An explicit Eulerian method for multiphase flow with contact line dynamics and insoluble surfactant

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ABSTRACT

The flow behavior of many multiphase flow applications is greatly influenced by wetting properties and the presence of surfactants. We present a numerical method for two-phase flow with insoluble surfactants and contact line dynamics in two dimensions. The method is based on decomposing the interface between two fluids into segments, which are explicitly represented on a local Eulerian grid. It provides a natural framework for treating the surfactant concentration equation, which is solved locally on each segment. An accurate numerical method for the coupled interface/surfactant system is given. The system is coupled to the Navier–Stokes equations through the immersed boundary method, and we discuss the issue of force regularization in wetting problems, when the interface touches the boundary of the domain. We use the method to illustrate how the presence of surfactants influences the behavior of free and wetting drops.

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1. Introduction

Microfluidics has become a very active area of research in fluid mechanics. In this area flows at very small scales are considered, and at these scales the effects of surface physics become increasingly important due to the large surface to volume ratio. The systems involved include effects from wetting, surfactants and other phenomena, and a rapid expansion of research objectives in computational mechanics has taken place to encompass modeling of such systems.

This interest in microfluidics is to a large extent motivated by the development of microfluidic devices. Here, the ability to create and manipulate small bubbles, or vesicles, is essential. A well known example is the so-called "lab-on-a-chip" – a broad term for integrated microfluidic devices that aim to perform advanced chemical synthesis or analysis on a single chip. Experimental investigations include work by Anna and collaborators [3,4] on microfluidic topics.

One might expect that the *multi-physics* modeling required for microfluidic applications would mostly be a fairly straight-forward matter of coupling existing solvers for the constituent physical systems. This is however not the case, since these systems present many specific challenges such as fluid–fluid interfaces, strong capillary forces, interface-solid contact lines, non-Newtonian stress

models and additional physical considerations, such as heating and the presence of surfactants. Several computational studies have been performed that take some of these features into account.

In this article we will discuss various computational aspects of microfluidic simulations. We discuss *interface tracking* from the point of view of domain decomposition and argue that it is natural to think of on-interface modeling of e.g. surfactants in terms of calculus on manifolds. Additionally, we shall bring modeling of wetting and contact line dynamics to fore, and consider a system involving both contact line dynamics and surfactants. First, though, we survey the diverse areas that we are concerned with.

1.1. Surfactants

Flow problems involving surfactants have captured the attention of many physicists for decades. A basic observation is that the presence of surfactants changes the surface tension in free-surface flows, and hence, among other things, the way drops form, break up and coalesce.

An example of huge practical importance is detergents, though physical interest in surfactants is much broader. We already mentioned that many microfluidic applications involve manipulation of drops or bubbles on small scales. If this is to be done with high precision, one must naturally understand the effect the presence of surfactants has on these operations, and if it can be used to improve them. Furthermore, there appears to be genuine interest from the medical community in the role that surfactants play in

vascular disorders, such as decompression sickness, see e.g. [10,74].

It comes as no surprise, then, that there is large interest in computational microflows and simulation of flows involving surfactants. It is not uncommon that 2D models are quite sound in this context, though there are certainly many applications where a full 3D model is required to accurately describe the flow. Regardless of dimensionality, the main computational tasks are: (i) flow modeling (solving e.g. Stokes or Navier–Stokes equations), (ii) interface dynamics (i.e. representing and evolving dynamic interfaces), and (iii) surfactant modeling (i.e. how surfactant concentrations on the interface, and possibly in the bulk fluid, interacts with the rest of the system).

The first two tasks, collectively denoted multi-phase flow methods, have been studied computationally in a remarkable volume of work, as summarized in a recent review by Wörner [68]. Prominent surveys for each of the main families of methods are (level-set methods) Sethian and Smereka [55], (front-tracking) Tryggvason et al. [66], (volume fraction methods) Scardovelli and Zaleski [54] and (phase field methods) Anderson et al. [2]. The reader is assumed a certain familiarity with these methods.

Before the third task (surfactants) is considered, it is appropriate to note that the established interface-tracking methods, coupled to flow equations, pose numerical challenges which must be carefully considered. One issue has to do with time-stability, and originates from the coupling of flow equations to interface dynamics via the surface tension force, which is proportional to the interface curvature. This proportionality necessitates differentiation of the interface, and magnifies errors in models such as the Continuum Surface Force (CSF) model [9], which underpins level-set, front tracking and volume-fraction methods. Much effort has been devoted to addressing this issue and successful solution strategies now exist, see for example Ceniceros and Fisher [12] and Sussman and Ohta [60].

