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Efficient energy stable numerical schemes for a phase field moving contact line model

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ABSTRACT

In this paper, we present two efficient energy stable schemes to solve a phase field model incorporating moving contact line. The model is a coupled system that consists of incompressible Navier–Stokes equations with a generalized Navier boundary condition and Cahn–Hilliard equation in conserved form. In both schemes the projection method is used to deal with the Navier–Stokes equations and stabilization approach is used for the non-convex Ginzburg–Landau bulk potential. By some subtle explicit–implicit treatments, we obtain a linear coupled energy stable scheme for systems with dynamic contact line conditions and a linear decoupled energy stable scheme for systems with static contact line conditions. An efficient spectral-Galerkin spatial discretization method is implemented to verify the accuracy and efficiency of proposed schemes. Numerical results show that the proposed schemes are very efficient and accurate.

1. Introduction

Phase-field/diffuse-interface models, whose origin can be traced back to Rayleigh [29] and Waals [41], have become one of the major tools to deal with many dynamical processes in material/biological morphology, in particular, the multiphase fluid systems that we are interested in this paper. The typical phase field model can be described by either the Allen–Cahn equation (see Bray [2]) or the Cahn–Hilliard equation (Cahn and Hilliard, [4]) based on energetic variational approaches. 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. A particular advantage of the phase-field approach is that the derived models are usually well-posed nonlinear partial differential equations that satisfy thermodynamics-consistent energy dissipation laws, which makes it possible to carry out mathematical analysis and further design numerical schemes which satisfy corresponding discrete energy dissipation laws. Thus phase field models recently have been the subject of many theoretical and numerical investigations (cf., for instance, [5,8,12–14,19,21,24,31,33,35–38,43]).

When the fluid–fluid interface touches a solid wall, it creates a moving contact line (MCL) problem that exists in many physical processes, for instance, wetting, coating, painting, etc. In this situation, it is well-known that the no-slip boundary condition for the Navier–Stokes equations is no longer applicable, otherwise, a non-physical velocity discontinuity will occur

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at the MCL (see e.g. [9,10,26]). Simulations by Koplik et al. [22,23], Thompson and Robbins [39], among others, using Molecular Dynamics (MD) showed that nearly complete slip happens near the MCL. To investigate the complex behavior at MCLs, microscopic-macroscopic hybrid simulations were carried out by Hadjiconstantinou [17], Ren and E [30], etc. This approach is powerful but computationally expensive for macroscopic applications. On the other hand, a set of accurate boundary conditions for the MCL problem in the context of phase field model was derived by Qian et al. [27], where they proposed a general Navier boundary condition (GNBC) and a dynamic contact line condition for a macroscopic model consisting of the Navier–Stokes equations and the Cahn–Hilliard equation. An explicit numerical scheme, which dictates a very small time step, was used to solve the Cahn–Hilliard equation to compare the results with MD simulations.

Recently, several attempts were made to improve the numerical stability and efficiency of solving the Navier–Stokes and Cahn–Hilliard coupled system for MCL problems. In He et al. [18], the authors proposed an operator splitting method with a least-squares finite element method for one of the sub-steps. The authors of Dong [6] and Dong and Shen [7] constructed some decoupled schemes for systems with variable density, however they did not provide any theoretical proof of discrete energy law for the decoupled schemes with dynamic contact line conditions. In Gao and Wang [14,15], Salgado [31] and Aland and Chen [1], the authors developed some energy stable schemes for the moving contact line problem with constant and/or variable densities. However, their schemes require solving a coupled nonlinear system for the phase function and velocity.

In this paper, we consider a phase-field moving contact line model which is a conserved version of the model proposed by Qian et al. [27,28]. We construct two energy stable temporal schemes for this model. One is a linear coupled scheme for systems with dynamic contact line conditions, the other is a linear decoupled scheme for systems with static contact line conditions. We then implement a Fourier–Legendre Galerkin approximation to investigate the efficiency and accuracy for the two schemes.

