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A fast algorithm for simulating vesicle flows in three dimensions

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ABSTRACT

Vesicles are locally-inextensible fluid membranes that can sustain bending. In this paper, we extend the study of Veerapaneni et al. [S.K. Veerapaneni, D. Gueyffier, G. Biros, D. Zorin, A numerical method for simulating the dynamics of 3D axisymmetric vesicles suspended in viscous flows, Journal of Computational Physics 228 (19) (2009) 7233–7249] to general non-axisymmetric vesicle flows in three dimensions.

Although the main components of the algorithm are similar in spirit to the axisymmetric case (spectral approximation in space, semi-implicit time-stepping scheme), important new elements need to be introduced for a full 3D method. In particular, spatial quantities are discretized using spherical harmonics, and quadrature rules for singular surface integrals need to be adapted to this case; an algorithm for surface reparameterization is needed to ensure stability of the time-stepping scheme, and spectral filtering is introduced to maintain reasonable accuracy while minimizing computational costs. To characterize the stability of the scheme and to construct preconditioners for the iterative linear system solvers used in the semi-implicit time-stepping scheme, we perform a spectral analysis of the evolution operator on the unit sphere.

By introducing these algorithmic components, we obtain a time-stepping scheme that circumvents the stability constraint on the time-step and achieves spectral accuracy in space. We present results to analyze the cost and convergence rates of the overall scheme. To illustrate the applicability of the new method, we consider a few vesicle-flow interaction problems: a single vesicle in relaxation, sedimentation, shear flows, and many-vesicle flows.

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1. Introduction

Vesicles (also known as fluid membranes) 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 biomembrane mechanics. Vesicle-inspired mechanical models can be used to approximate red blood cell mechanics. For example, at equilibrium (i.e., in a quiescent fluid), 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 cell dynamics, formation of tank-treading ellipsoids and tumbling motion, are shared with vesicles [6,33,35].

The vesicle evolution dynamics is characterized by a competition between membrane elastic energy, surface inextensibility, vanishing in-plane shear resistance, and non-local hydrodynamic interactions. Simulation of vesicles is a challenging

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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.

In this paper, we present an algorithm for the simulation of general three-dimensional vesicle flows, extending our recent work on 2D [62] and 3D axisymmetric vesicles [61]. (To demonstrate the capabilities of our code, we depict a few time-snapshots from a 20-vesicle simulation in Fig. 1.)

To establish notation, we start with the standard PDE formulation of the problem:

$$
\begin{aligned}
& -\Delta \mathbf{v} + \nabla p = \mathbf{0} \quad \text{in } \mathbb{R}^3 \setminus \gamma \quad \text{(conservation of momentum in bulk fluid)},\\
& \operatorname{div} \mathbf{v} = 0 \quad \text{in } \mathbb{R}^3 \setminus \gamma \quad \text{(conservation of mass)},\\
& \operatorname{div}_\gamma \mathbf{v} = 0 \quad \text{on } \gamma \quad \text{(surface inextensibility)},\\
& [\![-p\mathbf{n} + (\nabla \mathbf{v} + \nabla \mathbf{v}^T)\mathbf{n}]\!] = \mathbf{f}_b + \mathbf{f}_\sigma \quad \text{on } \gamma \quad \text{(balance of momentum on the membrane)},\\
& \mathbf{v} - \mathbf{v}_\infty \to 0, \quad \text{if } \|\mathbf{x}\| \to \infty \quad \text{(far field condition)},\\
& \frac{\partial \mathbf{x}}{\partial t} = \mathbf{v} \quad \text{on } \gamma \quad \text{(membrane material point motion)}.
\end{aligned}
\tag{1}
$$

