Comment on "Heat transfer and fluid flow in microchannels and nanochannels at high Knudsen number using thermal lattice-Boltzmann method"

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In this Comment we reveal the falsehood of the claim that the lattice Bhatnagar-Gross-Krook (BGK) model "*is capable of modeling shear-driven, pressure-driven, and mixed shear-pressure-driven rarified* [sic] *flows and heat transfer up to* Kn = 1 *in the transitional regime*" made in a recent paper [Ghazanfarian and Abbassi, Phys. Rev. E **82**, 026307 (2010)]. In particular, we demonstrate that the so-called "Knudsen effects" described are merely numerical artifacts of the lattice BGK model and they are unphysical. Specifically, we show that the erroneous results for the pressure-driven flow in a microchannel imply the false and unphysical condition that $6\sigma\mathrm{Kn} < -1$, where Kn is the Knudsen number $\sigma = (2 - \sigma_v)/\sigma_v$ and $\sigma_v \in (0, 1]$ is the tangential momentum accommodation coefficient. We also show explicitly that the defects of the lattice BGK model can be completely removed by using the multiple-relaxation-time collision model.

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In a recent paper [1], Ghazanfarian and Abbassi (GA hereafter) use the energy conserving lattice Boltzmann equation (LBE) with two sets of distribution functions to simulate "*gaseous flow and heat transfer in planar microchannel and nanochannel with different wall temperatures in transitional regime* $0.1 \leqslant \mathrm{Kn} \leqslant 1$." The paper includes four test cases in two dimensions (2D): (a) the Fourier flow, (b) the Couette flow, (c) the Poiseuille flow, and (d) mixed shear-pressure-driven flow in the developing and fully developed regions. Based on their numerical results, the authors conclude that the lattice Boltzmann (LB) method they employed "*is capable of modeling shear-driven, pressure-driven, and mixed shear-pressure-driven rarified* [sic] *flows and heat transfer up to* Kn = 1 *in the transitional regime*." In this Comment we would like point out that the results presented by GA in the paper [1] are erroneous and the above claim is false.

Both the LB model and the flows studied by GA [1] are well understood. The lattice Boltzmann model used by GA is the lattice Bhatnagar-Gross-Krook (BGK) equation with the so-called "diffuse scattering" boundary conditions (DSBCs) [2]. By using a *second-order* Taylor expansion of the Maxwellian equilibrium distribution in the flow velocity $\boldsymbol{u}$ (cf. Eq. (3) in [1]), the LB model used by GA is a solver for near incompressible Navier-Stokes equations. That is, in principle the LB model is incapable of solving the Boltzmann equation, which is required for flows in the transitional flow regime with the Knudsen number $\mathrm{Kn} \sim 1$. The reasons are obvious. First, under the diffusive scaling $\delta_t \sim \delta_x^2 \sim \varepsilon^2$ [3–5], the LBE with a fixed set of discrete velocities tied to the underlying lattice, however large that may be, converges to the following equation [4]:

$$\partial_t f_i + \frac{1}{\varepsilon}\boldsymbol{\xi}_i \cdot \nabla f_i = \frac{1}{\varepsilon^2} J_i, \qquad (1)$$

which is different from the Boltzmann equation. Moreover, the LBE solves the pressure p and the velocity $\boldsymbol{u}$ with first-order and second-order spatial accuracy, respectively, and first-order temporal accuracy [4]. That is, the LBE so formulated cannot solve the evolution equations of the moments of the distribution function f beyond the second order in ε — it is inherently a second-order Navier-Stokes solver and not a solver for kinetic equations. In addition, the LBE lacks the necessary symmetries required by the higher-order tensorial moments as a direct consequence of its discrete nature, unless a large number of discrete velocities are used [6]. This limits the validity of the LBE to the slip-flow regime at best but not beyond. While the lattice Boltzmann equation in general, as formulated in [1], is bounded by the aforementioned limitations, regardless of specifics in its collision model or implementations, there are additional defects which are specifically inherent to the lattice BGK model used by GA [1] and others [7], and it is these defects that lead to the erroneous results of GA [1], which will be discussed in detail in this Comment.

