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Efficient numerical methods for multiple surfactant-coated bubbles in a two-dimensional stokes flow

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ABSTRACT

We present efficient and highly accurate numerical methods to compute the deformation of surfactant-coated, two-dimensional bubbles in a slow viscous flow. Surfactant acts to locally alter the surface tension and thereby change the nature of the interface motion. In this paper, we restrict our attention to the case of a dilute insoluble surfactant. The convection–diffusion equation for the surfactant concentration on the interface is coupled with the Stokes equations in the fluid domain through a boundary condition based on the Laplace-Young condition. The Stokes equations are first recast as an integral equation and then solved using a fast-multipole accelerated iterative procedure. The computational cost per time-step is only $O(N \log N)$ operations, with N being the number of discretization points on the interface. The bubble interfaces are described by a spectral mesh and is advected according to the fluid velocity in such a manner so as to preserve equal arc length spacing of marker points. This equal arc length framework has the dual advantage of dynamically maintaining the spatial mesh and allowing efficient, implicit treatment of the stiffest terms in the dynamics. Several phenomenologically different examples are presented.

1. Introduction

Surface active agents (surfactants), whether present as impurities or deliberately added, critically alter the dynamics of multiphase flow systems. Surfactant molecules typically consist of hydrophilic heads and hydrophobic tails, and thus they tend to adhere to, and accumulate on, interfaces between fluids. Their impact is to locally lower the surface tension and thereby alter the dynamics, often critically. Important phenomenological effects that may be influenced by surfactant include bubble or droplet creation by tip streaming, cusp formation, and drop coalescence or breakup. Not surprisingly, surfactant can play an important role in many industrial and biomedical applications such as drug delivery, hydro-desulfurization of crude oil, polymer blending, paints and plastic production, emulsifications, or pulmonary functioning.

Computationally modeling these flows is very challenging. The interfacial surface tension depends on the surfactant concentration through a possibly-nonlinear equation of state. Nonuniform capillary (normal) and Marangoni (tangential) stresses are induced in the fluid, which significantly affects the deformation of the interface. The evolution equation for the surfactant concentration is stiff; surfactant diffuses by molecular mechanisms and is transported along the interface by fluid convection. There may be adsorption/desorption of interfacial surfactant to/from the bulk of the fluid. This evolution

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equation is coupled with the equations governing the fluid motion, and this coupling is highly nonlinear. The shape of the interface can become very complex: regions of high curvature might develop and/or topological changes may occur.

Numerically investigating the often-subtle phenomenological changes caused by the presence of surfactant (for example, whether a cusp forms in finite time, when and where surfactant caps form, the conditions required for tip streaming) clearly require a high degree of spatial and temporal accuracy. However, depending on the methods used, requiring higher accuracy may be achievable only at the expense of the size of problem that can be investigated. Even with significant advances in computer architecture, this trade-off continues to be negotiated. Recent examples in the literature support this point. Xu et al. [37] present a level set/immersed interface method for two-dimensional interfaces with insoluble surfactants. They present examples of up to four drops in a shear flow, with both a linear and nonlinear equation of state. Their methods include novel techniques to correct the characteristic loss of mass often seen in level set methods. However, even with these corrections, the change in drop area or surfactant mass can be up to 1%, with computational costs preventing the refinement needed for further accuracy. Integral equation methods are more amenable to numerical methods that can achieve high spatial accuracy, however, standard implementations [3,26] can be very costly to compute. Not surprisingly, interfaces are often left under-resolved. For example [26] reports numerical oscillations in the interface shape due to inadequate spatial resolution and in [3], quantities were conserved to only 0.5%. The linearity of the Stokes equations can be exploited by a variety of analytic techniques. Seigel and co-authors [31] use slender-body theory to examine the conditions required for tip streaming in a single axisymmetric bubble, presenting analytical results valid in certain regimes, only.

In this paper, we hope to provide motivation that when suitably chosen numerical methods are coupled with modern, fast, algorithms, it is possible to retain a high degree accuracy without sacrificing efficiency. Here, we present highly-accurate and efficient numerical methods for computing the motion of inviscid interfaces (bubbles) in a two-dimensional Stokes flow in the presence of an insoluble surfactant. We employ integral equation methods based on the complex variable theory for the biharmonic equation and further developed by Kropinski [16,17] for studying interfacial motion in a Stokes flow. The discretization of the integral equations is spectrally-accurate, and the iterative solution is accelerated by using the fast multipole method (FMM) [5,27] to compute the matrix–vector products. With N points in the discretization of the boundary, the integral-equation solve requires only $O(N)$ operations, versus standard implementations of iterative schemes (for example [20]) which require $O(N^2)$ operations. For the motion of the interface, we employ the ideas of Hou et al. [13] and recast the evolution equations into an equal arc length frame. In this manner, we are able to dynamically maintain marker points at equal arc length intervals. More importantly, we can easily remove the stiffness caused by the diffusion term in the surfactant transport equation, since an implicit treatment of this term becomes explicit in Fourier space. The dynamics, then, are amenable to efficient treatment by high-order, semi-implicit methods such as the IMEX Runge–Kutta methods discussed in [2].

There are a variety of other analytical and computational approaches, each having their unique advantages and disadvantages. Integral equation methods are a natural choice for Stokes flow, and we are by no means the first to adopt this approach (a non-exhaustive list includes [3,9,20,25,39]). In most of these studies, a cubic spline or a lower-order representation is used to describe the interface. Siegel [29,30] exploits the complex-variable theory for the biharmonic to derive analytical and semi-analytical methods (largely limited to studying a single bubble); these provide useful examples to verify other numerical methods. Methods that naturally handle topological changes (for example, drop breakup or coalescence) include level set and volume of fluid methods. For example, Xu et al. [37] use at a level set method to look at insoluble surfactants on droplets. Yang et al. [38] develop a hybrid level-set/front-tracking method to research interface problems for unstructured triangular grids. These methods are excellent for handling complicated, multi-component environments, but they tend to be low-order accurate. There has been recent work using the full Navier–Stokes equations [8,18,22]: however, these nascent studies are low-order accurate and simulations typically involve only a small number of bubbles or drops.

There are a number of limitations in the physical model we investigate here:

- It is in two-dimensions.
- We do not consider the case of droplets containing fluid of a different viscosity.
- We consider the case, only, of insoluble surfactant with a linear constitutive relation between surfactant concentration and surface tension (although a nonlinear relationship can easily be substituted for the linear one).
- We cannot deal with topological changes.

While the physical model is limited, we believe our methods are useful for two reasons. First, our techniques are highly accurate and they will serve as a useful benchmark for other methods that are developed to solve more complicated models. Second, we feel this paper serves as a preliminary step in demonstrating the philosophy that by coupling modern fast algorithms with well-conditioned integral equations, it is possible to develop highly accurate and efficient tools for investigation problems of scientific interest. While the problems presented in this paper may be of limited scientific scope, currently, the methods can and will be extended to include, for example, three-dimensions (the fast multipole method has already been adapted to handle the potentials associated with the Stokes equations in three-dimensions [35]) and/or drops with different viscosity ratios ([16] includes this effect, albeit in the clean flow case, only).

We begin in the next section by outlining the governing equations for inviscid interfaces in a Stokes flow and the convection–diffusion equation for an insoluble surfactant. We show how the two are coupled through the Laplace-Young condition and an equation of state that relates surface tension to surfactant concentration. In Section 3, we outline the