

A New Multiscale Coarse-Grain Methodology: the Self-Consistent Force-Matching Method

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In recent years, coarse-grained molecular modeling and simulation have gained tremendous interest in attempting to extend the accessible time- and length-scale of molecular simulations. A major concern though, is how to determine the CG force fields that accurately represent the thermodynamic and molecular properties of the system of interest. A new computational method is developed to calculate the pair potentials between coarse-grained particles from the structural properties observed in an all-atom MD simulation or experiment. In other words, we aim to tackle the inverse problem of statistical mechanics. This method is based on a force matching method that minimizes the difference in forces between all-atom and coarse-grain models. It has recently been shown that the force matching method corresponds to the Yvon-Born-Green (YBG) equation that describes the hierarchical connection between the two-body and three-body correlation functions of simple liquids. However, the lack of self-consistency prevents the reproduction of desired structural correlation functions. By designing a stable and efficient iterative procedure, we propose to solve the YBG equation self-consistently to retrieve interaction potentials from given structural properties. The implication of such capability in molecular design will be addressed. This self-consistent force-matching (SCFM) method is applied to develop the coarse-grained force fields of water, ethane, hexane, and ethanol from all-atom molecular dynamics simulations. By reproducing pair distribution functions, we also found that the agreement of three-body correlation functions between all-atom and coarse-grained simulations is improved. The SCFM method will be contrasted with the commonly inverse Monte Carlo strategy in developing coarse-grain potential. The issues of transferability of coarse-grain force fields and the thermodynamic and dynamic consistency of coarse-grained simulations will also be discussed.