The "diffuse scattering" boundary conditions used by GA can be recast as combinations of the bounce-back (BB) and specular-reflective (SR) boundary conditions (BCs) [8]. For athermal (or isothermal, as referred by GA) flows, the lattice BGK (LBGK) model with various BCs can be solved analytically for the Poiseuille flow when the streamwise direction aligns with the lattice line and the flow is driven by a constant body force [8–13]. It is well understood that the LBGK model with the bounce-back type of boundary conditions, including the DSBCs, is inaccurate to deal with the Dirichlet boundary condition. Specifically, the precise locations where the Dirichlet boundary condition is satisfied depend on the relaxation parameter τ in the LBGK model [8–14]. Consequently, the effective channel width H also depends on τ. In particular, this defect of the LBGK model with the bounce-back type of BCs has been studied in detail analytically and numerically for the microchannel flow [8] and other cases [13–15]. It has been shown repeatedly [8,16,17] that the results of the 2D microchannel flow obtained by using the LBGK with the bounce-back type of BCs are indeed erroneous not only quantitatively, but also *qualitatively*, as attested by the results of GA [1], which will be further dissected later in this Comment.

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The flow through a long microchannel in 2D has been studied extensively [18–23]. The analytic solution of the compressible isothermal flow through a long microchannel in 2D can be obtained by solving the steady, isothermal compressible Navier-Stokes equations in 2D perturbatively. The small parameter $\varepsilon := H/L \ll 1$ is the aspect ratio of the channel height H and the channel length L (cf. e.g., [18]). The dimensionless parameters in the flow are the Reynolds number Re, the Mach number Ma, and the Knudsen number Kn, all defined by the outlet flow conditions:

$$\mathrm{Re} := \frac{\rho_{\mathrm{out}} U_{\mathrm{out}} H}{\mu},$$
$$\mathrm{Ma} := \frac{U_{\mathrm{out}}}{\sqrt{\gamma R T}},$$
$$\mathrm{Kn} = \sqrt{\frac{\pi\gamma}{2}}\frac{\mathrm{Ma}}{\mathrm{Re}} = \sqrt{\frac{\pi R T}{2}}\frac{\mu}{H p_{\mathrm{out}}},$$

where ρ_{out} and U_{out} are the averaged density and the averaged streamwise velocity at the channel outlet, μ is the dynamic viscosity, γ is the heat capacity ratio, and R and T are the gas constant and temperature, respectively. The equation of state for an ideal gas $p = \rho R T$ is also used in the analysis. It must be emphasized that the above relationship between Kn, Ma, and Re is basically the von Kármán relationship based on the Navier-Stokes equation, which implies that Kn must be small, that is, $\mathrm{Kn} = O(\varepsilon)$, $\varepsilon \ll 1$, and $\mathrm{Re} = O(\varepsilon^{\alpha})$, $\alpha \geqslant 0$, thus $\mathrm{Ma} = O(\varepsilon^{1+\alpha})$.

The compressible Navier-Stokes equations are analyzed with the following boundary conditions. At the walls, the spanwise velocity v vanishes and the streamwise velocity u is governed by a first-order slip velocity model [24]:

$$u|_{\mathrm{wall}} = \sigma \mathrm{Kn} H \partial_y u|_{\mathrm{wall}}, \quad \sigma := \frac{(2-\sigma_v)}{\sigma_v}, \tag{2}$$

where $\sigma_v \in (0, 1]$ is the tangential momentum accommodation coefficient, which is assumed to be 1 here (hence $\sigma = 1$). The averaged pressures at the inlet and outlet are p_{in} and p_{out}, respectively. In the leading orders of ε, the solutions for the pressure $p(x)$ along the channel center line, the streamwise velocity $u(y)$, and the spanwise velocity $v(y)$ are

$$p(x) = [a^2 + (1+2a)x + \vartheta(\vartheta+2a)(1-x)]^{1/2} - a, \tag{3a}$$
$$u(x,y) = -\frac{\varepsilon \mathrm{Re}}{8\gamma \mathrm{Ma}^2} p' \left(1 - 4y^2 + 4\sigma\frac{\mathrm{Kn}}{p}\right), \tag{3b}$$
$$v(x,y) = -\frac{\varepsilon^2 \mathrm{Re}}{8\gamma \mathrm{Ma}^2}\frac{1}{p}\left[\frac{1}{2}(p^2)''\left(1 - \frac{3}{4}y\right) + 4\sigma \mathrm{Kn} p''\right] y, \tag{3c}$$

