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3D phase-field simulations of interfacial dynamics in Newtonian and viscoelastic fluids

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ABSTRACT

This work presents a three-dimensional finite-element algorithm, based on the phase-field model, for computing interfacial flows of Newtonian and complex fluids. A 3D adaptive meshing scheme produces fine grid covering the interface and coarse mesh in the bulk. It is key to accurate resolution of the interface at manageable computational costs. The coupled Navier–Stokes and Cahn–Hilliard equations, plus the constitutive equation for non-Newtonian fluids, are solved using second-order implicit time stepping. Within each time step, Newton iteration is used to handle the nonlinearity, and the linear algebraic system is solved by preconditioned Krylov methods. The phase-field model, with a physically diffuse interface, affords the method several advantages in computing interfacial dynamics. One is the ease in simulating topological changes such as interfacial rupture and coalescence. Another is the capability of computing contact line motion without invoking ad hoc slip conditions. As validation of the 3D numerical scheme, we have computed drop deformation in an elongational flow, relaxation of a deformed drop to the spherical shape, and drop spreading on a partially wetting substrate. The results are compared with numerical and experimental results in the literature as well as our own axisymmetric computations where appropriate. Excellent agreement is achieved provided that the 3D interface is adequately resolved by using a sufficiently thin diffuse interface and refined grid. Since our model involves several coupled partial differential equations and we use a fully implicit scheme, the matrix inversion requires a large memory. This puts a limit on the scale of problems that can be simulated in 3D, especially for viscoelastic fluids.

1. Introduction

Interfacial dynamics is scientifically intriguing because of the coupling between hydrodynamics in the bulk and deformation of the interfaces. It is also taking on more practical significance with the recent technological advances in microengineering and miniaturization. For example, drop and bubble dynamics has been a key element in designing microfluidic devices [1], where the smaller length scales accentuates the interfacial forces. From a computational standpoint, the moving internal boundaries present a numerical challenge, and two classes of methods have been developed to meet it: interface

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tracking and interface capturing [2]. The former deploys grid points or markers on the interface that track it each time step [3–5]. The latter uses an auxiliary scalar field that distinguishes the fluid components. Thus, the onus of managing a moving grid is replaced by that of computing a convection or convection–diffusion equation for the scalar field, typically on an Eulerian grid. Each approach has its advantages and limitations.

The phase-field method to be discussed in this paper is an interface-capturing method. It is distinguished from other methods in its class by having a physical origin in a diffuse interface where the two fluid components mix to a limited extent and store a mixing energy. Thus, the phase-field parameter ϕ has a well defined physical meaning; its profile in the diffuse interface may be related to van der Waals-type of long range forces [6], and the mixing energy gives rise to interfacial tension [7]. Because of its energy-based formalism and the physical picture of the diffuse–interface model, it has some unique features among interface-capturing methods [8]: (i) The evolution of the interface is self-consistent and requires no ad hoc intervention such as the re-initialization in level set methods. (ii) The theory has an energy law that ensures well-posedness in numerical computation [9,10]. (iii) The variational framework easily integrates interfacial treatment and non-Newtonian rheology, as the latter is almost always derivable from a microstructural free energy [11]. (iv) It regularizes singular events on the interfaces such as breakup [12], coalescence [6] and moving contact lines [13,14].

In recent years, several groups have successfully applied the phase-field method to two-phase flow simulations [e.g. [7,15–18]]. These computations demonstrated that for the results to be quantitatively accurate, two conditions have to be met. First, the interface should be sufficiently thin so that the theoretical model approaches the so-called sharp-interface limit [19]. Second, this thin region must be adequately resolved by fine mesh; it typically requires some 10 grid points. Otherwise, the interfacial layer is subject to unphysical distortions, the interfacial tension is inaccurate and the results are unreliable. Thus, interfacial resolution is the bottleneck for phase-field computations. To address this issue, we have developed AMPHI, a finite-element algorithm on an unstructured grid that is adaptively refined and coarsened as the interface moves [20]. It has been applied so far to drop-interface partial coalescence [21], drop formation in microfluidic channels [12], cell motion in capillary [22], defect dynamics in nematic liquid crystals [23] and defect-mediated self-assembly of microdrops [24]. In particular, we have taken advantage of the variational formalism of the model to incorporate the non-Newtonian rheology of complex fluids.

With a few exceptions [e.g. [18,25]], prior phase-field computations are in 2D planar and axisymmetric geometries. In many situations, the two-dimensionality constitutes a serious drawback. Not only are there quantitative differences between 2D and 3D dynamics, as is expected, but they sometimes differ qualitatively. One example is the capillary instability of a thread in 3D contrasted with the stability of a 2D sheet. Besides, the most interesting feature of the physical problem might be accessible only in 3D. For instance, the stratified flow of two fluid components in a pipe is subject to distortion of the interface. A particularly intriguing phenomenon is viscous encapsulation, whereby the less viscous component encircles the more viscous one [26]. In this geometry, a lubrication approximation that ignores the variation along the axis of the pipe will decouple the shear of the primary flow and the secondary flow in the cross-section that would distort the interface [27]. Hence, viscous encapsulation in stratified Newtonian fluids can only be probed by fully 3D computations. Finally, applications to engineering problems will inevitably involve complex 3D geometries.

This work represents an extension of the two-dimensional AMPHI to a full 3D version AMPHI3D. It involves upgrading the solver and mesh generation modules to 3D, and properly integrating the two. In this paper, we will describe the theoretical models and computational algorithm, and present solutions of benchmark problems as validation. As before, we are especially interested in interfacial dynamics of complex fluids with non-Newtonian rheology. If our recent 2D computations illustrated the potential of the AMPHI algorithm, the 3D version promises a broader range of applications, with opportunities to explore intriguing physics in more complex problems.

2. Theory and numerical method

2.1. Diffuse interface model

The diffuse–interface method as applied to two-phase flows has been described by a number of authors [15,16,28]. Yue et al. [7,11] have shown how the model can be extended to non-Newtonian fluids, and developed the AMPHI algorithm in two dimensional geometries based on finite elements with adaptive meshing [20]. The main ideas of the 3D algorithm are close to those in 2D. In this section, we will briefly summarize these ideas and give the governing equations, using the mixture of a Newtonian and an Oldroyd-B fluid as an example. The method accommodates other types of complex fluids such as nematic liquid crystals [11,23,24,29,30], but we will confine this paper to Newtonian–Newtonian and Newtonian–Oldroyd-B mixtures.

Consider a Newtonian fluid in contact with an immiscible viscoelastic Oldroyd-B fluid. Their interface may intersect a solid wall to produce a three-phase contact line. The moving contact line presents a well-known stress singularity, and the diffuse interface provides a particularly attractive regularization scheme. Thus, we will include the contact line in the general formulation, and compute the spreading drop as one of the benchmark problems. In the diffuse interface framework, the Newtonian and Oldroyd-B components mix to some extent in a very thin interfacial region and store a mixing energy f_{mix}. In addition, each component interacts with the solid substrate with a fluid–solid surface energy f_w. An Oldroyd-B fluid is a dilute suspension of polymer chains, modeled as linear Hookean dumbbells, in a Newtonian solvent [31]. Thus, there is