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Mesosopic Methods in Engineering and Science

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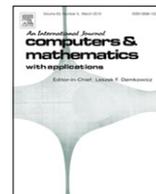
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Editorial

Mesososcopic methods in engineering and science

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, because of 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; macroscopic theory is therefore inadequate, yet microscopic theory may be impractical because it requires computational capabilities far beyond our present 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, which 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 and thereby substantially extend 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 Seventh ICMMES Conference was held at the University of Alberta, Edmonton, Canada, July 12–16, 2010. This special issue of the *Computers and Mathematics with Applications* devoted to this conference includes eleven selected and peer-reviewed papers on a wide range of topics related to the focused areas of ICMMES, in particular, the lattice Boltzmann (LB) method. There are three papers on the theory and numerical analysis of the LBE, which deal with interpretation and derivation of the lattice Boltzmann method using Strang splitting [1], stable LB schemes with a dual entropy approach in one dimension [2], out-flow boundary conditions in the LBE [3], and optimal relaxation collisions for LB methods [4]. Other papers deal with numerics and applications of the LB methods including a lattice Boltzmann study of gas flows in a long micro-channel [5], LB simulation of turbulent flow laden with finite-size particles [6], on enhanced nonlinear free surface flow simulations with a hybrid LBM-VOF model [7], finite element LB simulations of free surface flow in a concentric cylinder [8], spectral-element discontinuous Galerkin LB simulation of flow past two cylinders in tandem with an exponential time integrator [9], multi-GPU implementation of the LB method [10], benchmark quality LB simulations of thermal convective flows in two dimensions [11], and LB simulation of a mannequin's thermal plume in a small room [12]. The usefulness of the LB method is attested by the wide range of applications.

The editors would like to thank the referees who helped to review the papers in this special issue. The organizers of the ICMMES-2010 and the ICMMES SCIENTIFIC COMMITTEE would like to acknowledge the generous support from School of Energy and The Environment at University of Alberta, the National Science Foundation of USA (Grant CBETS-1029428), DBR Technology Center Schlumberger and the Office of Research at Old Dominion University.

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