where p is normalized by p_{out}, both u and v are normalized by U_{out}, x and y are normalized by L and H, respectively. Hence $x \in [0, 1]$ and $y \in [-1/2, +1/2]$; $p' := dp/dx$, $p'' := d^2p/dx^2$, $\vartheta := p_{\mathrm{in}}/p_{\mathrm{out}} > 1$, and $a := 6\sigma \mathrm{Kn} > 0$. Clearly, the pressure $p(x)$, which is of $O(1)$, deviates from the solution of the incompressible Navier-Stokes equation, which is a straight line, that is, $p_0 := \vartheta - (\vartheta - 1)x$. The streamwise velocity u, which is of $O(\varepsilon)$, is predominantly a parabola with a slip velocity linearly proportional to Kn. The spanwise velocity v, which is of $O(\varepsilon^2)$, is antisymmetric about the channel center line $y = 0$. In most papers, if not all, which use the LBGK model to simulate the microchannel flow, only $u(y)$ and $p(x)$ are shown, but rarely $v(y)$ (cf. [7,8] and references therein); few demonstrate the convergence of the results as the mesh resolution N is increased, with fixed Re, Ma, and Kn.

The deviation of $p(x)$ from its (normalized) incompressible counterpart $p_0(x) = \vartheta - (\vartheta - 1)x$ is

$$\delta p(x) := [a^2 + (1+2a)x + \vartheta(\vartheta+2a)(1-x)]^{1/2} - (a+\vartheta) + (\vartheta-1)x, \tag{4}$$

and the gradient of $\delta p(x)$ is

$$\delta p'(x) = \frac{(1+2a) - \vartheta(\vartheta+2a)}{2[a^2 + (1+2a)x + \vartheta(\vartheta+2a)(1-x)]^{1/2}} + (\vartheta - 1). \tag{5}$$

By solving the equation of $\delta p'(x) = 0$, that is,

$$(1+a)^2 - (\vartheta+a)^2 = 2(1-\vartheta)[a^2 + (1+2a)x + \vartheta(\vartheta+2a)(1-x)]^{1/2}, \tag{6}$$

we see that $\delta p(x)$ has a unique maximum located at

$$x_{\mathrm{c}} = \frac{1}{2} + \frac{(\vartheta - 1)}{4(\vartheta + 2a + 1)}, \tag{7}$$

and $1/2 < x_{\mathrm{c}} < 3/4$ for $1 < \vartheta < \infty$. Because

$$\delta p'(0) = \frac{(\vartheta-1)^2}{2(\vartheta+a)} > 0, \tag{8a}$$
$$\delta p'(1) = -\frac{(\vartheta-1)^2}{2(1+a)} < 0, \tag{8b}$$

therefore $\delta p(x)$ is *positive* and convex in the interval $0 \leqslant x \leqslant 1$. This has been confirmed by experiments [25–27], direct Monte Carlo simulations (DSMC) [16], and the MRT-LB scheme [8].

The MRT-LB model with various BCs can be solved analytically for the Poiseuille flow [8], which is a *perfect* parabola linearly superposed with a slip velocity at the boundary depending on specifics of particle-boundary interactions. With the DSBCs, the slip velocity U_{s} measured at the $\delta_x/2$ beyond the last fluid nodes is [8]

$$U_{\mathrm{s}} = \frac{G\delta_t}{4}\left[\left(\frac{1}{s_q} - \frac{8-s_\nu}{2-s_\nu}\right) + 6N_y\right], \tag{9}$$

where G is the constant acceleration, N_y is the number of grid points across the channel, and s_ν and s_q are the relaxation rates of the shear-stress and the energy-flux moments [28]. For LBGK model, $s_\nu = s_q = 1/\tau$, thus

$$U_{\mathrm{s}} = \frac{G\delta_t}{4}\left[\left(\tau - \frac{8\tau-1}{2\tau-1}\right) + 6N_y\right]. \tag{10}$$

With $G = 8\nu U_{\mathrm{m}}/H^2$, $H = N_y\delta_x$, $\nu = c_s^2(\tau - 1/2)\delta_t$, $\mathrm{Re} = U_{\mathrm{m}}H/\nu$, and $\mathrm{Ma} = U_{\mathrm{m}}/c_s$, Eq. (10) can be rewritten as

$$\frac{U_{\mathrm{s}}}{U_{\mathrm{m}}} = 2\left(\frac{\mathrm{Ma}}{\mathrm{Re}}\right)^2\left[1 + \frac{6N_y(2\tau-1) - 5\tau}{(2\tau-1)^2}\right]. \tag{11}$$

In the LB simulations, both Re and Ma remain as constants, and so does Kn. As the resolution N_y increases, so does τ, in order to maintain a constant Re. Consequently the slip velocity U_{s} depends on both τ and N_y. This shows that the slip velocity obtained by the LBGK model is indeed a numerical artifact.

