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Coarse-grained model for lipid bilayer membranes and vesicles[1]
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We present a coarse-grained model for simulation studies of lipid bilayer membranes and vesicles. We separately track the behavior of the leaflets in each bilayer, allowing us to model the mechanics of vesicles and a rich array of other phases, topologies, and defect structures. Each particle in the coarse-grain model represents a patch of lipid molecules and carries a vector degree of freedom, representing the local average lipid chain orientation. Particles interact via a pair potential depending on separation distance and relative chain orientation. Solvent is treated as implicit, and membrane fluctuations are modeled via a Langevin thermostat. Resulting bilayer structures show liquid-like diffusion within each leaflet. We show that bilayer vesicles coalesce spontaneously from a random initial state, even though no spontaneous curvature is imposed by the model. We also explore the transition from vesicles to lamellar phases as a function of increasing density. We discuss potential application to the study of vesicle fission and fusion.

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