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A note on the lattice Boltzmann method beyond the Chapman-Enskog limits

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Abstract. – A non-perturbative analysis of the Bhatnagar-Gross-Krook (BGK) model kinetic equation for finite values of the Knudsen number is presented. This analysis indicates why discrete kinetic versions of the BGK equation, and notably the lattice Boltzmann method, can provide semi-quantitative results also in the non-hydrodynamic, finite-Knudsen regime, up to $Kn \sim \mathcal{O}(1)$. This challenges the pessimistic stance, according to which the lattice Boltzmann method should only be used for strictly hydrodynamic purposes. It may also help the interpretation of recent simulations of microflows, which show satisfactory agreement with continuum kinetic theory in the moderate-Knudsen regime.

In the last decade, the lattice Boltzmann (LB) method has developed into a very flexible and effective numerical method for the simulation of a large variety of complex flows, mostly in the macroscopic domain [1–3]. Fueled by relentless progress in micro, nano and bio-sciences, the recent years have witnessed a growing interest in exploring the possibility to enrich LB in the direction of describing micro-structured flows [4, 5].

The LB method is based on a stylized stream-and-collide microscopic dynamics of fictitious particles, located on the nodes of discrete lattices and interacting according to local collision rules that drive the system towards a local equilibrium [2, 3]. Mathematically:

$$f_i(\vec{x} + \vec{c}_i\Delta t, t + \Delta t) - f_i(\vec{x}, t) = -\omega\Delta t \left[f_i(\vec{x}, t) - f_i^{(eq)}(\vec{x}, t)\right],$$

where $f_i(\vec{x}, t)$ is the probability to find a particle at position $\vec{x}$ and time t, moving along the lattice direction defined by the discrete speeds $\vec{c}_i$ $(i = 1, ..., b)$. The second term at the r.h.s. of the above equations denotes relaxation towards a local equilibrium, the lattice analogue of a Maxwellian distribution in continuum kinetic theory:

$$f_i^{eq}(\vec{x}, t) = nw_i \left(1 + \beta\vec{c}_i \cdot \vec{u} + \frac{\beta^2}{2}[(\vec{c}_i \cdot \vec{u})^2 - u^2]\right).$$

In the above, $n(\vec{x}, t)$ is the fluid density, $\vec{u}$ the flow speed, $\beta = 1/c_s^2$ is the inverse square speed of sound, and w_i a discrete set of weights normalized to unity. Finally, ω indicates a typical time-scale relaxation (frequency relaxation) to local equilibrium, and governs the kinematic viscosity of the LB macroscopic fluid [2,6,7]. More general versions account for multiple-time relaxation [8–10], but the simpler single-time (BGK) relaxation form will be sufficient for our present purposes.

By taking suitable averages over molecular speeds, it can be shown that the resulting macroscopic quantities obey the Navier-Stokes equation of continuum mechanics. The fluid and current density are given by a linear superposition of the discrete distributions f_i:

$$n(\vec{x},t) = \sum_{i=1}^{b} f_i(\vec{x},t), \qquad \vec{J}(\vec{x},t) = \sum_{i=1}^{b} \vec{c}_i f_i(\vec{x},t). \tag{1}$$

In order for those quantities to satisfy the exact hydrodynamic equations, it is required that the macroscopic fields do not vary appreciably on the scale of the mean free path λ and the lattice spacing Δx. Based on the consolidated Chapman-Enskog background [11], one might be led to conclude that the range of applicability of LB methods is bounded by the domain of validity of the Chapman-Enskog method [12], the implication being that LB can only be used for strictly hydrodynamic purposes. Yet, such a restrictive stance is challenged by a number of recent numerical simulations [13–20] which clearly show that, by using appropriate boundary conditions, LB can reproduce some salient features of flows beyond the hydrodynamic regime, such as the onset of slip flow at finite-Knudsen numbers.

In this letter, we wish to propose a theoretical explanation for this rather unexpected validity of LB in the beyond-Chapman-Enskog region. Our analysis is based on a non-perturbative solution of the lattice BGK (LBGK) equation, which overcomes the restrictions imposed to the standard Chapman-Enskog multiple scale analysis and extensions thereof [21, 22]. This non-perturbative character sets our work apart also from very recent and systematic work on the finite-Knudsen behaviour of lattice-BGK models [23].

Our analysis is confined to the bulk region of the flow, giving for granted that the use of proper boundary conditions is crucial to obtain correct results in actual LB simulations of microflows [24].

