Journal of Computational Physics 231 (2012) 5788–5804

Contents lists available at SciVerse ScienceDirect

Journal of Computational Physics

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

A time-stepping scheme involving constant coefficient matrices for phase-field simulations of two-phase incompressible flows with large density ratios

S. Dong *, J. Shen

Department of Mathematics, Purdue University, West Lafayette, IN 47907, United States

ARTICLE INFO

Article history:
Received 11 November 2011
Accepted 28 April 2012
Available online 18 May 2012

Keywords:
Phase field approach
Time stepping scheme
Spectral element method
Large density ratio
Cahn–Hilliard equation

ABSTRACT

We present an efficient time-stepping scheme for simulations of the coupled Navier–Stokes Cahn–Hilliard equations for the phase field approach. The scheme has several attractive characteristics: (i) it is suitable for large density ratios, and numerical experiments with density ratios up to 1000 have been presented; (ii) it involves only constant (time-independent) coefficient matrices for all flow variables, which can be pre-computed during pre-processing, so it effectively overcomes the performance bottleneck induced by variable coefficient matrices associated with the variable density and variable viscosity; (iii) it completely de-couples the computations of the velocity, pressure, and the phase field function. Strategy for spectral-element type spatial discretizations to overcome the difficulty associated with the large spatial order of the Cahn–Hilliard equation is also discussed. Ample numerical simulations demonstrate that the current algorithm, together with the Navier–Stokes Cahn–Hilliard phase field approach, is an efficient and effective method for studying two-phase flows involving large density ratios, moving contact lines, and interfacial topology changes.

1. Introduction

The essential idea of the (diffusive) phase field approach for two-phase flows is to use a phase field function to describe the two-phase system, and to replace the (sharp) fluid interface with a thin smooth transition layer (i.e. diffuse interface) connecting the two immiscible fluids. The phase field function varies continuously over the transition layer and is mostly uniform in the bulk phases. The concept of a diffuse interface can be traced back to Rayleigh [21] and van der Waals [28] over a century ago; see [1] for a review of related aspects.

Among different formulations of phase fields, the energetic variational formulation (see e.g. [18,17]) is particularly attractive. With this formulation, the two-phase flow is characterized by the free energy of the system. The Cahn–Hilliard [3] free energy is the most commonly used in this regard. The governing equations for the two-phase system can be derived by the classical procedure of Lagrangian mechanics based on the least action principle. They consist of a single unified incompressible Navier–Stokes equation for the entire flow domain, which includes phase field-dependent density/viscosity and a phase field-dependent force term representing the surface tension effect, coupled with the convective Cahn–Hilliard equation which describes the evolution of the phase field function.

* Corresponding author.
E-mail address: sdong@math.purdue.edu (S. Dong).

0021-9991/$ - see front matter © 2012 Elsevier Inc. All rights reserved.
http://dx.doi.org/10.1016/j.jcp.2012.04.041

The phase field-based approach exhibits favorable properties in several aspects compared to other related methods. For example, because this approach is physically motivated and the two-phase system is characterized by a free energy, different physical effects, such as complex rheology, can be accounted for by a suitable modification of the free energy. This appears to be a key advantage compared to other interface-capturing methods such as level set, volume of fluids and front tracking [19,23,22,27]. The phase field approach can also handle moving contact lines with ease because of the diffuse interface involved within [1,14], while for other approaches the moving contact line problem appears to be considerably challenging. This approach can also naturally capture morphological and topological changes of the interface such as breakup, coalescence and reconnection, and it employs a single unified set of governing equations formulated over the entire domain, which can be solved on a fixed grid in a purely Eulerian fashion.

