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Preface

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PREFACE

DCDS-S SPECIAL ISSUE ON MESOSCOPIC METHODS AND THEIR APPLICATIONS TO CFD

Matter, conceptually classified into fluids and solids, can be completely described by the microscopic physics of its constituent atoms or molecules. However, for most engineering applications, a macroscopic or continuum description has usually been sufficient due to the large disparity between the spatial and temporal scales relevant to these applications and the scales of the underlying molecular dynamics. In this case, the microscopic physics merely determines material properties such as the viscosity of a fluid or the elastic constants of a solid. These material properties cannot be derived within the macroscopic framework, but the qualitative nature of the macroscopic dynamics is usually insensitive to the details of the underlying microscopic interactions.

The traditional picture of the role of microscopic and macroscopic physics is now being challenged as new multi-scale and multi-physics problems begin to emerge. For example, in nano-scale systems, the assumption of scale separation breaks down; thus, macroscopic theory is inadequate, yet microscopic theory may be impractical because it requires computational capabilities far beyond our current reach. This new class of problems poses unprecedented challenges to mathematical modeling as well as numerical simulation and requires new and non-traditional analysis and modeling paradigms. Methods based on mesoscopic theories, which connect the microscopic and macroscopic descriptions of the dynamics, provide a promising approach. They can lead to useful models, possibly requiring empirical inputs to determine some of the model parameters that are sub-macroscopic yet indispensable to the relevant physical phenomena.

The area of complex fluids focuses on materials such as suspensions, emulsions, and gels, where the internal structure is relevant to the macroscopic dynamics. An important challenge will be to construct meaningful mesoscopic models by extracting all the macroscopically relevant information from the microscopic dynamics.

There already exist a few mesoscopic methods such as the Lattice Gas Cellular Automata (LGCA), the Lattice Boltzmann Equation (LBE), Discrete Velocity Models (DVM) of the Boltzmann equation, Gas-Kinetic Schemes (GKS), Smoothed Particle Hydrodynamics (SPH), and Dissipative Particle Dynamics (DPD). Although these methods are sometimes designed for macroscopic hydrodynamics, they are not based upon the Navier-Stokes equations; instead, they are closely related to kinetic theory and the Boltzmann equation. These methods are promising candidates to effectively connect microscopic and macroscopic scales, thereby substantially extending the capabilities of numerical simulations. For this reason, they are the focus of the International Conferences on Mesoscopic Methods in Engineering and Science (ICMMES, <http://www.icmmes.org>).

The eighteenth ICMMES Conference was held at the University of La Rochelle, La Rochelle, France, from June 28 to July 1, 2022. This special issue of Discrete

and Continuous Dynamical Systems–Series S (DCDS-S), devoted to this conference, includes 8 selected and peer-reviewed papers on different topics related to the focus areas of ICMMES covering theory and numerical analysis of the LBE and its boundary conditions [1, 2, 3, 4], large-eddy simulations using the LBE [5, 6], and numerics and models for multi-phase and multi-component fluids [7, 8].

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