

1163-45-1351

Rolf J Ryham* (rryham@fordham.edu), Fordham University, Department of Mathematics, JMH 401, Bronx, NY 10458, and **Szu-Pei Fu**, **Yuan-Nan Young** and **Bryan Quaife**. *Hydrodynamics of small unilamellar vesicles (sUVs) simulated using a hybrid approach*. Preliminary report.

In this talk we simulate the hydrodynamics of small unilamellar vesicles (sUVs) using a hybrid approach that is shown to capture the formation of sUVs in a solvent (SIAM J Multiscale Model. Simul., vol 18, pp. 79-103). In this hybrid formulation, the non-local interactions between the coarse-grained lipid molecules are described by a hydrophobicity functional, giving rise to forces and torques (between lipid particles) that dictate the motion of both particles and the fluid flow in the viscous solvent. Both the hydrophobic and hydrodynamic interactions between the coarse-grained amphiphilic particles are formulated into integral equations, which allow for accurate and efficient numerical simulations in both two- and three-dimensions. We validate our hybrid coarse-grained model by reproducing various physical properties of a lipid bilayer membrane, and use this simulation tool to examine how a small unilamellar vesicle behaves under a planar shear flow, and investigate the collective dynamics of sUVs under a shear flow. Finally we also examine the possibility of membrane rupture by extreme flowing conditions. (Received September 15, 2020)