Another thing to point out is that interface representation imposes natural limitations. For instance, in level-set methods, the location of the interface is not known (as the method is implicit), and in front-tracking the interface is represented in a pointwise sense. These are two extremes that will pose distinct challenges to further modeling. There have been many attempts to marry the strengths of two methods (or eliminating notable drawbacks) in hybrid methods, such as the work by Sussman and Puckett [61,59], Aulisa et al. [5], Enright et al. [22], and Gaudlitz and Adams [24]. These methods add mathematical and practical complexity to already quite complicated methods. Sophisticated methods exist that treat interface jump conditions, such as variations on the Immersed Interface method (IIM) by LeVeque and collaborators [38,39,36], including level-set methods. Additional challenges arise in these methods – while they are seen as more accurate (no unphysical "smearing"), the aforementioned stability issues are more severe.

That is not to say that multi-phase simulations are intractable – to the contrary. Much work has gone into efficient implementations of these methods that produce very impressive computational results [35,56,43]. The preceding remarks aim to remind that, numerically and in basic modeling terms, multi-phase flow is still a field where the motivation for more research is large.

Proceeding to surfactants, the macroscopic model considers a concentration of surfactants *on* an interface that is governed by convection and diffusion. The basic coordinate-free equation is well known, (derived in plain terms by Wong et al. [67] following [57]),

$$\frac{D\rho}{Dt} + \rho(\nabla_s \cdot \mathbf{u}) = D_\Gamma \nabla_s^2 \rho. \tag{1}$$

Here, we simply note that we are dealing with a reaction–diffusion PDE on the interface which is non-linearly coupled to the interface

itself – see Section 3 for a complete statement. Additionally, when the surfactants are soluble, there can be a surfactant concentration in the bulk fluid and an exchange mechanism at the interface, see e.g. Jin et al. [29].

Of particular interest among recent work is the method by Muradoglu and Tryggvason [44]. We wish to highlight this as a valuable computational tool – the results they present, as well as subsequent work [43], clearly justifies this. Rather than being primarily a physical investigation, they set out to give a general computational method for axisymmetric cases that they then validate against theory and experiments. They build upon the well-established *finite difference/front-tracking* (FD/FT) method by Tryggvason et al. [66], and add the surfactant treatment (including soluble surfactants) as a bolt-on to the existing multiphase flow solver; the solver strategy is simply to interleave Euler-forward (first order) time steps of the interface, surfactants and flow. All time-stepping is first-order accurate, but the time step is constrained by stability to be $\Delta t \sim \Delta x^2$, because the diffusive term in the surfactant Eq. (1) is handled explicitly.

A method with many similarities is given by Zhang et al. [74], in a paper that predates Muradoglu and Tryggvason by about two years. It is, again, a front-tracking method for the axially symmetric case, where the emphasis is more clearly on an application – which is blood flow.

Implicit interface tracking methods have been extended to include surfactants on the interface, such as the level-set method by Xu et al. [69,70] and various VOF methods [52,28,19]. The main concern in such methods is conservation of surfactant; [69] is largely concerned with modifications that deal with this. Other implicit methods recently proposed include phase-field (Cahn–Hilliard) methods by Liu and Zhang [41] and Teigen et al. [62], as well as a "smoothed particle hydrodynamics" method by Adami et al. [1].

In the realm of viscous (Stokes) flow, a method for the full 3D problem was introduced early, namely the boundary-integral method by Yon and Pozrikidis [71]. Booty and Siegel [8] give a boundary integral method that couples to a method for solving a bulk surfactant transport–diffusion equation (in the limit of weak diffusion); and they are able to resolve a thin layer around the interface with large surfactant gradients.

1.2. Wetting and contact line dynamics

The intersection line of two immiscible fluids with a solid is called the contact line, which in two dimensions reduces to a contact point. Wetting generally refers to the case of a liquid–gas–solid system when the gas is displaced by the liquid, and hence the contact line is moving. Applications involving wetting and contact line dynamics appear in many industrial processes, both macroscopic (oil recovery, reactor cooling, coating) and microscopic (drop manipulation in lab-on-a-chip devices), and is clearly of great practical importance.

In the static case when the contact line is immobile, the equilibrium (or static) contact angle[1] θ_s formed between the fluid–fluid interface and the solid surface (cf. Fig. 1) is determined by Young's equation,

$$\sigma_1 - \sigma_2 - \sigma \cos \theta_s = 0, \tag{2}$$

which states that the surface tensions σ_1, σ_2, σ at the fluid–fluid and solid–fluid interfaces are in horizontal equilibrium when the contact line is at rest [16].

If the static case can be treated with relative ease; quite the opposite can be said about the dynamic case, when the contact line

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[1] In this work we consider only the apparent/macroscopic contact angle, see e.g. de Gennes [16] for an extensive treatment.