Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 318 (2017) 1005–1029
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Linear and unconditionally energy stable schemes for the binary fluid–surfactant phase field model

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Received 11 December 2016; received in revised form 3 February 2017; accepted 7 February 2017
Available online 22 February 2017

Highlights

- We use the "Invariant Energy Quadratization" approach to transform the free energy functional into an equivalent, quadratic form by introducing new variables. Based on the reformulated system, we develop a first and a second order semi-discretized scheme in time for the system, in which all nonlinear terms are treated semi-explicitly.
- The resultant semi-discretized schemes consist of a linear elliptic equation system at each time step, where the coefficient matrix operator is symmetric positive definite and thus the system can be solved efficiently. We further prove that the proposed schemes are unconditionally energy stable, i.e. thermodynamically consistent in the discrete case.
- Convergence test together with 2D and 3D numerical simulations are presented after the semi-discrete schemes are fully discretized in space using the Fourier-Spectral method to demonstrate the stability and the accuracy of the proposed schemes.
- Moreover, the new schemes are the first such *linear* and *accurate* schemes with *unconditional energy stability* for the nonlinear coupled multivariate model.

Abstract

In this paper, we consider the numerical solution of a binary fluid–surfactant phase field model, in which the free energy contains a nonlinear coupling entropy, a Ginzburg–Landau double well potential, and a logarithmic Flory–Huggins potential. The resulting system consists of two nonlinearly coupled Cahn–Hilliard type equations. We develop a first and a second order time stepping schemes for this system using the "Invariant Energy Quadratization" approach; in particular, the system is transformed into an equivalent one by introducing appropriate auxiliary variables and all nonlinear terms are then treated semi-explicitly. Both schemes are linear and lead to symmetric positive definite systems in space at each time step, thus they can be efficiently solved. We further prove that these schemes are unconditionally energy stable in the discrete sense. Various 2D and 3D numerical experiments are performed to validate the accuracy and energy stability of the proposed schemes.

Keywords: Phase-field; Fluid-surfactant; Cahn–Hilliard; Energy stability; Ginzburg–Landau; Flory–Huggins

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http://dx.doi.org/10.1016/j.cma.2017.02.011
0045-7825/

1. Introduction

Surfactants are some organic compounds that can reduce the surface tension of the solution and allow for the mixing of immiscible liquids. A typical well-known example of immiscible liquids is the mixture of oil and water. There are many studies on modeling and numerical simulations for investigating the binary fluid–surfactant system. In the pioneering work of Laradji et al. [1,2], the diffuse interface approach, or called the phase field method, was first used to study the phase transition behaviors of the monolayer microemulsion system, formed by surfactant molecules. The phase field method is a well-known effective modeling and simulation tool to resolve the motion of free interfaces between multiple material components. About its recent developments in advanced algorithms and computational technologies, we refer to [3–21] and references cited therein.

A variety of binary fluid–surfactant phase field (BFS-PF) models had been well investigated in the past two decades, see [1,2,18,22–25]. In [1,2], two phase field variables are introduced to represent the local densities of the fluids, as well as the local concentration of the surfactant, respectively. There are two types of nonlinear energy terms in the model, including (i) the phenomenological Ginzburg–Landau (G–L) double well potential for the density variable to describe the phase separation behaviors of the fluid mixture, and (ii) the nonlinear coupling entropy term to ensure the high fraction of the surfactant near the fluid interface. Subsequently, the authors in [23] developed a modified model by adding an extra diffusion term and a G–L type potential for the concentration variable, in order to improve the stability. In [22] the logarithmic Flory–Huggins (F–H) potential was added in order to restrict the range of the concentration variable, while the nonlinear coupling entropy is essentially the same as that in [1,2,23]. A slightly different nonlinear coupling entropy was presented in [24], which could penalize the concentration to accumulate along the fluid interface. In [25], the authors further modified the model in [24] by adding the F–H potential for the local concentration variable as well.

Numerically, it is a challenging issue to develop unconditionally energy stable schemes to discretize the stiff nonlinear terms for the phase field type models, where the stiffness is originated from the thin interface thickness parameter. As a matter of fact, the simple fully-implicit or explicit type discretizations will induce very severe time step size constraint (called conditionally energy stable) on the interfacial width [26–28], so they are not efficient in practice. Many efforts had been done in this direction in order to remove this type of time step size constraint (cf. [10,26,27,29,29–51]). About these developed numerical techniques, we give a detailed discussion in Section 3. Moreover, we emphasize that the "unconditional" here only means the schemes have no constraints on the time step size from stability point of view. However, large time step size will definitely induce large errors in practice. This fact motivates us to develop more accurate schemes, e.g., the second order time stepping schemes while preserving the unconditional energy stability in this paper.

In addition to the stiffness issue from the interfacial width, we must notice that a particular specialty of the BFS-PF system is the strong *nonlinear couplings* between multiple phase field variables, that increases the complexity for algorithm developments to a large extent. Therefore, although a variety of phase field fluid–surfactant models had been developed for over twenty years, there are very few successful attempts in designing efficient and energy stable schemes for them. Recently, in [52], Gu et al. had developed a first order in time, nonlinear scheme to solve a particular BFS-PF model developed in [24,25] based on the convex splitting approach, where the convex part of the free energy potential is treated implicitly while the concave part is treated explicitly. Except an assumption that the approximate solutions always (accidentally) sit inside the domain of the logarithmic functional (such an assumption is often hard to hold in practical simulations), their arguments about the convex–concave decomposition for the coupling potential are not valid as well since it is not sufficient to justify the convexity of a function with multiple variables from the positivity of second order partial derivatives. In addition, their scheme is only of first order in time, and its computational cost is relatively expensive due to the nonlinear nature.

Therefore, in this paper, the main purpose is to develop some more efficient and effective numerical schemes to solve the particular BFS-PF model that had been developed in [24,25] since this model is a typical representative of nonlinearly coupled multivariate fluid–surfactant models. We expect that our schemes can combine the following three desired properties, i.e., (i) *accurate* (second order in time); (ii) *stable* (the unconditional energy dissipation law holds); and (iii) *easy to implement and efficient* (only need to solve some fully *linear* equations at each time step). To achieve such a goal, instead of using traditional temporal discretization approaches like simple implicit, stabilized explicit, convex splitting, or other various tricky Taylor expansions to discretize the nonlinear potentials, we adopt the so-called *Invariant Energy Quadratization* (IEQ) method, which is a novel approach and had been successfully applied for other gradient flow models with various nonlinear potentials in the author's recent work (cf. [39,53–58]).