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An accurate integral equation method for simulating multi-phase Stokes flow

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ABSTRACT

We introduce a numerical method based on an integral equation formulation for simulating drops in viscous fluids in the plane. It builds upon the method introduced by Kropinski in 2001 [17], but improves on it by adding an interpolatory quadrature approach for handling near-singular integrals. Such integrals typically arise when drop boundaries come close to one another, and are difficult to compute accurately using standard quadrature rules. Adapting the interpolatory quadrature method introduced by Helsing and Ojala in 2008 [11] to the current application, very general drop configurations can be handled while still maintaining stability and high accuracy. The performance of the new method is demonstrated by some challenging numerical examples.

1. Introduction

There is a rapidly growing research area within fluid mechanics referred to as “micro-fluidics”, which is partly driven by the strong trend to miniaturize equipment for chemical analysis and synthesis. One emerging technology is “droplet micro-fluidics” in which an aqueous sample is emulsified into droplets and dispersed in a continuous oil phase [13,33]. At these small scales, viscous forces dominate, inertial effects are negligible, and the Reynolds numbers are very small. With pico-liter sized droplets, the surface to volume ratio is large, and the interface dynamics is becoming increasingly important.

Over the years, numerous numerical methods have been developed for the simulation of immiscible multiphase flow. In a sharp interface mathematical description of two immiscible fluids on the continuum level, the fluid–fluid interface is assumed to be infinitesimally thin. Surface forces are singularly supported on the interfaces separating the two fluids, leading to a discontinuity in pressure and velocity gradients across the fluid interfaces. Due to these difficulties, it still remains a challenge to perform highly accurate simulations of immiscible multiphase flow.

The dominant class of methods in the literature is what is often called interface tracking or interface capturing methods. In these methods, the Navier–Stokes or Stokes equations are solved on a computational grid or mesh, that is not required to conform to the fluid–fluid interfaces, and the interfaces are represented separately. Surveys of the main families of methods can be found in (Level-set methods) Sethian and Smereka [34], (Front-tracking) Tryggvason et al. [36] and (Volume of Fluid methods) Scardovelli and Zaleski [32].

The most commonly used approach of including the effect of the singular surface tension force in the fluid solver is to solve the Navier–Stokes equations with regularized surface tension force, an idea that was introduced for elastic interfaces by Peskin already in 1977 [27]. This smears the solution at the interface over a thin region, and velocities will never be

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better than first order accurate close to the interface, even if constructions based on specific choices of regularized delta functions can allow for higher orders of accuracy away from the interface [35].

In order to increase the accuracy close to the interface, methods that avoid regularization and instead directly enforce jump conditions at the interface have been developed, starting with the Immersed Interface (IIM) method [20] and the extended finite element (XFEM) method [6]. These methods can achieve second order accuracy, but issues remain, such as possible ill-conditioning in XFEM depending on how interfaces intersect the underlying grid. This remains an area of active research, with new promising ideas [37].

The Stokes equations for multiphase flow can be reformulated as boundary integral equations containing integrals over the fluid–fluid interfaces, see e.g. [2,26,28,41]. The above mentioned issues are then avoided – there is no underlying volume grid to couple to, jumps in solutions are naturally taken care of, and viscosity ratios between fluids enter only in coefficients of the equations.

When the Stokes equations are reformulated as boundary integral equations, the dimension of the equations and hence the number of unknowns in the discretized problem is reduced. The drawback is that these discretizations result in dense linear systems, making them very costly to solve. This can be addressed by the use of acceleration techniques such as either a fast multipole (FMM) method [9,38] or FFT-based methods [31,21,22].

