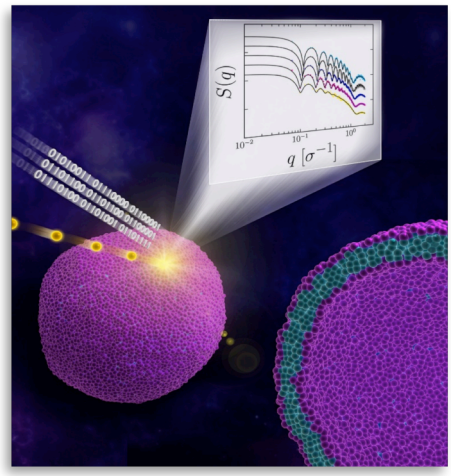
Bridging Simulations with Neutron Scattering Yields New Capabilities to Probe Lipid Bilayers

Achievement: Coarse-grained molecular dynamics calculations provide transformative capabilities to corroborate and extend neutron scattering studies of lipid bilayer membranes.



Schematic illustration of our new computational modeling capability for understanding dynamics of bilayer lipid membranes and for predicting neutron scattering results.

Significance and Impact: The ability to precisely probe the length and time scales that underlie ionic and molecular transport in lipid bilayers opens new opportunities to explore long-standing problems in membrane physics.

Research Details:

- Our protocol for coarse-grained molecular dynamics can accurately mimic neutron scatting experiments (SANS and NSE) on lipid bilayer membranes.
- This capability led to the discovery of additional dynamical modes corresponding to membrane thickness fluctuations.

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Overview:

This work demonstrates a coarse-grained MD simulation approach that mimics neutron scattering data from large unilamellar lipid vesicles over a range of bilayer rigidities. While experimental observations of membrane structure and dynamics are limited in both spatial and temporal resolution, computer simulations when appropriately quantified/calibrated are able to intimately resolve dynamics and structure, enabling accurate interpretation of experimental results and a detailed molecular understanding of complex lipid bilayer membranes. In particular, the synergy between neutron scattering experiments and molecular simulations offers opportunities for new discoveries in membrane physics, as the length and time scales probed by molecular dynamics (MD) simulations parallel those of experiments. Specifically, in this work we have simulated vesicle form factors and membrane thickness fluctuations determined from small angle neutron scattering (SANS) and neutron spin echo (NSE) experiments, respectively. Our simulations accurately reproduce trends from experiments and thereby lay the groundwork for studies of more complex membrane systems.