2010

Mesoscopic Methods in Engineering and Science

Alfons Hoekstra

Li-Shi Luo
Old Dominion University, lluo@odu.edu

Manfred Krafczyk

Original Publication Citation

Hoekstra, A., Luo, L. S., & Krafczyk, M. (2010). Mesoscopic methods in engineering and science. *Computers & Mathematics with Applications, 59*(7), 2139-2140. doi:10.1016/j.camwa.2009.10.029

Computers and Mathematics with Applications 59 (2010) 2139–2140

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

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 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 for effectively connecting microscopic and macroscopic scales and 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 Fifth ICMMES Conference was held in the University of Amsterdam, Amsterdam, The Netherlands, June 16–20, 2008. This special issue of *Computers and Mathematics with Applications* devoted to this conference includes twenty six selected papers on a wide range of topics related to the focus areas of ICMMES: Theory and numerical analysis of the LBE and its boundary conditions [1–4], large-eddy simulations using the LBE [5,6], numerics and models for multi-phase and multi-component fluids [7–10], complex fluids in porous media [11–14], biological [15] and non-Newtonian flows [16], nano-scale thermal conduction in silicon [17], multi-scale and hybrid approaches for complex fluids and soft matter [18–20], implementation of LBE algorithms on GPU [21], and various applications in computational fluid dynamics including mixing layers in shallow water equations [22], sound generation [23,24], forced convection [25], and heat transfer [25,26]. The usefulness of the LBE method is attested to by the wide range of applications.

The editors would like to thank the referees who have helped to review the papers in this special issue. The organizers of the ICMMES-2008 and the ICMMES Scientific Committee would like to acknowledge the support from The University of Amsterdam, The National Science Foundation of the United States under the Grant CBET 0827259, Old Dominion University, Foundation for Fundamental Research on Matter of the Netherlands, J.M. Burgerscentrum Research School for Fluid Mechanics, Netherlands Organisation for Scientific Research, Norit Process Technology B.V., OSPT Research School Process Technology, Shell Nederland B.V., and NEC Europe Ltd.

References

[1] F. Dubois, P. Lallamand, M. Tekitek, On superconvergent lattice Boltzmann boundary scheme, Comput. Math. Appl. 59 (2010) 2141–2149.
[2] M. Rheinländer, On the stability-structure for lattice Boltzmann schemes, Comput. Math. Appl. 59 (2010) 2150–2167.

