Abstract Submitted
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Brownian dynamics simulations of lipid bilayer membrane with hydrodynamic interactions in LAMMPS[1] SZU-PEI FU, YUAN-NAN YOUNG, New Jersey Institute of Technology, ZHANGLI PENG, University of Notre Dame, HONGYAN YUAN, University of Rhode Island — Lipid bilayer membranes have been extensively studied by coarse-grained molecular dynamics simulations. Numerical efficiencies have been reported in the cases of aggressive coarse-graining, where several lipids are coarse-grained into a particle of size $4 \sim 6$ nm so that there is only one particle in the thickness direction. Yuan *et al.* proposed a pair-potential between these one-particle-thick coarse-grained lipid particles to capture the mechanical properties of a lipid bilayer membrane (such as gel-fluid-gas phase transitions of lipids, diffusion, and bending rigidity). In this work we implement such interaction potential in LAMMPS to simulate large-scale lipid systems such as vesicles and red blood cells (RBCs). We also consider the effect of cytoskeleton on the lipid membrane dynamics as a model for red blood cell (RBC) dynamics, and incorporate coarse-grained water molecules to account for hydrodynamic interactions. The interaction between the coarse-grained water molecules (explicit solvent molecules) is modeled as a Lennard-Jones (L-J) potential. We focus on two sets of LAMMPS simulations: 1. Vesicle shape transitions with varying enclosed volume; 2. RBC shape transitions with different enclosed volume.

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