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Supplemental Information

Toward Hydrodynamics with Solvent Free Lipid Models: STRD Martini

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Supplemental Information: Toward hydrodynamics with solvent free lipid models: STRD MARTINI

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Supplemental Results.

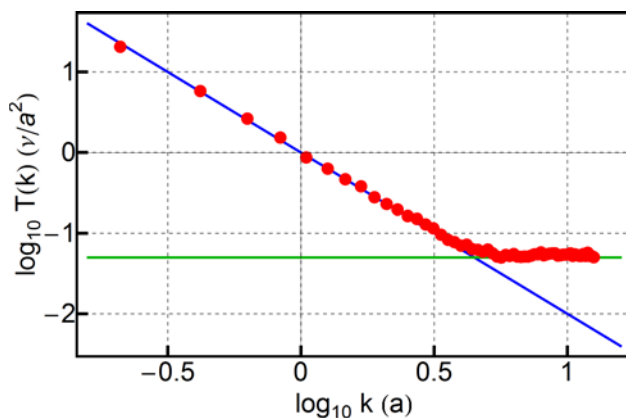


Figure S1. As demonstrated by Huang et al (32), transverse velocity correlations between SRD particles decay exponentially, and the time integrals $T(k,t)$ of the normalized correlation functions converge to values that depend only on the wavenumber. For small k , the $1/(vk^2)$ relationship resembles the Oseen tensor (blue). Below a certain length scale, $T(k)$ reaches a plateau equal to half the collision interval (green). This is the minimum length scale at which the SRD algorithm resolves hydrodynamics. For the parameters selected in this figure, the minimum length scale is 2.77 nm, or 1.39 times the size of a collision cell. Selected SRD parameters are $m = 72$ amu, $a = 2.0$ nm, $\tau = 200$ fs, $\alpha = 180^\circ$, and $N = 1 \text{ nm}^{-3}$.

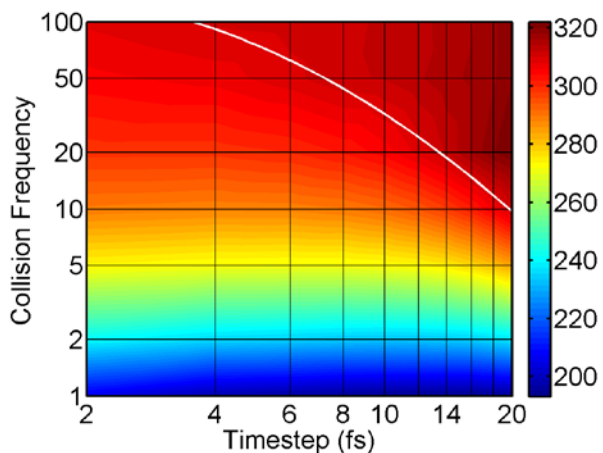


Figure S2. Applying a thermostat to only SRD particles leads to a difference in equilibrium temperature between the membrane and SRD fluid. When collisions occur too frequently, energy is removed from the membrane and dissipated in the SRD fluid by the thermostat. If the MD timestep and collision frequency are chosen with care, the temperature difference will vanish (white contour). Selected SRD parameters are $m = 72$ amu, $a = 1.0$ nm, $\alpha = 90^\circ$, and $N = 3.7$ nm⁻³. These simulations were performed using the direct MPC coupling method, but a similar result is found if the WCA coupling method is used.

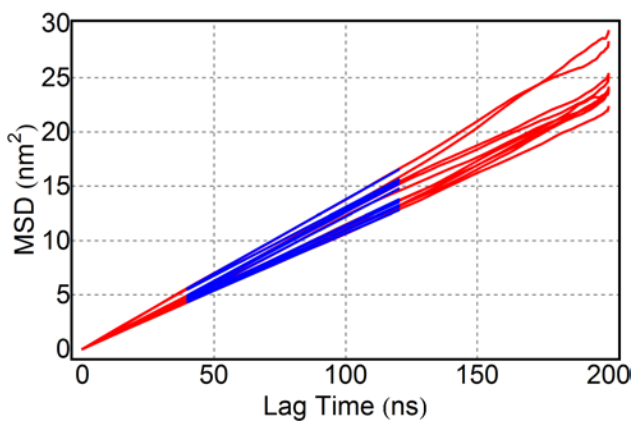


Figure S3. Example of independent fits to lipid mean squared displacements from nonoverlapping trajectory segments to obtain diffusion constants and error bars. Ten 200 nsec trajectory segments from a single 2000 nsec trajectory obtained at 0.47 cP are shown. The slope m of the red region was obtained by least squares and the diffusion constant estimated by $D = m/4$.