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Molecular-detailed simulation of red blood cells in Stokes flows[1]

ZHANGLI PENG, QIANG ZHU, UC San Diego — The red blood cell (RBC) membrane consists of a lipid bilayer and a cytoskeleton. By coupling a multiscale approach of RBC membranes with a boundary element method (BEM) for the exterior and interior fluids, we developed a numerical capacity to relate the fluid-structure interaction of RBCs in Stokes flows with detailed mechanical loads inside its molecular architecture. Our multiscale approach includes three models: in the whole cell level, a finite element method (FEM) is employed to model the lipid bilayer and the cytoskeleton as two distinct layers of continuum shells; the mechanical properties of the cytoskeleton are obtained from a molecular-based model; the spectrin, a major protein of the cytoskeleton, is simulated using a constitutive model. BEM is applied to predict the exterior and interior Stokes flows, and is coupled with the FEM of the membrane through a staggered coupling algorithm. Using this method, we simulated the tumbling and tank-treading behaviors of RBCs in shear flows, and investigated the RBC dynamics in capillary flows. The structural deformation of the cytoskeleton and the interaction force between the lipid bilayer and the cytoskeleton are predicted.

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