Numerical simulations of giant vesicles in more complex Stokes flows and discretization considerations of the boundary element method

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Quantifying the dynamics and rheology of soft biological suspensions such as red blood cells, vesicles, or capsules is paramount to many biomedical and computational applications. These systems are multiphase flows that can contain a diverse set of deformable cells and rigid bodies with complex wall geometries. For this thesis, we are performing several numerical simulations using boundary element methods (BEM) for biological suspensions in biomedically relevant conditions. Each simulation is devised to answer fundamental questions in modeling these systems.

Part of this thesis centers around the fluid mechanics of giant unilamellar vesicles (GUVs), fluid droplets surrounded by a phospholipid bilayer. GUVs are important to study because they mimic the dynamics of anuclear cells and are commonly used as a basis for artificial cells. The dynamics of vesicles in simple shear or extensional flows have been extensively studied. However the conditions seen in microfluidic devices or industrial processing are not always described by steady shear or extensional flows alone, and require more investigation. In our first study, we investigate the shape stability of osmotically deflated vesicles in a general linear flow (i.e., linear combinations of extensional and rotational flows). We modeled the vesicles as a droplet with an incompressible interface with a bending resistance. We simulated a range of flow types from purely shear to purely extensional at viscosity ratios ranging from 0.01 to 5.0 and reduced volumes (measured asphericity, higher is more spherical) from 0.60 to 0.70. The vesicle's viscosity ratio appears to play a minimal role in describing its shape and stability for many mixed flows, even in cases when significant flows are present in the vesicle interior. We find in these cases that the bending critical capillary number for shape instabilities collapse onto similar values if the capillary number is scaled by an effective extensional rate. These results contrast with droplet studies where both viscosity ratio and flow type have significant effects on breakup. Our simulations suggest that if the flow type is not close to pure shear flow, one can accurately quantify the shape and stability of vesicles

using the results from an equiviscous vesicle in pure extension. Only when the flow type is nearly shear flow, do we start to see deviations in the observations discussed above. In this situation, the vesicle's stationary shape develops a shape deviation, which introduces a stabilizing effect and makes the critical capillary number depend on the viscosity ratio.

Continuing with our research on single vesicle dynamics, we have performed simulations and experiments on vesicles in large amplitude oscillatory extensional (LAOE) flows. By using LAOE we can probe the non-linear extension and compression of vesicles and how these types of deformation affect dilute suspension microstructure in time-dependent flows through contractions, expansions, or other complex geometries. Our numerical and experimental results for vesicles of reduced volumes from 0.80 to 0.95 have shown there to be three general dynamical regimes differentiated by the amount of deformation that occurs in each half cycle. We have termed the regimes: symmetrical, reorienting, and pulsating in reference to the type of deformation that occurs. We find the deformation of the quasispherical vesicles in the microfluidic experiments and boundary element simulations to be in quantitative agreement. The distinct dynamics observed in each regime result from a competition between the flow frequency, flow time scale, and membrane deformation timescale. Using the numerical results, we calculate the particle coefficient of stresslet and quantify the nonlinear relationship between average vesicle stress and strain rate. We additionally present some results on the dynamics of tubular vesicles in LAOE, showing how the experiments suggest the vesicles undergo a shape transformation over several strain rate cycles. Broadly, our work provides new information regarding the transient dynamics of vesicles in time-dependent flows that directly informs bulk suspension rheology.

Our most recent project deals with the accuracy of discretized double layer integrals for Stokes flow in the boundary element method. In the fluid mechanics literature, the chosen parameterization, meshing procedure, and singularity handling are often selected arbitrarily or based on a convergence study where the number of elements is decreased until the relative error is sufficiently low. A practical study on the importance of each of these parameters to the accurate calculation of physically relevant results, such as the particle stresslet, could alleviate some of the guesswork required. The analytical formulas for the eigenfunctions/eigenvalues of the double layer operator of an ellipsoidal particle in a quadratic flow were recently published[1], providing an analytical basis for testing boundary element method discretization accuracy. We use these solutions to examine the local and global errors produced by changing the interpolation order of the geometry and the double-layer density. The results show that the local errors can be significant even when the global errors are small, prompting additional study on the distribution of local errors. Interestingly, we find that increasing the interpolation orders for the geometry and the double layer density does not always guarantee smaller errors. Depending on the nature of the meshing near high curvature regions, the number of high aspect ratio elements, and the flatness of the particle geometry, a piecewise-constant density can exhibit lower errors than piecewise-linear density, and there can be little benefit from using curved triangular elements. Overall, this study provides practical insights on how to appropriately discretize and parameterize three-dimensional (3D) boundary-element simulations for elongated particles with prolate-like and oblate-like geometries.

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[1] C. P. Martin, S. Wang, and S. Kim, “Surface tractions on an ellipsoid in stokes flow: Quadratic ambient fields,” Physics of Fluids, vol. 31, no. 2, p. 021 209, 2019.