations in one, two and three dimensions, Phys. A 347 (2005) 429–443.
[6] D.J. Eyre, Unconditionally gradient stable time marching the Cahn–Hilliard equation, in: J. Bullard, R. Kalia, M. Stoneham, L.-Q. Chen (Eds.), Computational and Mathematical Models of Microstructural Evolution, The Materials Research Society, 1998a.
[7] D.J. Eyre, An unconditionally stable one step scheme for gradient systems, Unpublished article, 1998b.
[8] D. Furihata, Finite difference schemes for $\frac{\partial u}{\partial t} = \left(\frac{\partial}{\partial x}\right)^\alpha \frac{\delta g}{\delta u}$ that inherit energy conservation or dissipation property, J. Comput. Phys. 156 (1999) 181–205.
[9] D. Furihata, A stable and conservative finite difference scheme for the Cahn–Hilliard equation, Numer. Math. 87 (4) (2001) 675–699.
[10] R. Glowinski, Numerical Methods for Nonlinear Variational Problems, Springer, New York, NY, 1984.
[11] R. Glowinski, Finite element methods for incompressible viscous flow, in: Handbook of Numerical Analysis, vol. 9, North-Holland, Amsterdam, 2003, pp. 3–1176.
[12] R. Glowinski, G. Guidoboni, T.-W. Pan, Wall-driven incompressible viscous flow in a two-dimensional semi-circular cavity, J. Comput. Phys. 216 (1) (2006) 76–91.
[13] R. Glowinski, H.B. Keller, L. Reinhart, Continuation-conjugate gradient methods for the least squares solution of nonlinear boundary value problems, SIAM J. Sci. Stat. Comp. 4 (6) (1985) 793–832.
[14] Y. He, Y. Liu, T. Tang, On large time-stepping methods for the Cahn–Hilliard equation, Appl. Numer. Math. 57 (2007) 616–628.

[15] J.W. Choi, H.G. Lee, An unconditionally gradient stable numerical method for solving the Allen–Chan equation, Phys. A 388 (2009) 1791–1803.
[16] J. Koplik, J.R. Banavar, J.F. Willemsen, Molecular dynamics of poiseuille flow and moving cantact lines, Phys. Rev. Lett. 60 (1988) 1282–1285.
[17] J. Koplik, J.R. Banavar, J.F. Willemsen, Molecular dynamics of fluid flow at solid surfaces, Phys. Fluids A 1 (1989) 781–794.
[18] Q. Du, Numerical analysis of a continuum model of phase transition, SIAM J. Numer. Anal. 28 (5) (1991) 1310–1322.
[19] T. Qian, X. Wang, P. Sheng, Molecular scale contact line hydrodynamics of immiscible flows, Phys. Rev. E 68 (2003) 016306.
[20] T. Qian, X. Wang, P. Sheng, Power-law slip profile of the moving contact line in two phase immiscible flows, Phys. Rev. Lett. 63 (2004) 094501.
[21] T. Qian, X. Wang, P. Sheng, A variational approach to the moving contact line hydrodynamics, J. Fluid Mech. 564 (2006) 333–360.
[22] R. Glowinski, Numerical Methods for Nonlinear Variational Problems, Springer, 2008.
[23] J. Shen, X. Yang, A phase-field model and its numerical approximation for two-phase incompressible flows with different densities and viscosities, SIAM J. Sci. Comput. 32 (3) (2010) 1159–1179.
[24] S.M. Wise, C. Wang, An energy-stable and convergent finite-difference scheme for the phase field crystal equation, SIAM J. Numer. Anal. 47 (3) (2009) 2269–2288.
[25] Z. Sun, A second-order accurate linearized difference scheme for the two-dimensional Cahn–Hilliard equation, Math. Comp. 64 (212) (1995) 1463.
[26] P.A. Thompson, W. Brinckerhoff, M.O. Robbins, Microscopic studies of static and dynamic contact angles, J. Adhesion Sci. Tech. 7 (1993) 535–554.
[27] P.A. Thompson, M.O. Robbins, Simulations of contact-line motion: slip and the dynamic contact angle, Phys. Rev. Lett. 63 (1989) 766–769.
[28] X. Wang, T. Qian, P. Sheng, Moving contact line on chemically patterned surfaces, J. Fluid Mech. 605 (2008) 59–78.
[29] X. Yang, J. Feng, C. Liu, J. Shen, Numerical simulation of jet pinching-off and drop formation using an energetic phase-field method, J. Comput. Phys. 218 (2006) 417–428.
[30] Z. Hu, S.M. Wise, Stable and efficient finite-difference nonlinear-multigrid schemes for the phase filed crystal equation, J. Comput. Phys. 228 (2009) 5323–5339.