“Multiscale Mechanics and Modeling of Fluid Materials”

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Abstract:

Multiscale mechanics is ubiquitous in fluid materials such as paint, starch and blood. To understand, explore and exploit such mechanism, we have adopted a computational approach with an emphasis on high performance computing, and it is complemented by semi-analytical approaches. In particular, we model soft materials such as particulate and colloidal multiphase suspension flows at individual scales, and study the dynamics and rheology of these non-Newtonian fluids. For this research line, we adopt a top-down/continuum perspective and thermal fluctuations differentiate whether it is a macroscopic or mesoscopic description. The corresponding numerical methods adopted are smoothed particle hydrodynamics (SPH) and smoothed dissipative particle dynamics (SDPD). We also consider a bottom-up perspective by systematically coarse-graining (CG) systems with atomic details into models with much reduced degrees of freedom. One of the rigorous CG strategies we employ is the Mori-Zwanzig (MZ) projection formalism from non-equilibrium statistical mechanics. One advantage of the MZ methodology is that not only the static, but also the dynamic properties of the detailed model can be reproduced accurately by the CG simulations. The corresponding numerical methods are molecular dynamics (MD), CG-MD, and dissipative particle dynamics (DPD). Furthermore, we also develop and

analyze coupling strategies to simulate two or multiple scales concurrently on the fly, such as hybrid simulations of particle dynamics and continuum mechanics. To facilitate the method developments and popularize further their applications, we have released a few high performance software packages. Along the different research lines, we emphasize various applications such as blood cells related to the efforts of modeling and algorithm developments.