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Simulating liquid-liquid phase separation and lipid transport on the Anton special purpose machine EDWARD LYMAN, Department of Physics and Astronomy and Department of Chemistry and Biochemistry, University of Delaware, LOGAN SANDAR, Department of Physics and Astronomy, University of Delaware, ALEXADER SODT, RICHARD W. PASTOR, Laboratory of Computational Biology, National Heart, Lung, and Blood Institute — We present simulation data for a bilayer composed of a ternary mixture of cholesterol, dioloeoyl phosphatidylcholine and dipalmitoyl phosphatidylcholine. The composition is chosen to be in the two-phase region and the temperature in the vicinity of the miscibility transition. Using the Anton special purpose computer to generate continuous trajectories longer the ten microseconds—which admits complete mixing of the lipids—we observe robust liquid-liquid phase coexistence. The time-and ensemble-averaged mean squared displacement (MSD) displays anomalous scaling on timescales less than 50 nsec and normal diffusion on longer timescales. The short-time anomalous scaling is explained by a mode-coupling argument[Flenner et al Phys Rev E 79:011907(2009)]. The per-lipid MSD's suggest that a few lipids remain associated with the liquid ordered domain for the duration of the simulation, suggesting a possible mechanism for anomalous transport on experimentally accessible timescales.

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