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Mesoscopic Methods in Engineering and Science

Christian Jansen

Manfred Krafczyk

Li-Shi Luo

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Preface

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. 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. A key distinctive feature of mesoscopic or kinetic methods is the modeling of the so-called the "fast" non-hydrodynamic modes or microscopic degrees of freedom, which are encapsulated in transport coefficients in continuum theories. The mesoscopic or kinetic methods maintain a very limited number of non-hydrodynamic modes, so that the dissipation is realized through either the fluctuation–dissipation mechanism, *i.e.*, Green-Kubo type formula, or the relaxation of these modes. 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 Thirteenth ICMMES was held in Hamburg University of Technology, Hamburg, Germany, July 18–22, 2016 (http://www.icmmes.org/icmmes2016). This special issue of the *Computers and Mathematics with Applications* devoted to this conference includes twelve selected and peer-reviewed papers on a wide range of topics related to the focused areas of ICMMES. The papers included in this special issue are all related to the lattice Boltzmann equation (LBE) and its applications. In particular, they are about the numerical analysis and implementations of the LBE [1–5], and the applications for blofluid system [6], complex fluids [7–9], fluid–structure interactions [10], thermal flows [11], and turbulence flow [12].

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Christian Janßen
Institute for Fluid Dynamics and Ship Theory (FDS), Hamburg University of Technology, Am Schwarzenberg-Campus 4, 21073 Hamburg, Germany
E-mail address: christian.janssen@tuhh.de.
URL: http://www.tuhh.de/fds.

Manfred Krafczyk
Institut für rechnergestützte Modellierung im Bauingenieurwesen (iRMB), Technische Universität Braunschweig, Pockelsstr. 3, 38106 Braunschweig, Germany
Institute for Computational Modeling in Civil Engineering, Technische Universität Braunschweig, Pockelsstr. 3, 38106 Braunschweig, Germany
E-mail address: kraft@irmb.tu-bs.de.
URL: http://www.irmb.tu-bs.de.

Li-Shi Luo
Beijing Computational Science Research Center, Beijing 100193, China
Department of Mathematics & Statistics, Old Dominion University, Norfolk, VA 23529, USA
E-mail addresses: lluo@odu.edu, lluo@csrc.ac.cn.
URL: http://www.lions.odu.edu/~lluo.