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Fast Equilibration of Coarse-Grained Polymeric Liquids

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Abstract

The study of macromolecular systems may require large computer simulations that are too time consuming and resource intensive to execute in full atomic detail. The integral equation coarse-graining approach by Guenza and co-workers enables the exploration of longer time and spatial scales without sacrificing thermodynamic consistency, by approximating collections of atoms using analytically-derived soft-sphere potentials. Because coarse-grained (CG) characterizations evolve polymer systems far more efficiently than the corresponding united atom (UA) descriptions, we can feasibly equilibrate a CG system to a reasonable geometry, then transform back to the UA description for a more complete equilibration. *Automating* the transformation between the two different representations simultaneously exploits CG efficiency and UA accuracy. By iteratively mapping back and forth between CG and UA, we can quickly guide the simulation towards a configuration that would have taken many more time steps within the UA representation alone. Accomplishing this feat requires a diligent workflow for managing input/output coordinate data between the different steps, deriving the potential at runtime, and inspecting convergence. In this paper, we present a lightweight workflow environment that accomplishes such *fast equilibration* without user intervention. The workflow supports automated mapping between the CG and UA descriptions in an iterative, scalable, and customizable manner. We describe this technique, examine its feasibility, and analyze its correctness.

Keywords: atomistic simulation, coarse-graining, scientific workflows, polymeric liquids, LAMMPS

1 Introduction

Despite considerable advancements in hardware and software technologies for supporting large-scale molecular simulations, computational chemists are confined to simulating relatively small systems compared to most laboratory experiments and real world bulk measurements. This