Abstract Submitted
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Stirring a Low Reynolds Number MARTINI[1] ANDREW ZGORSKI, EDWARD LYMAN, University of Delaware — Hydrodynamic interactions are an important component of lipid membrane dynamics. A proper molecular dynamics simulation of lateral diffusion in a membrane requires coupling to hydrodynamic flows in the surrounding solvent. In the low Reynolds number limit, the interactions mediated by these flows are long-ranged. When periodic boundary conditions are used with typical simulation sizes, these interactions lead to finite-size effects that inhibit diffusion. The system sizes required to adequately simulate lateral diffusion are computationally prohibitive when using explicit solvent models due to the number of pairwise solvent-solvent interactions. However, implicit solvent models entirely neglect hydrodynamic momentum transport. To remedy this, we have supplemented the Dry MARTINI implicit solvent model with an efficient mesoscopic particle-based hydrodynamic model called Stochastic Rotation Dynamics (SRD). Our implementation allows for fine control over fluid properties of the solvent, such as viscosity and Reynolds number, and includes a thermostat for the solvent that produces canonical energy fluctuations without interfering with the mesoscopic hydrodynamic flows.

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