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Dynamic simulation of locally inextensible vesicles suspended in an arbitrary two-dimensional domain, a boundary integral method

Abtin Rahimian [a], Shravan Kumar Veerapaneni [b], George Biros [a,*]

[a] School of Computational Science and Engineering, College of Computing, Georgia Institute of Technology, Atlanta, GA 30332, United States
[b] Courant Institute of Mathematical Sciences, New York University, New York, NY 10003, United States

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ABSTRACT

We consider numerical algorithms for the simulation of hydrodynamics of two-dimensional vesicles suspended in a viscous Stokesian fluid. The motion of vesicles is governed by the interplay between hydrodynamic and elastic forces. Continuum models of vesicles use a two-phase fluid system with interfacial forces that include tension (to maintain local "surface" inextensibility) and bending. Vesicle flows are challenging to simulate. On the one hand, explicit time-stepping schemes suffer from a severe stability constraint due to the stiffness related to high-order spatial derivatives in the bending term. On the other hand, implicit time-stepping schemes can be expensive because they require the solution of a set of nonlinear equations at each time step.

Our method is an extension of the work of Veerapaneni et al. [S.K. Veerapaneni, D. Gueyffier, D. Zorin, G. Biros, A boundary integral method for simulating the dynamics of inextensible vesicles suspended in a viscous fluid in 2D, Journal of Computational Physics 228(7) (2009) 2334–2353], in which a semi-implicit time-marching scheme based on a boundary integral formulation of the Stokes problem for vesicles in an unbounded medium was proposed.

In this paper, we consider two important generalizations: (i) confined flows within arbitrary-shaped stationary/moving geometries; and (ii) flows in which the interior (to the vesicle) and exterior fluids have different viscosity. In the rest of the paper, we will refer to this as the "*viscosity contrast*". These two problems require solving additional integral equations and cause nontrivial modifications to the previous numerical scheme. Our method does not have severe time-step stability constraints and its computational cost-per-time-step is comparable to that of an explicit scheme. The discretization is pseudo-spectral in space, and multistep BDF in time. We conduct numerical experiments to investigate the stability, accuracy and the computational cost of the algorithm. Overall, our method achieves several orders of magnitude speed-up compared to standard explicit schemes.

As a preliminary validation of our scheme, we study the dependence of the inclination angle of a single vesicle in shear flow on the viscosity contrast and the reduced area of the vesicle, the lateral migration of vesicles in shear flow, the dispersion of two vesicles, and the effective viscosity of a dilute suspension of vesicles.

* Corresponding author.
E-mail addresses: rahimian@gatech.edu (A. Rahimian), shravan@ims.nyu.edu (S.K. Veerapaneni), gbiros@acm.org, biros@seas.upenn.edu (G. Biros).

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1. Introduction

Vesicles are closed lipid membranes suspended in a viscous medium. The mechanical deformation of vesicles and their interaction with viscous fluids are thought to play an important role in many biological phenomena [13,31] and are used experimentally to understand properties of biomembranes [30]. In addition, vesicle mechanics have been used as models for the motion of red and white blood cells [19,22], whose quantitative description will help in better understanding blood rheology.

In this article, we focus on numerical schemes for continuum models of vesicle dynamics. This is a challenging problem because the motion and shape of the vesicles must be determined dynamically from a balance of interfacial forces with fluid stresses. The shape dynamics of fluid vesicles is governed by the coupling of the flow within the membrane of the vesicle with the hydrodynamics of the surrounding bulk fluid. Following our previous work on vesicle flows [34], we present a semi-implicit numerical scheme for the simulation of the motion of arbitrarily shaped vesicles that can have a viscosity contrast with the background fluid. We also extend our formulation to handle interior flows and interaction of vesicles with other moving particles with prescribed motion.

Our method is based on an integral equation formulation. In particulate flow problems involving vesicles, the elastic and incompressibility properties of their membranes must be resolved and the numerical schemes must be modified in order to accommodate these properties and to solve the resulting set of equations. Details of the boundary integral formulation for elastic interfaces and incompressible vesicles can be found in the works of Pozrikidis [24,25].

The overwhelming majority of works on particulate flows uses explicit schemes that pose severe restrictions on the time step. In contrast, semi-implicit methods result in two to three orders of magnitude larger step size that is almost independent of the spacial grid size [34]. In contrast to stencil-based methods (e.g. finite element methods), integral equation formulations avoid discretization of the overall domain and instead discretize only the vesicle-boundary and the boundary of the enclosing domain. This is the main reason that integral equations have been used extensively for vesicle, and more generally, particulate and interfacial flow simulations [25].

1.1. Contributions

The boundary integral formulation coupled to the shape dynamics results in an integro-differential equation that is constrained by the local inextensibility. Extending our previous work [34], we use semi-implicit time-stepping, fast summation schemes, and spectral discretization in space. The combination of these approaches for flows with interface singularities is not unique. However, we are unaware of any previous analysis and application of implicit time-stepping schemes combined with fast solvers to vesicles that have a viscosity contrast with the surrounding fluid and are interacting with confined boundaries. These improvements enable the simulation a large number of interacting vesicles, as described in Sections 3 and 4, and depicted in Fig. 1.

The main contributions of this paper are:

- The extension of the techniques developed in [14,20,34] to vesicle flows in confined geometry and vesicles with viscosity contrast.
- The numerical investigation of the stability and accuracy of the time-stepping schemes.
- A preliminary validation of our methodology by comparing our numerical results to results in the literature.

In particular, for validation, we investigate (i) the dependence of vesicles' inclination angle in shear flow on viscosity contrast and reduced area; (ii) the lateral migration of vesicles in shear flow due to collision; and (iii) the rheology of a dilute suspension of vesicles.

1.2. Limitations

The most significant limitation of our method is that the number of Fourier modes used to represent the vesicle membrane and the time step are not chosen adaptively. The former is a minor limitation (in 2D) but the latter is quite significant. Our spectral discretization (which we combine with a special high-order scheme for singular integrals) in space [34] results in discretization errors that are dominated by the time-stepping scheme. In our experiments, 64–128 Fourier modes in space are typically sufficient to fully resolve the shapes of the vesicles in the flow regimes we have examined. For more concentrated suspensions, adaptive schemes combined with a posteriori estimates may be necessary.

We solve the discretized system of equations using the Generalized Minimum Residual Method (GMRES) [29] with an appropriate set of preconditioners, which are based on the spectral properties of the operators. Nonetheless, for very small viscosity contrasts $\nu \ll 1$ (see Table 1 for its definition), the spectral properties of the operators change and a generic preconditioner, as we use here, fails to fully compensate for the poor conditioning of the operators.

1.3. Related work

Vesicles are used, theoretically and experimentally, to investigate the properties of biological membranes [30], blood cells [19,22], and drug-carrying capsules [32].