321c The Multi-Scale Simulation Challenge for Biomolecular Systems

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A multi-scale theoretical and computational methodology will be presented for describing biomolecular assemblies across multiple length- and time-scales. The approach provides an interface between atomistic molecular simulations, mesoscale dynamics, and continuum mechanics. The underlying methodology couples atomistic-level simulations with mesoscale simulations which, in turn, can be bridged to continuum-level modeling where necessary. A new and systematic multi-scale coarse-graining strategy for linking the atomistic-scale interactions to the mesoscale will also be presented. Applications of the overall methodology will be given for biomembrane systems, as well as for cellular cytoskeleton filaments and nucleic acids if time allows.