Integrating molecular simulation with neutron scattering to study flexible biological systems

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Neutron scattering will address frontier challenges in biological research by providing crucial information about the three-dimensional (3D) structure and dynamics of biological systems, which underpins the molecular basis of biological processes. Small-angle neutron scattering (SANS) is an ideal technique to investigate dynamic and flexible biosystems, whose importance in cellular function is increasingly recognized. However, a critical factor limiting the impact of SANS is the interpretation of experimental data on flexible systems. The specific challenge is to determine the "conformational ensemble" i.e., the 3D structures that give rise to the experimental SANS signal. Overcoming this challenge requires the integration of SANS with high performance molecular dynamics simulation. We discuss targeted computational methods that scale on the supercomputers and permit interpretation of SANS data with realistic physical models.