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Thermodynamic forces in coarse-grained simulations[1]

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Atomically detailed molecular dynamics simulations have profoundly advanced our understanding of the structure and interactions in soft condensed phases. Nevertheless, despite dramatic advances in the methodology and resources for simulating atomically detailed models, low-resolution coarse-grained (CG) models play a central and rapidly growing role in science. CG models not only empower researchers to investigate phenomena beyond the scope of atomically detailed simulations, but also to precisely tailor models for specific phenomena. However, in contrast to atomically detailed simulations, which evolve on a potential energy surface, CG simulations should evolve on a free energy surface. Therefore, the forces in CG models should reflect the thermodynamic information that has been eliminated from the CG configuration space. As a consequence of these thermodynamic forces, CG models often demonstrate limited transferability and, moreover, rarely provide an accurate description of both structural and thermodynamic properties. In this talk, I will present a framework that clarifies the origin and impact of these thermodynamic forces. Additionally, I will present computational methods for quantifying these forces and incorporating their effects into CG MD simulations. As time allows, I will demonstrate applications of this framework for liquids, polymers, and interfaces.

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