Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 326 (2017) 144–174
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Mass conservative and energy stable finite difference methods for the quasi-incompressible Navier–Stokes–Cahn–Hilliard system: Primitive variable and projection-type schemes

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Received 26 February 2017; received in revised form 8 August 2017; accepted 11 August 2017
Available online 18 August 2017

Highlights

- Two novel staggered grid finite difference methods are provided.
- Discrete mass conservation is naturally satisfied due to the discretization.
- Energy stability is achieved at the fully discrete level for both methods.
- An efficient nonlinear multigrid solver is designed for solving the two methods.

Abstract

In this paper we describe two fully mass conservative, energy stable, finite difference methods on a staggered grid for the quasi-incompressible Navier–Stokes–Cahn–Hilliard (q-NSCH) system governing a binary incompressible fluid flow with variable density and viscosity. Both methods, namely the primitive method (finite difference method in the primitive variable formulation) and the projection method (finite difference method in a projection-type formulation), are so designed that the mass of the binary fluid is preserved, and the energy of the system equations is always non-increasing in time at the fully discrete level. We also present an efficient, practical nonlinear multigrid method – comprised of a standard FAS method for the Cahn–Hilliard equation, and a method based on the Vanka-type smoothing strategy for the Navier–Stokes equation – for solving these equations. We test the scheme in the context of Capillary Waves, rising droplets and Rayleigh–Taylor instability. Quantitative comparisons are made with existing analytical solutions or previous numerical results that validate the accuracy of our numerical schemes. Moreover, in all cases, mass of the single component and the binary fluid was conserved up to 10^{-8} and energy decreases in time.

Keywords: Energy stability; Staggered finite differences; Multigrid; Binary fluid flow; Variable density; Phase-field method

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http://dx.doi.org/10.1016/j.cma.2017.08.011

1. Introduction

Phase-field, or diffuse-interface models [1,2], have now emerged as a powerful method to simulate many types of multiphase flows, including drop coalescence, break-up, rising and deformations in shear flows [3–8], contact line dynamics [9–11], thermocapillary effects [12,13], and tumor growth [14,15]. Phase-field models are based on models of fluid free energy which goes back to the work of Cahn and collaborators [16,17]. The basic idea is to introduce a phase variable (order parameter) to characterize the different phases that vary continuously over thin interfacial layers and is mostly uniform in the bulk phases. Sharp interfaces are then replaced by the thin but nonzero thickness transition regions where the interfacial forces are smoothly but locally distributed in the bulk fluid. One set of governing equations for the whole computational domain can be derived variationally from the free energy, where the order parameter fields satisfy an advection–diffusion equation (usually the advective Cahn–Hilliard equations) and is coupled to the Navier–Stokes equations through extra reactive stresses that mimic surface tension.

The classical phase-field model, the Model H [18], was initially developed for simulating a binary incompressible fluid where components are density matched, and was later generalized for simulating binary incompressible fluids with variable density components [19–27], in which some models, however, do not satisfy the Galilean invariance or are not thermodynamic consistency. As the phase-field model can be derived through a variational procedure, thermodynamic consistency of the model equations can serve as a justification for the model. In addition, this approach ensures the model compatible with the laws of thermodynamics, and to have a strict relaxational behavior of the free energy, hence the models are more than a phenomenological description of an interfacial problem. Lowengrub and Truskinovsky [25] and Abels et al. [19] extended the Model H to a thermodynamically consistent model for variable density using two different modeling assumptions on the phase variable (mass concentration [25] or volume fraction [19]) and the velocity field (mass averaged [25] or volume averaged velocity [19]). Although the two models are developed to represent the same type of flow dynamics, the resulting equations have significant differences due to the underlying modeling choices. In particular, the quasi-incompressible NSCH model (q-NSCH) developed by Lowengrub and Truskinovsky [25] adopts a mass-averaged velocity, and the fluids are mixing at the interfacial region which generates the changes in density. Such a system was called quasi-incompressible, which leads to a (generally) non-solenoidal velocity field ($\nabla \cdot \boldsymbol{u} \neq 0$ but was given through the quasi-incompressibility condition) and an extra pressure term appears in the Cahn–Hilliard equation comparing to Model H. In the model of Abels et al. [19], a solenoidal (divergence-free) velocity field is obtained due to the volume-averaged mixture velocity modeling assumption. However the mass conservation equation of their model is modified by adding a mass correction term. Most recently, another quasi-incompressible phase-field model [28] was developed to study the binary fluid with variable density, where the volume fraction is employed as the phase variable leading to a different free energy.

Solving the q-NSCH model is quite a challenging problem. The CH equation is a fourth order nonlinear parabolic PDE, which contains an extra pressure term; the solution of the phase variable varies sharply through the thin diffuse-interface region where the velocity field is non-solenoidal; the variable density is a non-linear function of the phase variable; the NS and CH equations are strongly coupled, which further increases the mathematical complexity of the model and that makes it difficult to design provably stable numerical schemes. Recently, it has been reported that thermodynamic consistency can serve as not only a critical justification for the phase-field modeling, but also an important criterion for the design of numerical methods. When the thermodynamic consistency is preserved at the discrete level, it guarantees the energy stability of the numerical method and also the accuracy of the solution, especially for the case where a rapid change or a singularity occurs in the solution, such as occurs in non-Newtonian hydrodynamic systems [29,30]. Therefore it is highly desirable to design such an energy stable method for the q-NSCH model, which dissipates the energy (preserve thermodynamic consistency) at the discrete level. Many time-discrete or fully discrete level energy stable methods [24,30–34] have been presented for the other types of NSCH models for binary incompressible fluid with the solenoidal velocity field. However for the q-NSCH model presented by Lowengrub and Truskinovsky [25] or the other quasi-incompressible type models with the non-solenoidal velocity, relatively few time-discrete energy stable methods are available [3,27,35]. Very recently, a C^0 finite element method for the q-NSCH system with a consistent discrete energy law was presented by Guo et al. [3], where interface topological transitions are captured and the quasi-incompressibility is handled smoothly. At the fully discrete level, however, there are no available energy stable numerical methods for the q-NSCH model.

Another important criterion for the method design is to guarantee mass conservation of the binary incompressible fluid at the fully discrete level. Due to appearance of the diffusion term and numerical dissipation introduced in discretization of the convective term in the Cahn–Hilliard equation, the total mass of the binary fluid is usually not