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Systematic Coarse-graining of Molecular Dynamics Simulations

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Coarse-grained (CG) models can provide a computationally efficient means to study biomolecular and other soft matter processes involving large numbers of atoms that are correlated over distance scales of many covalent bond lengths and at long time scales. Systematic variational coarse-graining methods based on information from molecular dynamics simulations of finer-grained (e.g., all-atom) models provide attractive tools for the systematic development of CG models. Examples include the multiscale coarse-graining (MS-CG) and relative entropy minimization methods, and results from the former theory will be presented in this talk. In addition, a new approach will be presented that is appropriate for the "ultra coarse-grained" (UCG) regime, e.g., at a coarse-grained resolution that is much coarser than one amino acid residue per CG particle in a protein. At this level of coarse-graining, one is faced with the possible existence of multiple metastable states "within" the CG sites for a given UCG model configuration. I will therefore describe newer systematic variational UCG methods specifically designed to CG entire protein domains and subdomains into single effective CG particles. This is accomplished by augmenting existing effective particle CG schemes to allow for discrete state transitions and configuration-dependent resolution. Additionally, certain aspects of this work connect back to single-state force matching and open up new avenues for method development. This general body of theory and algorithm provides a formal statistical mechanical basis for the coarse-graining of fine-grained molecular dynamics simulation data at various levels of CG resolution. Representative applications will be described as time allows.