Discretizations with a so-called Nyström method will be of high accuracy, given that the errors in the numerical integration are kept small. The integrands can however be weakly singular or singular and special quadrature is needed to obtain high accuracy. The case of *near singularity* occurs when the evaluation point is close to the interface but not on it, such as when it is located on an interface nearby. In Stokes flow, interfaces will get arbitrarily close, as the fluid layer between them can slowly drain, but they do not collide. For the singular case, a large gain in accuracy can be obtained by local modifications to a quadrature rule in the vicinity of the singularity [1,15,24], modifications that are specific to the class of singular functions that is considered. One can also introduce a mapping that removes the principal singularity, see e.g. [4]. Asymptotic expansions and singularity removal are used in a recent development for axisymmetric Stokes flow to design a quadrature rule that handles the singular integration [26]. These methods are however not applicable for nearly singular integrals. Mappings can however still be used even though they do not remove the singularity. A polar grid can be centered around the closest point on the surface of integration, possibly with a transformation to also cluster points in this area [4,14,39,40] to increase the accuracy of the quadrature. Another approach is to use an interpolatory procedure in addition to the singular integration to handle the nearly singular case [29,39]. Helsing and Ojala [11] have developed an interpolatory scheme that offers very high accuracy in the nearly singular case for the integral kernels of Laplace's equation in 2D. Another method for two-dimensional problems that offers an accuracy of second to third order in the grid spacing of the boundary curve can be found in [3] and yet another new and promising development is the so-called QBX method, designed for the 2D Helmholtz equation in [16].

In this paper we present a numerical scheme for simulating Stokes flow capable of handling very general drop configurations while maintaining high accuracy. We will use the integral equation formulation from Kropinski, [17], and by adapting the interpolatory quadrature introduced in [11], we are able to allow drops to be arbitrarily close to each other without losing stability or accuracy. This is the main novelty of the paper, and it allows for drop simulations that were previously infeasible.

The structure of this paper is as follows: in Section 2 we discuss the specific problem we are solving and introduce its integral equation formulation. In Section 3, we describe the interpolatory quadrature approach we will use, and in Section 4 we discuss the numerical method in some detail. In Section 5 we demonstrate how the solver performs for some drop configurations, and lastly, in Section 6 some options for future extensions of the solver are outlined.

2. Problem statement

Consider an infinite expanse of fluid in the plane with viscosity μ_0 containing n drops Ω_k with boundary Γ_k and viscosity $\mu_k = \lambda_k \mu_0$ for $k = 1, 2, \ldots, n$. The surrounding fluid resides in Ω_0. All viscosities are positive and we set Γ to be the union of all Γ_k (see Fig. 1). Assuming zero Reynolds number flow, the equations governing the flow are the Stokes equations

$$\mu_0 \Delta \mathbf{u}_0 = \nabla p_0, \quad \nabla \cdot \mathbf{u}_0 = 0, \quad \mathbf{x} \in \Omega_0, \tag{1}$$

$$\mu_k \Delta \mathbf{u}_k = \nabla p_k, \quad \nabla \cdot \mathbf{u}_k = 0, \quad \mathbf{x} \in \Omega_k, \quad k = 1, \ldots, n, \tag{2}$$

where $\mathbf{u}_0$ and p_0 is the velocity and pressure in the surrounding fluid and $\mathbf{u}_k$ and p_k is the velocity and pressure in drop k. In this paper, the flow will be driven by surface tension only, and we will assume that the n drops will not be in contact with each other, only with the surrounding fluid. The boundary conditions at the drop boundaries are therefore continuity of the velocity and a jump in normal stress proportional to the curvature. On the boundary of drop k we write this latter condition as

$$-(p_0 - p_k)\mathbf{n} + 2(\mu_0 \boldsymbol{\varepsilon}_0 - \mu_k \boldsymbol{\varepsilon}_k)\mathbf{n} = -\sigma \kappa \mathbf{n}, \tag{3}$$

where $\mathbf{n}$ is the outward unit normal, σ is the surface tension coefficient, κ is the curvature and $\boldsymbol{\varepsilon}$ is the 2×2 rate of strain tensor with elements

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right). \tag{4}$$