“Reducing the Cost of Molecular Dynamics Simulations”

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Abstract:

To extend the Molecular Dynamics simulations to larger spatiotemporal length and time scales one can simplify the representation of the simulated system, i.e, perform a coarse-grained simulation. However, such models involve several often a priori made assumptions, i.e., the level of coarse-graining and the model complexity. We show how this issue can be addressed with Bayesian statistical framework [1] for the case of coarse-grained models of water [2]. Another route to cost reduction is to perform a multiscale simulation where the atomistic and coarse-grained representations are concurrently coupled. We showcase some recent applications: a protein embedded in an atomistic/supramolecular water [3] and a DNA molecule in a hybrid atomistic/implicit solvent [4].

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