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Preface: theory, methods, and applications of mesoscopic modeling*

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With increasing attention to complex fluids and soft matter, we have witnessed a fast-growing research in mesoscopic modeling and simulation in the past decades. The development of mesoscopic methods offers many potential opportunities as well as challenges in modeling of complex materials for diverse applications. Despite significant progress in the past decade, mesoscopic methods are still under development. New formulation in the models, novel theoretical interpretations, and innovative numerical algorithms often appear in literature. These mesoscopic methods have been already applied to a large number of problems, including polymer and colloidal suspensions, multiphase fluids, biological materials, and blood rheology. New applications of mesoscopic modeling in different areas are still emerging.

This special issue aims to highlight the developments of different mesoscopic methods, algorithms, and their applications to complex fluids and soft matter. Many interesting phenomena at the mesoscopic scale are beyond the capability of atomistic simulations, while important mesoscopic discrete features and thermal fluctuations cannot be captured by mean-field theories. To this end, mesoscopic methods can seamlessly bridge the gap between microscopic atomistic dynamics and macroscopic bulk behavior because they are grounded in both macroscale and microscale models. This special issue showcases the most up-to-date and exciting research in both bottom-up (from atomistic models to coarse-grained representations) and top-down (from continuum descriptions to fluctuating hydrodynamics) mesoscopic methods, developments of new algorithms as well as applications.

In the first paper, Li et al.[1] review bottom-up mesoscopic methods with applications to biological systems, and discuss the effectiveness and versatility of particle-based mesoscopic methods in simulations of biological processes involving significant topological changes. Nikolov et al.[2] present a new application of mesoscopic modeling. They use a bottom-up approach, dissipative particle dynamics (DPD), to simulate swelling kinetics of polymeric microgels, and investigate the effect of different solvent conditions on the bulk modulus of microgels.

To explore hydrodynamic behavior of DPD fluids, Bian et al.[3] analyze current correlation functions of DPD in Fourier space with comparison to results of molecular dynamics (MD) and

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linearized hydrodynamic equations. They quantify the length scales where DPD is still valid but the hydrodynamic solution fails. Using the same method of analysis, Azarnykh et al.[4] investigate the behavior of a DPD fluid within different scaling regimes, and demonstrate that DPD follows Langevin dynamic within the particle regime at scales smaller than cut-off radius of particle interactions, but differs from Langevin dynamics for the collective regime that the length scale is larger than the decorrelation length of particles.

In the fifth paper, Ellero and Español[5] provide a comprehensive review of a top-down approach, the smoothed dissipative particle dynamics (SDPD) method, covering both fundamental and technical aspects of SDPD. Faure and Stoltz[6] present new stable and accurate schemes to improve the stability of SDPD simulation by introducing a Metropolis step in the integration of the non-conservative parts.

In addition to these Lagrangian methods, Wang et al.[7] present a new fluctuating hydrodynamic method based on the finite volume method for fluid-structure interactions in confined channels, ellucidating the role of confinement on the dynamics of microstructure subjected to hydrodynamics coupling and thermal fluctuations. Jin et al.[8] use the lattice Boltzmann method (LBM) to resolve intermittent behaviors on small scales in isotropic turbulent flows, and show that the scaling of spatial structure functions (up to ten orders) is consistent with the experimental measurements and theoretical results. This provides a solid basis for using LBM to study more complex processes that are sensitive to small scales and mesoscale structures in turbulent flows.

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