0898-1221/$ – see front matter
doi:10.1016/j.camwa.2009.10.029

[3] Z.X. Yang, Pressure condition for lattice Boltzmann methods on domains with curved boundaries, Comput. Math. Appl. 59 (2010) 2168–2177.
[4] C.-H. Liu, K.-H. Lin, H.-C. Mai, C.-A. Lin, Thermal boundary conditions for thermal lattice Boltzmann simulations, Comput. Math. Appl. 59 (2010) 2178–2193.
[5] P. Sagaut, Toward advanced subgrid models for lattice Boltzmann-based large-eddy simulation: Theoretical formulations, Comput. Math. Appl. 59 (2010) 2194–2199.
[6] M. Weickert, G. Teike, M. Sommerfeld, Investigation of the LES WALE turbulence model within the lattice Boltzmann framework, Comput. Math. Appl. 59 (2010) 2200–2214.
[7] C. Janßen, M. Krafczyk, A lattice Boltzmann approach for free surface flow simulations on non-uniform block-structured grids, Comput. Math. Appl. 59 (2010) 2215–2235.
[8] A. Kupershtokh, Criterion of numerical instability of liquid state in LBE simulations, Comput. Math. Appl. 59 (2010) 2236–2245.
[9] P.M. Dupuy, M. Fernandino, H.A. Jakobsen, H.F. Svendsen, Using Cahn–Hilliard mobility to simulate coalescence dynamics, Comput. Math. Appl. 59 (2010) 2246–2259.
[10] A. Kuzmin, A.A. Mohamad, Multirange multi-relaxation time Shan–Chen model with extended equilibrium, Comput. Math. Appl. 59 (2010) 2260–2270.
[11] H. Gao, C.Q. Qiu, D. Fan, Y. Jin, L.-P. Wang, Three-dimensional microscale flow simulation and colloid transport modeling in saturated soil porous media, Comput. Math. Appl. 59 (2010) 2271–2289.
[12] G.X. Shi, H. Gao, V.I. Lazouskaya, Q.J. Kang, Y. Jin, L.-P. Wang, Viscous flow and colloid transport near air–water interface in a microchannel, Comput. Math. Appl. 59 (2010) 2290–2304.
[13] E.S. Boek, M. Venturonli, Lattice-Boltzmann studies of fluid flow in porous media with realistic rock geometries, Comput. Math. Appl. 59 (2010) 2305–2314.
[14] A.G. Yiotis, M.E. Kainourgiakis, E.S. Kikkinides, A.K. Stubos, Application of the lattice-Boltzmann method to the modeling of population blob dynamics in 2D porous domains, Comput. Math. Appl. 59 (2010) 2315–2325.
[15] H. Hatzikirou, L. Brusch, C. Schaller, M. Simon, A. Deutsch, Prediction of traveling front behavior in a lattice-gas cellular automaton model for tumor invasion, Comput. Math. Appl. 59 (2010) 2326–2339.
[16] G. Pingen, K. Maute, Optimal design for non-Newtonian flows using a topology optimization approach, Comput. Math. Appl. 59 (2010) 2340–2350.
[17] P. Heino, Lattice-Boltzmann finite-difference model with optical phonons for nanoscale thermal conduction, Comput. Math. Appl. 59 (2010) 2351–2359.
[18] O. Henrich, D. Marenduzzo, K. Stratford, M.E. Cates, Domain growth in cholesteric blue phases: Hybrid lattice Boltzmann simulations, Comput. Math. Appl. 59 (2010) 2360–2369.
[19] E.M. Kotsalis, J.H. Hanasaki, J.H. Walther, P. Koumoutsakos, Non-periodic molecular dynamics simulations of coarse grained lipid bilayer in water, Comput. Math. Appl. 59 (2010) 2370–2373.
[20] J.H. Lee, B. Dünweg, J. Schumacher, Multiscale modelling strategy using the lattice Boltzmann method for polymer dynamics in a turbulent flow, Comput. Math. Appl. 59 (2010) 2374–2379.
[21] F. Kuznik, C. Obrecht, G. Rusaouen, J.-J. Roux, LBM based flow simulation using GPU computing processor, Comput. Math. Appl. 59 (2010) 2380–2392.
[22] H.W. Liu, M.Y. Lam, M.S. Ghidaoui, Numerical study of temporal shallow mixing layers using BGK-based schemes, Comput. Math. Appl. 59 (2010) 2393–2402.
[23] M. Hiraishi, M. Tsutahara, R.C.K. Leung, Numerical simulation of sound generation in a mixing layer by the finite difference lattice Boltzmann method, Comput. Math. Appl. 59 (2010) 2403–2410.
[24] S. Tajiri, M. Tsutahara, H. Tanaka, Direct simulation of sound and under water sound generated by a water drop hitting a water surface using the finite difference lattice Boltzmann method, Comput. Math. Appl. 59 (2010) 2411–2420.
[25] A.A. Alamyane, A.A. Mohamad, Simulation of forced convection in channel with extended surfaces by lattice Boltzmann method, Comput. Math. Appl. 59 (2010) 2421–2430.
[26] S. Gokaltun, G.S. Dulikravich, Lattice Boltzmann computations of incompressible laminar flow and heat transfer in a constricted channel, Comput. Math. Appl. 59 (2010) 2431–2441.

Alfons Hoekstra [1]
Section of Computational Science, Informatics Institute, Faculty of Science, University of Amsterdam, Kruislaan 403, 1098 SJ Amsterdam, The Netherlands
E-mail address: A.G.Hoekstra@uva.nl.
URL: http://staff.science.uva.nl/~alfons/.

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

Manfred Krafczyk [2]
Institut für rechnergestützte Modellierung im Bauingenieurwesen, Technische Universität Carola-Wilhelmina zu Braunschweig, Pockelsstraße 3, 38106 Braunschweig, Germany
E-mail address: kraft@irmb.tu-bs.de.
URL: http://www.irmb.tu-bs.de.

* Corresponding editor. Tel.: +1 757 683 5295; fax: +1 757 683 3885.
[1] Tel.: +31 20 5257543.
[2] Tel.: +49 531 391 7588; fax: +49 531 391 7599.