Predictive Fluctuating Hydrodynamics Simulations of Interacting Particles via Mesoscopic Coarse-Graining

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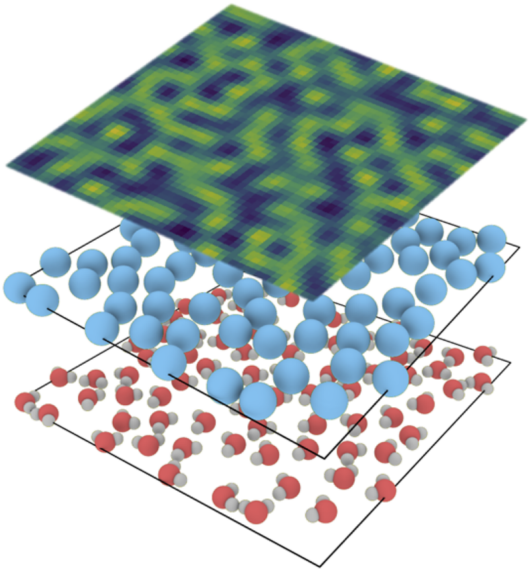

Fluctuating hydrodynamics provides a powerful theoretical framework for describing transport and collective behavior in liquids, including processes such as diffusion, phase separation, and molecular self-assembly that occur at mesoscopic scales beyond the reach of conventional particle-based simulations. However, establishing a direct and predictive connection between mesoscopic fluctuating hydrodynamic models and the underlying molecular dynamics remains a significant challenge due to the large separation of spatiotemporal scales and the limitations of conventional top-down modeling approaches. While analytical microscopic mappings have been proposed for density dynamics under Langevin processes, the singular mathematical nature of the resulting density fields raises concerns about the validity and practical utility of the associated stochastic partial differential equations, particularly for direct numerical implementation.

In this work, we present a systematic mesoscopic coarse-graining framework that enables numerical simulations of fluctuating hydrodynamics for interacting liquids. The heart of our approach consists of bottom-up coarse-graining of the Dean-Kawasaki description of microscopic density dynamics onto mesoscopic grids. Starting from particle-level molecular dynamics simulations as microscopic input, we derive a coarse-grained stochastic partial differential equation in which the resolution is controlled by scaling analysis. We further demonstrate that this methodology systematically incorporates key microscopic correlations into coarse-grained density fields by determining the effective mesoscale interactions renormalized at the grid scale. By elucidating how coarse-graining influences structural and dynamical correlations at the mesoscopic level, this framework enables numerical field-theoretic simulations of fluids at larger length and time scales with substantially reduced computational cost. Altogether, this work establishes a practical computational route for connecting molecular simulations with fluctuating hydrodynamic models, enabling predictive multiscale simulations of complex condensed phase systems across molecular and mesoscopic length scales.

References:

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