2. A Navier–Stokes Cahn–Hilliard coupled model in conserved form

We consider the moving contact line dynamics of a two-phase incompressible, immiscible fluid in a physical domain denoted by Ω with boundary Γ. It is showed in [27,28] that this problem can be modeled by a Navier–Stokes Cahn–Hilliard coupled system (NSCH) with a general Navier boundary condition. A non-dimensional, conserved version of the system is given below.

Incompressible Navier–Stokes equations for hydrodynamics:

$$R(\boldsymbol{u}_t + \boldsymbol{u}\cdot\nabla\boldsymbol{u}) = \Delta\boldsymbol{u} - \nabla p - B\phi\nabla\mu, \tag{2.1}$$

$$\nabla\cdot\boldsymbol{u} = 0, \tag{2.2}$$

$$\boldsymbol{u}\cdot\boldsymbol{n} = 0 \quad \text{on } \Gamma, \tag{2.3}$$

$$l(\phi)(\boldsymbol{u}_\tau - \boldsymbol{u}_w) + \partial_n\boldsymbol{u}_\tau - BL(\phi)\nabla_\tau\phi = 0 \quad \text{on } \Gamma. \tag{2.4}$$

Cahn–Hilliard equation for the dynamics of phase variable:

$$\phi_t + \nabla\cdot(\boldsymbol{u}\phi) = M\Delta\mu, \tag{2.5}$$

$$\mu = -\varepsilon\Delta\phi + f(\phi), \tag{2.6}$$

$$\partial_n\mu = 0 \quad \text{on } \Gamma, \tag{2.7}$$

$$\phi_t + \boldsymbol{u}_\tau\cdot\nabla_\tau\phi = -\gamma L(\phi) \quad \text{on } \Gamma. \tag{2.8}$$

In the above system, the unknowns are: $\boldsymbol{u}$ – the fluid velocity, p – the pressure, ϕ – the phase-field variable, μ – the chemical potential. The function $L(\phi)$ in Eq. (2.8) is given by

$$L(\phi) = \varepsilon\partial_n\phi + g'(\phi), \tag{2.9}$$

where $g(\phi)$ is the boundary interfacial energy; $l(\phi)\geq 0$ is a given coefficient function; the function $f(\phi) = F'(\phi)$, with $F(\phi)$ being the Ginzburg–Landau bulk potential. More precisely, F and g are defined as

$$F(\phi) = \frac{1}{4\varepsilon}\left(\phi^2-1\right)^2, \qquad g(\phi) = -\frac{\sqrt{2}}{3}\cos\theta_s\sin\left(\frac{\pi}{2}\phi\right), \tag{2.10}$$

where θ_s is the static contact angle. In Eqs. (2.1)–(2.9), bold face letters denote vector variables, ∇ denotes the gradient operator, $\boldsymbol{n}$ is the outward normal direction on boundary Γ, scalar operator $\partial_n = \boldsymbol{n}\cdot\nabla$ is the partial derivative along direction $\boldsymbol{n}$, τ is the boundary tangential direction, and vector operator $\nabla_\tau = \nabla - (\boldsymbol{n}\cdot\nabla)\boldsymbol{n}$ is the gradient along tangential direction, $\boldsymbol{u}_w$ is the boundary wall velocity, $\boldsymbol{u}_\tau$ is the boundary fluid velocity in tangential direction. From (2.3), we have $\boldsymbol{u} = \boldsymbol{u}_\tau$ on boundary Γ.

There are six non-dimensional parameters in this system. R is the Reynolds number, B denotes the strength of the capillary force comparing to the Newtonian fluid stress, M is the mobility coefficient, γ is a boundary relaxation coefficient, $l(\phi)$ is the ratio of domain size to boundary slip length, ε is the ratio between interface thickness and domain size. Similar