Abstract Submitted
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Simulation of lipid bilayers using coarse grained methods MARK STEVENS, Sandia National Labs — There are many important biological processes involving lipid bilayers on times scales beyond that accessible by atomistic simulations. We have developed coarse-grained, bead-spring models of lipid molecules to treat membrane fusion, domain formation and the general physical characteristics of lipid bilayers. A key aspect of these coarse-grained models is that the liquid nature of a bilayer is explicitly present in the simulations; the lipids diffuse far beyond their neighbors in contrast to atomistic simulations. With these models self-assembly into a bilayer starting from a random configuration of lipids and solvent is readily simulated. We have performed extensive simulations to characterize these lipid models in single component lipid bilayers. For a variety of tail lengths, the area per lipid as a function of temperature has been calculated; the liquid-gel transition has been characterized. Models have been developed for a variety of lipids including double bonds in the lipid tails. Simulation results will be presented for fusion and domain formation.

Mark Stevens
Sandia National Labs

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