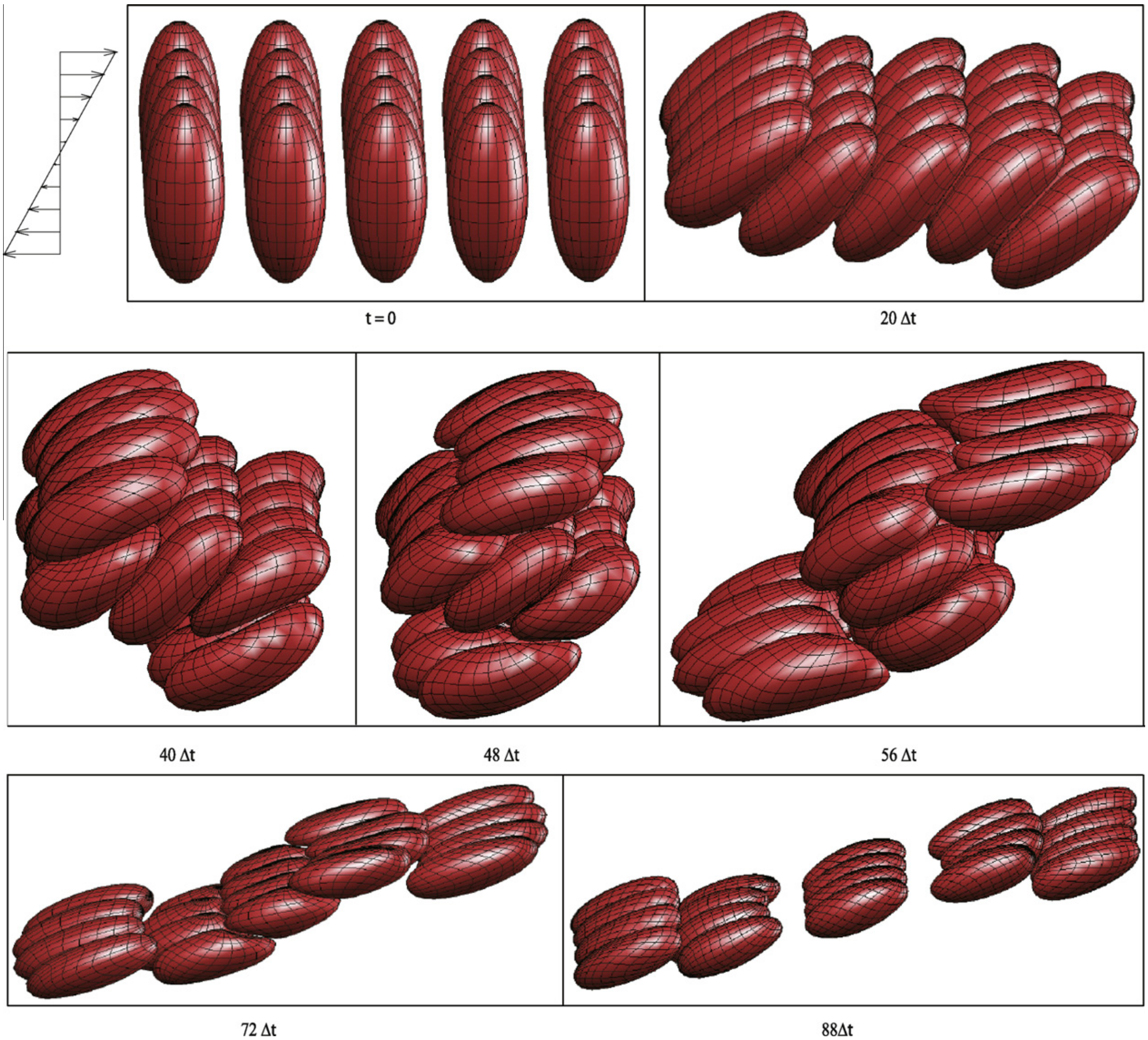

Fig. 1. Snapshots of 20 vesicles suspended in a simple shear flow with $\chi = 18$. Initially, each vesicle has a non-equilibrium 2–1 ellipsoidal shape and they are arranged in a rectangular lattice. The number of spatial discretization points is $338 (p = 12)$ and the average wall-clock time is 110 s per time-step on a 2.33 GHz Xeon workstation with 4 GB of RAM.

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