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Formation of vesicles in a viscous solvent: A hybrid coarse-grain/continuum approach SZU-PEI FU, ROLF RYHAM, Fordham University, YUAN-NAN YOUNG, New Jersey Institute of Technology — In this talk a theoretical model for long-range, hydrophobic attraction between amphiphilic particles (such as lipid molecules) is developed to quantify the macroscopic assembly and mechanics of a lipid bilayer membrane in solvents. The non-local interactions between amphiphilic particles are obtained from the first domain variation of a hydrophobicity functional, giving rise to forces and torques (between 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. Such hybrid coarse-grained model is validated by its capability to reproduce various physical properties of a lipid bilayer membrane. Furthermore we present simulation results of vesicle formation in both a quiescent flow and a pressure driven flow (as in the microfluidic jetting experiments). Finally we also illustrate how our hybrid model can be generalized to investigate the effects of local charges on the bending rigidity of a lipid bilayer membrane.

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