Simulation and validation of surfactant-covered droplets in two-dimensional Stokes flow

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There is growing interest in micro-scale bubble and drop dynamics, fueled by development of miniaturized equipment in chemical and biological analyses. At the micro-scale, the Reynolds number is small and the flow is well described by the linear Stokes equations. Additionally, due to the large surface to volume ratio of small droplets, surface tension forces are prominent. Surface tension may be modified with the addition of surface reacting agents (surfactants), thus the transportation of surfactants is of great interest.

In this project, we simulate the deformation of droplets in flows described by the Stokes equations. The droplets are covered with insoluble surfactants, i.e. the surfactants reside only on the droplet-fluid interfaces. The evolution of the interfaces is computed with a boundary integral equation method that allows us to solve Stokes equations to high accuracy, also for drops in close proximity to each other. For boundary integral methods, the numerical errors typically grow large when evaluating velocities very close to the interfaces. We employ a specialized method for numerical integration to avoid these issues [1], and can obtain a high accuracy for our entire domain. A pseuo-spectral solver for the surfactant concentration is used, allowing us to solve for the surfactants with spectral accuracy. We couple the methods of interface movement and surfactant concentration in time. Care is taken in the adaptivity of the timesteps and we show it maintains accuracy both in drop deformation and surfactant evolution.

In the special case of imposed linear strain flow, our results are validated against available analytic results for bubbles [2]. We show agreement with the analytic results both for clean and surfactant-covered bubbles. Analytical results further predict coinciding bubble/drop shapes independent of viscosity ratio for the cases with surfactants, which we also obtain in our numerical simulations.

References

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