Deciphering nanometer scale heterogeneity in ordered lipid phases using molecular simulation and small angle neutron scattering

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Our lab is interested in lipid correlations at the nanometer scale, that is, below the scale of disordered and ordered domains. This information will provide valuable information for how bilayers respond to stresses, especially curvature. We apply molecular dynamics and neutron scattering. As we see it, molecular dynamics supplies complete information but absolutely requires validation, while neutron scattering provides accurate but heavily filtered information for that validation. Although it depends on scattering contrast, the lateral correlation signal we seek is typically small compared with that of the bilayer form. Moreover, simulations use periodic boundary conditions, introducing spurious correlations. First I will present our lab's computational software that extracts useful lateral correlations from simulation, and then I will demonstrate the favorable comparisons of our simulations to small angle neutron scattering experiments.