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Dynamic Coarse-grained Modeling of Lipid Bilayer Membranes

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A coarse-grained approach capturing features at the level of of individual lipid molecules is presented for the study of dynamic phenomena related to bilayer membranes. The model takes into account molecular interactions between lipids, hydrodynamic coupling, and thermal fluctuations. The model is parameterized to have bending elasticity, compression moduli, and shear viscosity comparable to experimentally studied bilayer membranes. To carry-out simulation studies using the model, new stochastic computational methods are introduced based on fluctuating hydrodynamics. Using this approach, specific simulation results are presented which characterize how molecular level interactions contribute to bilayer mechanics (stiffness, tension, compressibility), bilayer rheology (shear viscosity, normal stress differences), and the mobility of bilayer embedded particles (single and pair diffusivity tensors). Applications of the bilayer model and computational methods to problems in cell biology are also discussed.