In contrast, for the MRT-LBE with the bounce-back-diffusive (BBD) boundary conditions, the slip velocity is [8]

$$U_s = \frac{G\delta_t}{4}\left[\left(\frac{1}{s_q} - \frac{8-s_\nu}{2-s_\nu}\right) + 6N_y\frac{(1-\beta)}{(1+\beta)}\right], \qquad (12)$$

where $0 \leqslant \beta \leqslant 1$, and $\beta = 1$ and 0 correspond to the bounce-back and diffusive boundary conditions, respectively. First and foremost, the MRT model allows the freedom to set $s_q = 8(2-s_\nu)/(8-s_\nu)$, so that the first term in U_s of Eq. (12) vanishes exactly. Second, by setting

$$\beta = \frac{3\mu - \mathrm{Kn}Hc\bar{\rho}_{\mathrm{out}}}{3\mu + \mathrm{Kn}Hc\bar{\rho}_{\mathrm{out}}}, \qquad (13)$$

where $c := \delta_x/\delta_t$, one has

$$U_s = \frac{\mathrm{ReKn}H}{3\delta_t U_{\mathrm{out}}}, \qquad (14)$$

which depends only on Kn and other relevant physical parameters [8]. The above result proves that the MRT model is imperative to obtain accurate and convergent results in slip-flow regime [8,29], because the LBE requires two *independent* relaxation rates to attain the consistent solution for the Poiseuille flow. We note that the LBGK models are only special cases of their MRT counterparts and that the implementation of the MRT models is just as simple as their LBGK counterparts. Thus, there is no reason not to use the MRT models.

As clearly exhibited in Fig. 6 of GA [1], when $\mathrm{Kn} = 1.0$, $\delta p(x)$ becomes negative and concave with $\delta p'(0) < 0$ and $\delta p'(1) > 0$, which is *physically* impossible, because that implies $a = 6\sigma\mathrm{Kn} < -\vartheta < -1$ [cf. Eqs. (1)]. In fact, $\delta p(x)$ already becomes *unphysical* when $\mathrm{Kn} = 0.8$, where $\delta p'(1) > 0$, which implies $6\sigma\mathrm{Kn} < -1$. Because $\vartheta := p_{\mathrm{in}}/p_{\mathrm{out}} > 1$, the defective symptom of $\delta p'(1) > 0$ (or equivalently $6\sigma\mathrm{Kn} < -1$) always appears first as Kn increases, as seen in [1] and a similar previous work [30].

Some comments are in order at this point. First, in principle simple slip-velocity models are invalid in the transitional flow region [31]. The LBGK model with the DSBCs used by GA implicitly assumes a slip-velocity model, which by definition is only valid for slip flows with small Knudsen number [31]. To accurately approximate flows in the transitional flow region, more sophisticated models are necessary [31]. Second, it is impossible for the LBE to resolve the Knudsen layer, because it is a Navier-Stokes solver. The LB solution is the exact *linear superposition* of a *perfect* parabola, that is, the solution of the incompressible Navier-Stokes equation, and a slip velocity at the channel walls [8], which is inconsistent with the Boltzmann solution in general (cf., e.g., Fig. 9-1 in [32]). Finally, we notice that a vast portion of the streamwise velocity profile $u(y)$ can be well approximated by a parabola, and this observation has been exploited to justify the claim that the LBGK model is capable of modeling rarefied flows in transitional flow regime with $\mathrm{Kn} \sim 1$ (cf. [1,7] and references therein), in spite of its fatal defects noted in the literature [8,14,16,17].

Our comments can be summarized as the following. First, for the Poiseuille flow with a constant body force, we can prove that the LBGK scheme with bounce-back type of boundary conditions, including the DSBCs used by GA [1], cannot yield the correct solution [8]. For the most part, the slip velocity obtained by using the LBGK model is a numerical artifact depending on both the relaxation parameter τ and the resolution N_y. Second, for the pressure driven compressible flow in a long channel, the LBGK scheme used by GA [1] yields *qualitatively unphysical* results in the transitional flow regime with $\mathrm{Kn} \sim 1$. In both cases we demonstrate that the MRT-LB model is imperative to obtain correct results [8]. The so-called "Knudsen effects" observed by GA [1] are merely numerical artifacts of the LBGK model or unphysical at times. The claim by GA that the LBGK model "is capable of modeling shear-driven, pressure-driven, and mixed shear-pressure-driven rarified [*sic*] flows and heat transfer up to $\mathrm{Kn} = 1$ in the transitional regime" is clearly false.

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