Systematic coarse-graining of molecular models by the Inverse Monte Carlo: Theory, practice and software.

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Molecular simulations of many phenomena related to biomolecular systems, soft matter and nanomaterials requires consideration of length scales above 10 nm and time scales longer than 1 mks, which necessitates the use of coarse-grained (low resolution) models, when each site of the model represents a group of atoms, and the solvent is often omitted. While many of coarse-grained models used in different studies in recent years relay on empirically parameterized interaction potentials, the multiscale approach is based on determination of coarse-grained potentials from atomistic (high resolution) simulations.

In this presentation a multiscale modeling approach based on the inverse Monte Carlo method is discussed, in which radial distribution functions (RDF) and distributions of internal degrees of freedom of molecular structure, obtained in high-resolution atomistic simulations, are used to reconstruct effective potentials which reproduce the same structural properties within low-resolution coarse-grained model. The statistical-mechanical equations expressing canonical properties such as RDFs in terms of potential parameters can be inverted and solved numerically according to the iterative Newton scheme [1]. The approach is illustrated on several examples of varying complexity: ionic solution; ionic liquids, coarse-grained lipid model, coarse-grained DNA model. We demonstrate further how effective potentials, derived exclusively from atomistic simulations, can be used to model such phenomena as lipid self-assembly, formations of vesicles and other ordered structures at varying lipid composition and concentration of different components. The problem of transferability and thermodynamical consistency of effective potentials obtained at different thermodynamic conditions is also discussed. Finally, a novel software MagiC [2] implementing the inverse Monte Carlo method for computation of effective potentials for coarse grained models of arbitrary structure from atomistic trajectories is presented.

[1] A. P. Lyubartsev, A.Mirzoev, L-J. Chen, A.Laaksonen *"Systematic coarse-graining of molecular models by the Newton inversion method"* Faraday Discussions, 2010, 144, 43 - 56.

[2] A.Mirzoev, A.P.Lyubartsev "*MagiC: Software package for multiscale modeling*", J.Chem.Theory and Computations, 2013, 9, 1512