

Abstract Submitted  
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**Development of a multi-resolution simulation approach** ANU NAGARAJAN, SILVINA MATYSIAK, University of Maryland, College Park, MD — The accurate representation of the aqueous environment in molecular dynamics simulations of medium to large systems poses a challenge in terms of simulation time scale and computational power. Multi-resolution simulation technique can be used to represent the solvent environment for simulating very large systems by splitting the system into nested regions. The different resolutions are combined to represent the solvent environment based on its physical relevance so that important regions of the solvent environment are in full atomistic representation and rest are in coarse-grained representation. Our method aims to represent the correct electrostatic properties in different representations and enable smooth transitions across the various resolutions. The ultimate goal of this work is to develop a multi-scale simulation method, for simulating bio-molecules in a multi-resolution solvent environment. This will allow us to gain the speed up necessary to simulate big macromolecular systems.

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