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Abstract for an Invited Paper
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Systematic Coarse-Graining of Biomolecular Systems

GREG VOTH, University of Utah

A multiscale theoretical and computational methodology will be presented for studying biomolecular systems across multiple length and time scales. The approach provides a systematic connection between all-atom molecular dynamics, coarse-grained modeling, and mesoscopic phenomena. At the heart of the methodology is the multiscale coarse-graining method for rigorously deriving coarse-grained models from the underlying molecular-scale forces. Applications of the multiscale approach will be given for membranes and proteins. Recent advances in coarse-graining large protein complexes will also be described along with key applications.