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Numerical methods for PDEs, Complex fluid dynamics simulations

The study of the incompressible flows with interfaces is of major interests among applied mathematics community. It plays an important role in numerous natural phenomena and industrial applications, especially, for the soft matter physics and hydrodynamics of micro-fluidic systems. We have successfully developed simple and efficient numerical schemes based on immersed boundary method for simulating fluid-surfactant and fluid-vesicle dynamics. Brief descriptions are as follows.

(I) **Interfacial flows with insoluble/soluble surfactant.** Surfactant are surface active agents that adhere to the fluid interface and affect the interface surface tension. Surfactant play an important role in many applications in the industries of food, cosmetics, oil, water purification , etc. In microsystems with the presence of interfaces, it is extremely important to consider the effect of surfactant since in such cases the capillary effect dominates the inertia of the fluids. We demonstrate the equilibrium for a hydrophobic drop with clean (dashed line) and contaminated interface (solid line) in Figure 1; the concentration distribution of a soluble droplet imposed to a flow is shown in Figure 2.

(II) **Vesicle hydrodynamics.** Vesicles dynamics in fluid flow has become a quite active research area recently in the communities of soft matter physics and computational fluid mechanics. Indeed, the understanding of vesicle behaviors in fluids might lead to a better knowledge of red blood cells in bloods since they both share some similar mechanical behaviors. It is well-known that the phospholipid membrane exhibits a resistance against area dilation and bending; therefore, it is natural to regard this membrane as an inextensible surface with mechanical properties defined by some energy functional. We have proposed a series of immersed boundary methods to simulate the dynamics of two- and three-dimensional inextensible vesicles in Navier–Stokes flows; for demonstration, the snapshots of a freely suspended vesicle in quiescent flow are shown in Figure 3.

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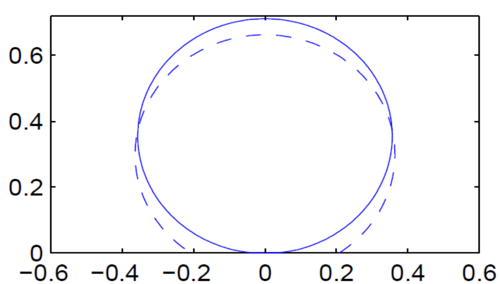

Figure 1

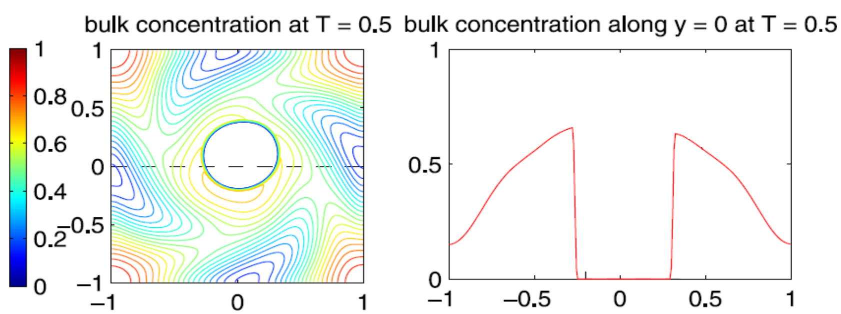

Figure 2

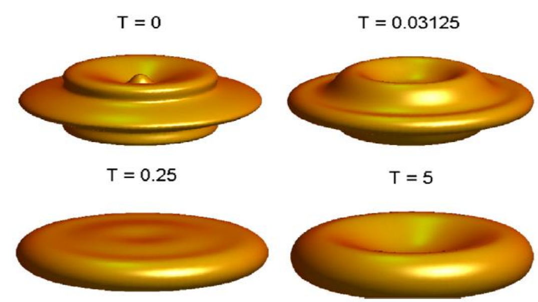

Figure 3