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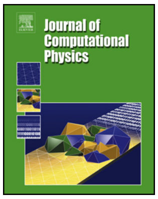

Low-resolution simulations of vesicle suspensions in 2D

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ABSTRACT

Vesicle suspensions appear in many biological and industrial applications. These suspensions are characterized by rich and complex dynamics of vesicles due to their interaction with the bulk fluid, and their large deformations and nonlinear elastic properties. Many existing state-of-the-art numerical schemes can resolve such complex vesicle flows. However, even when using provably optimal algorithms, these simulations can be computationally expensive, especially for suspensions with a large number of vesicles. These high computational costs can limit the use of simulations for parameter exploration, optimization, or uncertainty quantification. One way to reduce the cost is to use low-resolution discretizations in space and time. However, it is well-known that simply reducing the resolution results in vesicle collisions, numerical instabilities, and often in erroneous results.

In this paper, we investigate the effect of a number of algorithmic empirical fixes (which are commonly used by many groups) in an attempt to make low-resolution simulations more stable and more predictive. Based on our empirical studies for a number of flow configurations, we propose a scheme that attempts to integrate these fixes in a systematic way. This low-resolution scheme is an extension of our previous work [51,53]. Our low-resolution correction algorithms (LRCA) include anti-aliasing and membrane reparametrization for avoiding spurious oscillations in vesicles' membranes, adaptive time stepping and a repulsion force for handling vesicle collisions and, correction of vesicles' area and arc-length for maintaining physical vesicle shapes. We perform a systematic error analysis by comparing the low-resolution simulations of dilute and dense suspensions with their high-fidelity, fully resolved, counterparts. We observe that the LRCA enables both efficient and statistically accurate low-resolution simulations of vesicle suspensions, while it can be 10× to 100× faster.

1. Introduction

Vesicle suspensions are deformable capsules filled with and submerged in an incompressible fluid. Their simulation plays an important role in many biological applications [32,58], such as biomembranes [57] and red blood cells (RBCs) [19,29,40,43,49].

Here we discuss the numerical simulations of vesicle suspensions; specifically, algorithms that enable stable and accurate simulations at ***low-resolution spatio-temporal discretization***. Although many algorithmically optimal methods exist (see below), the costs remain prohibitively expensive for large vesicle suspensions. So, the basic question we try to address

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in this paper is the following. What is the minimum resolution required to recover different quantities of interest in the context of boundary integral equation methods for vesicle suspensions?

Understanding and improving low-resolution simulations will enable parametric studies and optimization (e.g., phase diagrams and design of microfluidic devices). Also many boundary integral equation codes use the empirical corrections we investigate here because convergence studies and high-resolution simulations are not possible. Further understanding these corrections and reducing the number of simulation parameters will be valuable for the community.

In our group, we have capability for both 2D and 3D simulations [51,55]. We have opted to study two-dimensional Stokesian suspensions since convergence studies in three dimensions for suspensions with a large number of vesicles can be extremely expensive [55]. In addition, two dimensional simulations are valuable on their own since they can reproduce experimentally observed flow physics in many regimes (e.g., motion of red blood cells in microchannels [13,29], margination of white blood cells in blood flow [12,13,17], and sorting of rigid particles and RBCs using deterministic lateral displacement technique [54,63,64]).

Background Vesicle flows are characterized by large deformations, local inextensibility of a vesicle's membrane, conservation of enclosed area due to the incompressibility of the fluid inside the vesicle, and stiffness related to tension and bending forces. These features make suspensions at low resolutions a challenging problem. In line with our previous work [51,52,55,59,60], and work of others [16,18,39,56,65–68], we use an integral equation formulation for the viscous interfacial flow [50]. Our previous results for simulating high-concentration vesicle suspensions in two dimensions [51,52] focus on accurate quadrature and high-order semi-implicit time stepping. The results in those papers rely on sufficient resolution and provide a robust framework for simulations. For example, vesicles do not collide because all hydrodynamic interactions are resolved with spectral accuracy. Thus, there is no need to introduce artificial repulsion forces between vesicles. We can accurately resolve long time horizon simulations for concentrated suspensions with roughly 96 or 128 points per vesicle. But in three dimensions such a resolution is prohibitively expensive. For example, a similar resolution using the 3D version of these algorithms [38] would require over 10,000 points per vesicle. Therefore, there is a need to use some empirical fixes to maintain stability in simulations, all the while accurately capturing the statistics of the underlying flow using as coarse discretization as possible. To measure the accuracy of the physics and statistics, we develop the algorithms in two dimensions so that we can compare with "ground truth" simulations performed at an adequate resolution. Demonstrating the effectiveness of these algorithms at low resolutions is the first step towards extending them to three dimensions.

Contributions Low-resolution simulations of vesicle suspensions can become unstable as a result of spurious oscillations in vesicles' shapes due to computing nonlinear terms, non-physical changes in vesicles' areas and arc-lengths, and vesicle collisions. We address these issues and develop a robust method by implementing some standard techniques and also introducing new schemes. We calibrate the parameters for these algorithms heuristically. We, then, investigate accuracy of our low-resolution simulations compared to the ground truth solutions. We also report the self-convergence of the low-resolution simulations without the ground truth. The numerical experiments help us develop a black-box solver that can capture underlying physics accurately using as coarse discretization as possible without having to adjust parameters other than the spatial and temporal resolution.

We summarize these contributions and our conclusions as follows:

- We introduce an efficient algorithm for determining an upsampling rate that is sufficient for controlling the aliasing errors caused by nonlinear terms, but not too large so that the computational costs are not unnecessarily inflated. Additionally, we formulate the reparametrization algorithm in [60] into two dimensions, which is necessary for low-resolution stability.
- Our previous adaptive time stepping work [53], which uses area-length errors in order to adjust the time step size, relied on asymptotic assumptions of the truncation error, which are not valid at the low resolutions. Since this result breaks down, we present a new variation of this scheme that can be used at all resolutions.
- A vesicle's area and arc-length are invariant in two-dimensional vesicle simulations (their counterparts are volume and surface area in the three-dimensional simulations). However, at low resolutions the errors can be extensive and hence result in unstable and non-physical flows in time scales much shorter than the target time horizons. Therefore, we present an efficient scheme to correct those errors without modifying the governing equations.
- Near-field (lubrication like) hydrodynamic interactions cannot be resolved accurately at low resolutions. This leads to non-physical collisions between vesicles. We detect collisions with spectral accuracy [51] and implement a short range repulsion force [23,62] to keep vesicles sufficiently separated. Unlike many other repulsion models requiring two parameters, our scheme is parameter-free, i.e., the repulsion length scale is set beforehand based on numerical experiments and the strength of the force is adaptive that guarantees no collision.
- We calibrate all the parameters of the LRCA heuristically and thereby develop a black-box solver with a single parameter. We test the solver in a real-world application of a microfluidic cell sorting device.