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Boundary integral method for the flow of vesicles with viscosity contrast in three dimensions

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ABSTRACT

We propose numerical algorithms for the simulation of the dynamics of three-dimensional vesicles suspended in viscous Stokesian fluid. Our method is an extension of our previous work (S.K. Veerapaneni et al., 2011) [37] to flows with viscosity contrast. This generalization requires a change in the boundary integral formulation of the solution, in which a double-layer Stokes integral is introduced, and leads to changes in the fluid dynamics due to the viscosity contrast of the vesicles, which can no longer be efficiently resolved with existing algorithms.

In this paper we describe the algorithms needed to handle flows with viscosity contrast accurately and efficiently. We show that a globally semi-implicit method does not have any time-step stability constraint for flows with single and multiple vesicles with moderate viscosity contrast and the computational cost per simulation unit time is comparable to or less than that of an explicit scheme. Automatic oversampling adaptation enables us to achieve high accuracy with very low spectral resolution. We conduct numerical experiments to investigate the stability, accuracy, and the computational cost of the algorithms. Overall, our method achieves several orders of magnitude speed-up compared to the standard explicit schemes.

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1. Introduction

Vesicles are closed phospholipid membranes suspended in a viscous solution. They are found in biological systems, and play an important role in intracellular and intercellular transport. Artificial vesicles are used in a variety of drug-delivery systems and in the study of biomembrane mechanics. Vesicle-inspired mechanical models can be used to approximate red blood cell mechanics. For example, at equilibrium, vesicles and healthy red blood cells have a biconcave shape that corresponds to a minimal membrane bending energy. Under nonequilibrium conditions, as experienced in a simple shear flow, the best-studied features of red blood cell dynamics, such as tank-treading and tumbling motions, are shared with vesicles [5,17,20].

The vesicle evolution dynamics is characterized by an interplay between membrane's elastic energy, surface inextensibility, vanishing in-plane shear resistance, and non-local hydrodynamic interactions. Simulation of vesicles is a challenging nonlinear free boundary value problem, not amenable to analytical solutions in all but a few simple cases; numerical simulations and experiments are the only options for the quantitative characterization of vesicle flows.

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In this paper, we present algorithms for the simulation of three-dimensional vesicle flows with contrast between the viscosity of the suspending fluid and that of the fluid enclosed inside each vesicle. This work is an extension of our previous work presented in [37].

1.1. Overview and contributions

Our method is based on Galerkin formulation corresponding to Lagrangian tracking of spectral collocation points placed on the membrane of the vesicle. We represent the vesicles in the spherical harmonic basis. For weakly-singular integrals, we use the high-order scheme proposed by Graham and Sloan [14] that enables accurate simulations with a small number of degrees of freedom per vesicle, compared to low-order schemes. For the position update in time, we present variants of semi-implicit marching scheme first derived for advection–diffusion equations [2] and then applied to integral-equation based fluid–structure interaction problems in [35].

The time-marching scheme requires the solution to a linear system of equations at each time step, which we perform using a Krylov iterative method, GMRES [33]. The problem of poor conditioning is addressed by a preconditioner based on the analytically-obtained spectrum of the operators on a unit sphere [37].

The main contributions of this article are:

- *Efficient and accurate treatment of vesicles with viscosity contrast.* The flow of vesicles with viscosity contrast requires introduction of a double-layer Stokes integral with the velocity as the density (Eq. (3a)). The resulting system behaves differently from the equal-viscosity case. As the viscosity contrast of vesicles increases, they behave more like rigid bodies, which causes the vesicles to get very close to each other under certain flow conditions. Due to this proximity, explicit or block implicit methods become inaccurate and unstable (Table 4). We propose and analyze a global implicit scheme, in which the interaction of vesicles is treated implicitly (Section 3.4). We show that the stable time step for this scheme is orders of magnitude larger than the explicit scheme and its computational cost (per unit time) is superior to that of the explicit or block implicit schemes (Table 5).
- *Galerkin formulation.* We use a Galerkin formulation for the boundary integral solution. In [37], we used pseudo-spectral method, which has the same accuracy as the Galerkin method, but requires twice as many variables (the grid points) compared to spherical harmonic coefficients used in the Galerkin method and, unlike our Galerkin method, leads to overdetermined systems.
- *Characterization and reduction of aliasing in differentiation.* As our simulations involve differentiation and sampling of various functions (such as the force distribution on the surface) that may not be band-limited, aliasing may occur. Specifically, under-sampled high-frequency components may contribute to the low-frequency content of various fields we compute. In order to facilitate simulations with a low spherical harmonics' truncation order, we introduce an algorithm (Algorithm 1) which automatically adjusts the upsampling rate of functions for differentiation. In addition to this, we use reparametrization of the surface (Algorithm 3) from [37].

1.2. Limitations

We restrict our attention to suspensions of vesicles in unbounded domains. We have ignored inertial terms, so the overall method is restricted to low Reynolds numbers. Only vesicles with spherical topology are considered and topological changes are not allowed. By restricting our attention to spherical topologies, we can use spherical harmonics as basis and compute singular quadratures with spectrally accuracy. For general topologies one could, for example, use the boundary representation and singular integral quadrature introduced in [41]. For singular integrals, [41] relies on the partition of unity functions, whose derivative magnitudes rapidly increase with order, and as a consequence high-order methods require a relatively large number of points. Other approaches such as phase-field method [9,10] are more suited for handling changes in topology.

Another important limitation of our scheme is the lack of adaptivity (both in space and time). This lack of adaptivity manifests itself in the evaluation of nearly-singular integrals and can cause vesicle–vesicle collisions when the viscosity contrast is high. Indeed, one can easily construct simulations with high viscosity contrast where our algorithms fail to resolve inter-vesicle interactions accurately.

In this article, we use a first-order time-stepping scheme. High-order backward difference (BDF) schemes for 2D vesicle simulation were presented in [32,36]. Their extension to our work entails the undesirable backward propagation of the reparametrization to previous time steps. A more attractive option is the spectral deferred correction (SDC) method, presented in [29,30] for 2D vesicles, where high-order solutions are iteratively constructed using a first-order scheme and only requires the previous time step (as opposed to BDF). SDC is well suited for high-order, adaptive time stepping and leverages the Globally-Implicit first-order scheme presented here.

1.3. Related work

This work is an extension of [37] and we refer the reader to [37] for a review of the related work on three-dimensional simulation of vesicles. The work of Graham and Sloan [14] on singular quadratures for the scalar Helmholtz operator, the

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