Editorial

Mesoscopic 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. An important challenge will be to construct meaningful mesoscopic models by extracting all the macroscopically relevant information from the microscopic dynamics.

There already exist 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 focuses of the INTERNATIONAL CONFERENCES ON MESOSCOPIC METHODS IN ENGINEERING AND SCIENCE (ICMMES, http://www.icmmes.org).

The second ICMMES Conference was held at THE HONG KONG POLYTECHNIC UNIVERSITY, Hong Kong, China, July 25–29, 2005. This special issue of the *Computer & Mathematics with Applications* devoted to this conference includes 26 selected papers mainly focusing on the LBE method, its theory and applications, and other methods including the smoothed particle hydrodynamics and molecular dynamics simulation. The maturity and usefulness of the kinetic methods are attested by the wide range of applications and the qualities of these simulations. Other nine papers presented during ICMMES-2005 have been published in a special issue of *International Journal of Computational Fluid Dynamics* (**20**(6):359–461 (2006)).

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