Overcoming the Multiscale Challenge for Biomolecular Systems

Gregory A. Voth

Department of Chemistry, James Franck Institute, and Institute for Biophysical Dynamics, The University of Chicago, Chicago, IL, USA

A multiscale theoretical and computational methodology will be discussed that can successfully describe biomolecular systems across multiple length and time scales. The overall approach provides a systematic connection between all-atom molecular dynamics, coarse-grained modeling, and mesoscopic phenomena. At the heart of the approach is a method for deriving coarse-grained models from protein structures and their underlying molecular-scale interactions. This particular aspect of the work has strong connections to the theory of renormalization, but it is more broadly developed and implemented for heterogeneous biomolecular systems. A critical component of the methodology is also its connection to experimental structural data such as cryo-EM or x-ray, thus making it "hybrid" in its character. Important applications of the multiscale approach to study key features of large multi-protein complexes such as the HIV-1 virus capsid, the actin-based cytoskeleton, and protein-mediated membrane remodeling will be presented as time allows.