When numerically simulating the coupled system of Navier–Stokes and Cahn–Hilliard equations, one faces several significant challenges. In particular, the case with large density ratio poses the foremost challenge. When the density ratio becomes very large (or very small) – for example, the air–water two phase system has a density ratio about 1000 – the commonly-used numerical schemes for incompressible Navier–Stokes equations face stability difficulties. Another main challenge is associated with the variable density and variable viscosity. Both the density and the viscosity change over time because they depend on the phase field function. Therefore, with usual formulations the coefficient matrices of the linear algebraic systems for the pressure and the velocity will be time-dependent. As a result, these coefficient matrices need to be re-computed every time step. This creates a severe bottleneck to the performance. Without a method to overcome this bottleneck, long-time production simulations will be severely hampered due to the high computational cost. A third challenge involves the couplings among the phase field function, the pressure, and the velocity. Algorithms that de-couple the computations of these variables would be highly preferred from the simulation perspective. Finally, somewhat unique to the spectral element (and also to finite element) type approach, which is our method of choice for spatial discretizations in this paper, the high spatial order (4th order) of the Cahn–Hilliard equation presents a special challenge, because derivatives of order two or higher does not exist in the discrete function space.

Largely owing to the difficulties posed by large density ratios, existing phase field simulations have been mostly confined to cases of matched density or small density ratios where a Boussinesq approximation can be used (which essentially uses a matched density for the two fluids); see e.g. [13,2,17,30,29,4,11,12]. The case with different densities for the two fluids is considered in a few studies with the phase field approach [16,5], which, however, all lead to linear algebraic systems with variable (time-dependent) coefficient matrices for the pressure and the velocity after discretization, resulting in a high computational cost. An energy-stable scheme has very recently been discussed in [26,25] with different fluid densities. The scheme results in a weakly coupled linear algebraic system for the velocity and the phase field function with variable coefficient matrices. However, most interestingly, only a Poisson equation needs to be solved for the pressure with this scheme, thanks to the adoption of a penalty formulation advocated by [8].

In this paper we present an algorithm for the phase field approach that overcomes the four aforementioned challenges. More specifically, the scheme is suitable for dealing with large density ratios, and numerical simulations with density ratios up to 1000 will be presented. The scheme involves only constant (time-independent) coefficient matrices for all flow variables, which can be pre-computed during pre-processing. This is a splitting scheme based on a velocity-correction type strategy (cf., for instance, [10,9]), and the computations for the pressure, velocity and the phase field are completely de-coupled. The difficulty caused by the high spatial order of the Cahn–Hilliard equation for spectral-element (and finite-element) type spatial discretizations is overcome by successively solving two Helmholtz type equations that are de-coupled from each other. Moreover, since the algorithm is based on a velocity-correction formulation, the usual inf-sup condition is not required and equal-order approximations for the velocity and pressure can be employed (cf. [9]).

The presented algorithm will be useful not only to the phase field approach, but more generally also applicable to other interface-capturing methods such as level set, volume of fluids and front tracking. For example, the performance bottleneck caused by the time-dependent coefficient matrices associated with variable density/viscosity also exists in these other interface-capturing methods. The strategies presented herein will be useful also to those situations.

We will also present benchmark test results to demonstrate the physical accuracy of the Navier–Stokes Cahn–Hilliard phase-field model. The study of this aspect seems to be lacking in the current phase-field literature.

2. Algorithm for Navier–Stokes/Cahn–Hilliard coupled system

2.1. Navier–Stokes/Cahn–Hilliard coupled system

Let $\Omega \subset \mathbb{R}^d$ ($d = 2$ or 3) denote the flow domain, and $\Gamma = \partial\Omega$ denote the boundary of Ω. Consider a mixture of two immiscible, incompressible fluids contained in Ω. Let ρ_1 and ρ_2 respectively denote the densities of the two fluids, and μ_1 and μ_2 denote their dynamic viscosities. With the phase field approach, this two-phase system is described by the following coupled system of equations:

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla p + \nabla\cdot\left[\mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T)\right] - \lambda\nabla\cdot(\nabla\phi\otimes\nabla\phi) + \mathbf{f}(\mathbf{x},t), \tag{1a}$$

$$\nabla\cdot\mathbf{u} = 0, \tag{1b}$$