

Comment on “Discrete Boltzmann Equation for Microfluidics”

In a recent Letter [1], Li and Kwok use a lattice Boltzmann equation (LBE) for microfluidics. Their main claim is that an LBE model for microfluidics can be constructed based on the “Bhatnagar-Gross-Krook [*sic*]” model by including “the equivalent external acceleration force exerting on the lattice particles by means of the electrostatic potential energy, intermolecular potential energy between pair of fluid molecules, and substrate potential energy due to interactions between the fluid and substrate.” The main result in [1] is Eq. (33); i.e., the slip velocity $U_s = [2\tau(\tau - 1)/(3\rho\nu)]F\delta_x^2$, where τ is the relaxation time in the Bhatnagar-Gross-Krook (BGK) model, F is the external force due to a mean-field potential, and δ_x is the lattice constant (or grid spacing). In this Comment we point out that the slip velocity is merely an artifact of the lattice BGK (LBGK) model [2–7]. Therefore, the claim that the LBGK model and Eq. (33) for U_s , in particular, show that “the slip velocity is directly proportional to the induced stress tensor due to the linear nanoscale heterogeneities on the substrate surface” and, thus, “a possible mechanism for fluid slip in microfluidic systems can result from the nanoscale heterogeneities on the substrate surface where the slip velocity is dependent on the gradient of the interaction potential energy between the fluid and substrate,” is false.

The error is well exemplified by the result that the slip velocity U_s is proportional to δ_x^2 , which merely indicates that formally the LBE scheme is second-order accurate. That is, with the flow properties fixed, the slip velocity vanishes as δ_x^2 when $\delta_x \rightarrow 0$. The kinetic nature of the LBE method manifests itself in precisely this phenomenon: hydrodynamic boundary conditions are difficult to satisfy on a grid point exactly, and this is well understood [2–7]. Moreover, the τ dependence of U_s is a defect of the LBGK model [5–7] rather than a physical effect as portrayed by Li and Kwok [1]. In essence, the artifacts in the LBGK model are misconstrued as physical effects by Li and Kwok [1].

We also emphasize that it is misleading to claim that the LBE method is better suited to simulate microfluidics than conventional computational fluid dynamics (CFD) methods. The mean-field approach simply cannot model intermolecular forces or any microscopic phenomena, and this fact cannot be escaped by the unprincipled introduction of a body force that is formally equivalent to the Lennard-Jones, or any other, potential. Intermolecular forces can be modeled only in the collision operator itself; physically they are entirely distinct from imposed external force fields [8,9]. It is physically implausible that flows of different substances (thus different molecular forces) should be distinguished by having different forcing terms in the Navier-Stokes equations. Consequently, the LBE method presently is capable only of modeling macroscopic hydrodynamics, which can also be dealt with by

conventional CFD methods. The fact that the *unique* LBE solution for Poiseuille flow is the standard Navier-Stokes parabolic profile proves this point unequivocally [3–7]. Contrary to the repeated claims made by Li and Kwok [1], conventional CFD methods can simulate slip and electrokinetically driven microflows [10], whereas presently the LBE method cannot even reproduce the Knudsen paradox (e.g., Ref. [10], p. 22)—the most direct and simplest effect of Knudsen slip.

Finally, we note that the material presented by Li and Kwok [1] concerning mean-field theory is ubiquitous in textbooks and that the Maxwell distribution including an external field is also standard [11,12]. Concerning the LBE method, there is considerable literature on the treatment of external forces [6–9,13,14] due to either mean-field or thermodynamic potentials [8,9], the kinetic nature of the slip velocity [2,4,7], and the analytic results related to various boundary conditions [4–7]. In particular, Eq. (33) in [1] is identical to Eq. (22) in [5]; i.e., $U_s = [16\tau(\tau - 1)/(3N^2)]U_c$, where $U_c = (N\delta_x)^2F/(8\rho\nu)$ and N is the number of grid points across the channel.

Comments from R. Rubinstein, P. Lellemand, and D. d’Humières and support from the U.S. AFOSR under Grant No. F49620-01-1-0142 are gratefully acknowledged.

Li-Shi Luo*

National Institute of Aerospace
144 Research Drive, Hampton, Virginia 23666, USA

Received 1 May 2003; published 1 April 2004

DOI: 10.1103/PhysRevLett.92.139401

PACS numbers: 47.11.+j, 82.20.Wt, 83.50.Ha, 85.85.+j

*Electronic addresses: luo@nianet.org;

<http://research.nianet.org/~luo>

- [1] B. Li and D. Kwok, Phys. Rev. Lett. **90**, 124502 (2003).
- [2] R. Cornubert, D. d’Humières, and D. Levermore, Physica (Amsterdam) **47D**, 241 (1991).
- [3] L.-S. Luo *et al.*, Phys. Rev. A **43**, R7097 (1991).
- [4] L.-S. Luo, J. Stat. Phys. **88**, 913 (1997).
- [5] X. He *et al.*, J. Stat. Phys. **87**, 115 (1997).
- [6] I. Ginzbourg and P. M. Alder, J. Phys. II (France) **4**, 191 (1994).
- [7] I. Ginzbourg and D. d’Humières, J. Stat. Phys. **84**, 927 (1996); Phys. Rev. E **68**, 066614 (2003); ITWM Report No. 38-2002, available at <http://www.itwm.fhg.de>.
- [8] L.-S. Luo, Phys. Rev. Lett. **81**, 1618 (1998).
- [9] L.-S. Luo, Phys. Rev. E **62**, 4982 (2000).
- [10] G. Em Karniadakis and A. Beskok, *Micro Flows* (Springer, New York, 2002).
- [11] K. Huang, *Statistical Mechanics* (Wiley, New York, 1963).
- [12] J. A. McLennan, *Introduction to Non-Equilibrium Statistical Mechanics* (Prentice-Hall, Englewood Cliffs, 1989).
- [13] A. Ladd and R. Verberg, J. Stat. Phys. **104**, 1191 (2001).
- [14] Z. Guo *et al.*, Phys. Rev. E **65**, 046308 (2002).