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Mesoscopic Methods in Engineering and Science

Chuguang Zheng

Jiding Lu

Zhaoli Guo

Li-Shi Luo
Old Dominion University

Manfred Krafczyk

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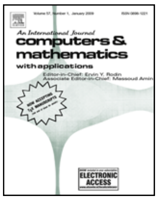

Editorial

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. 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 Sixth ICMMES Conference was held in the South China University of Technology (SCUT), Guangzhou City, China, July 13–17, 2009. This special issue of the *Computers and Mathematics with Applications* devoted to this conference includes twenty-eight selected and peer-reviewed papers on a wide range of topics related to the focused areas of ICMMES: Development of high-order LB algorithm [1]; theory and numerical analysis of LB models for advection–diffusion system [2,3] and axial-symmetric flows [4]; study of the connection between the LBE and the artificial compressibility method [5]; development of the LB scheme with non-uniform grids for large-eddy simulation (LES) of high-Reynolds-number flow in three dimensions [6]; development of LB algorithms with the immersed boundary method (IBM) for particulate flows [7] and fluid–structure interaction problems [8]; modeling and simulation of micro-flows [9,10], complex flows of fluid with realistic equation of state [11], free-surface flows [12], droplet collisions [13], cavitation [14], dendrite growth in convective flows [15], gas–solid two phase flows [16], and flow through porous media [17,18]; implementation of LB algorithms on general purpose graphic processing units (GPGPUs) [12,19,28]; gas-kinetic scheme (GKS) for liquid–gas mixture [20], compressible flows with various Mach and Knudsen numbers [21], and shallow water equation [22]; as well as other LB applications of computational fluid dynamics [23–27]. The usefulness of the LBE method is attested by the wide range of applications.

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Chuguang Zheng [1]
State Key Laboratory of Coal Combustion,
Huangzhong University of Science and Technology,
1037 Luoyu Road, Wuhan 430074, Hubei, China
E-mail address: cgzheng@mail.hust.edu.cn.

Jidong Lu [2]
School of Electric Power, South China University of Technology,
381 Tianhe Road, Guangzhou 510641, Guangdong, China
E-mail address: jdlu@scut.edu.cn.

Zhaoli Guo[3]
State Key Laboratory of Coal Combustion,
Huangzhong University of Science and Technology,
1037 Luoyu Road, Wuhan 430074, Hubei, China
E-mail address: zlguo@mail.hust.edu.cn.

Li-Shi Luo[*]
Department of Mathematics & Statistics, and Center for Computational Sciences,
Old Dominion University, Norfolk, Virginia 23529, USA
E-mail address: lluo@odu.edu.
URL: http://www.lions.odu.edu/~lluo.

Manfred Krafczyk[4]
Institut für rechnergestützte Modellierung im Bauingenieurwesen (iRMB),
Technische Universität Carola-Wilhelmina zu Braunschweig,
Mühlenpfordtstr. 4-5, 38106 Braunschweig, Germany
E-mail address: kraft@irmb.tu-bs.de.
URL: http://www.irmb.tu-bs.de.

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[*] Corresponding editor. Tel.: +1 757 683 5295, +1 757 864 8006; fax: +1 757 683 3885, +1 757 864 6134.
[1] Tel.: +86 27 87545526; fax: +86 27 87545526.
[2] Tel.: +86 20 87114081; fax: +86 20 87110613.
[3] Tel.: +86 27 87545526; fax: +86 27 87545526.
[4] Tel.: +49 531 391 7588; fax: +49 531 391 7599.