Multiscale Simulation of Protein Assemblies

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Abstract

Advances in theoretical and computational methodology will be presented that are designed to simulate complex (biomolecular and other soft matter) 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 these concepts are methods for deriving coarse-grained (CG) models from molecular structures and their underlying atomic-scale interactions. This particular aspect of the work has strong connections to the procedure of renormalization, but in the context of CG models it is developed and implemented for more heterogeneous systems. An important new component of our work has also been the concept of the "ultra-coarse-grained" (UCG) model and its associated computational implementation. In the UCG approach, the CG sites or "beads" can have internal states, much like quantum mechanical states. These internal states help to self-consistently quantify a more complicated set of possible interactions within and between the CG sites, while still maintaining a high degree of coarse-graining in the modeling. The presence of the CG site internal states greatly expands the possible range of systems amenable to accurate CG modeling, including quite heterogeneous systems such as aggregation of hydrophobes in solution, liquid-vapor and liquid-solid interfaces, and complex self-assembly processes such as large multi-protein complexes. Applications to experimentally important systems such as cytoskeleton actin filaments and HIV virions will be given.

Keywords: Ultra Coarse Grained, Coarse Grained, Beads, Biophysical Dynamics, Biomolecular, HIV, Cytoskeleton

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