Statistical mechanics of consistent coarse-grained models derived from experimental data

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Atomically detailed molecular dynamics (MD) simulations have tremendously advanced our understanding of biomolecular structure and dynamics. However, despite the rapid growth of computational power, atomistic MD simulations remain somewhat limited in scope. Many vital biological processes such as signal transduction and protein translation occur on timescales or across length-scales that are not effectively investigated with conventional atomistic simulations. Consequently, simulations of coarse-grained (CG) models have rapidly become an increasingly important tool for investigating complex biological systems. CG models are significantly more efficient than atomically detailed models because they require fewer interacting particles for simulating a given system and also because they allow a larger simulation time step. The greatest promise of CG modeling, though, may be the potential for tailoring a particular model to investigate a particular system. In other words, while atomistic MD simulations may provide a powerful "hammer" for investigating biomolecular systems, CG MD simulations may expand the computational "tool box" by providing a "wrench" with much greater flexibility.

The present talk discusses recent progress in CG modeling. We survey the motivation for CG modeling; we review a statistical mechanical framework for CG models that are "consistent" with an atomistic model; and we discuss a variational procedure for numerically implementing this framework. In the course of this analysis, we highlight the role of structural correlations in the process of developing consistent CG models. Finally, we demonstrate the potential for developing CG models directly from experimental data.