Let us refer for simplicity to the 1d-continuum Boltzmann equation, written in BGK [25] form:

$$\partial_t f(x,v,t) + v\partial_x f(x,v,t) = -\omega\left[f(x,v,t) - f^{(eq)}(x,v,t)\right],$$

where the local equilibrium $f^{(eq)}(x,v,t)$ depends on x and t via the local velocity and density fields. Let us now consider the exact solution as provided, for each given velocity v (see also [26]), by an integration along the particle trajectory, from t to $t+\Delta t$:

$$f(x+v\Delta t, t+\Delta t) = e^{-\omega\Delta t} f(x,t) + \omega e^{-\omega\Delta t}\int_0^{\Delta t} e^{s\omega} f^{(eq)}(x+vs, t+s)\mathrm{d}s, \tag{2}$$

being Δt a generic time increment corresponding to the lattice time step. The above expression is exact, but purely formal, until one specifies a concrete procedure to compute the integral at the right-hand side. Even though the quadratic dependence of $f^{(eq)}$ on f itself prevents an exact analytical solution, one can formally expand the integrand as

$$f^{(eq)}(x+vs, t+s) = \sum_{n=0}^{\infty} \frac{s^n D^n}{n!} f^{(eq)}(x,t), \tag{3}$$

where $D \equiv \partial_t + v\partial_x$ denotes the streaming operator. By inserting this expansion into (2), we can formally solve the integral exactly, and obtain:

$$f_{t+\Delta t} = e^{-\omega\Delta t} f_t + \frac{e^{D\Delta t} - e^{-\omega\Delta t}}{1 + D/\omega} f_t^{(eq)}, \tag{4}$$

where we have used the short-hand notation $f_{t+s} = f(x + vs, t + s)$. This expression invites a number of useful considerations. Let us first recast it in the symbolic propagator form:

$$f_{t+\Delta t} = P(\omega\Delta t) f_t + Q(\omega\Delta t, D\Delta t) f_t^{(eq)}, \tag{5}$$

where

$$P(\omega\Delta t) = e^{-\omega\Delta t} \tag{6}$$

is the propagator from time t to time $t + \Delta t$, and

$$Q(\omega\Delta t, D\Delta t) = \frac{e^{D\Delta t} - e^{-\omega\Delta t}}{1 + D/\omega} \tag{7}$$

co-propagates the influence of the equilibrium at time t on the solution at time $t + \Delta t$.

By neglecting the equilibrium variations on a scale Δt, *i.e.*

$$f_{t+t'}^{(eq)} \simeq f_t^{(eq)}, \qquad 0 \le t' \le \Delta t \tag{8}$$

the propagator $e^{D\Delta t}$ acting on $f^{(eq)}$ is such that

$$e^{D\Delta t} f_t^{(eq)} = f_t^{(eq)}. \tag{9}$$

This leads to a much simplified version of the integral equation in the limit $Df^{(eq)} \to 0$:

$$f_{t+\Delta t} = e^{-\omega\Delta t} f_t + (1 - e^{-\omega\Delta t}) f_t^{(eq)} \tag{10}$$

or, equivalently,

$$f_{t+\Delta t} = P(\omega\Delta t) f_t + Q_{LB}(\omega\Delta t) f_t^{(eq)}, \tag{11}$$

where we have defined the LB co-propagator as

$$Q_{LB}(\omega\Delta t) \equiv (1 - e^{-\omega\Delta t}). \tag{12}$$

The stick-to-equilibrium approximation (9) is tantamount to retaining only the zeroth order term in the Taylor expansion (3), and consequently it is expected to work only for small values of Δt in the integral of (2).

It is interesting to note that, already at this zeroth order level, and without any further assumption on ω, it is possible to identify a fully explicit discrete Boltzmann equation in BGK form. This reads:

$$f_{t+\Delta t} - f_t = -\omega_{LB}\Delta t (f_t - f_t^{(eq)}) \tag{13}$$

with relaxation frequency $\omega_{LB}\Delta t = (1 - e^{-\omega\Delta t})$.

It is now instructive to analyze the two extreme limits $\omega\Delta t \gg 1$ and $\omega\Delta t \ll 1$, in the exact solution (5) first, and then in the discrete lattice BGK solution (11). Let us begin with the former. Provided that the kinetic operator $D\Delta t$ remains bounded, we can identify the *enslaving* limit ($\omega\Delta t \gg 1$) characterized by

$$P(\omega\Delta t) = e^{-\omega\Delta t} \longrightarrow 0,$$

$$Q(\omega\Delta t, D\Delta t) = \frac{e^{D\Delta t} - e^{-\omega\Delta t}}{1 + D/\omega} \longrightarrow e^{D\Delta t}.$$

This is equivalent to enslave the solution to the local equilibrium, *i.e.* $f_{t+\Delta t} = f^{(eq)}_{t+\Delta t}$. The opposite situation ($\omega\Delta t \ll 1$) represents the *free-molecular* limit, in which one has

$$P(\omega\Delta t) = e^{-\omega\Delta t} \longrightarrow 1$$

$$Q(\omega\Delta t, D\Delta t) = \frac{e^{D\Delta t} - e^{-\omega\Delta t}}{1 + D/\omega} \longrightarrow 0$$

corresponding to a free-flow (collisionless) solution $f_{t+\Delta t} = f_t$.

A natural question arises on the nature of the same limits in the Lattice BGK equation (11). The effect on the streaming propagator is the same, since the streaming term is integrated *exactly* in the lattice version. There remains to inspect the behaviour of $Q_{LB}(\omega\Delta t)$ in the two aforementioned limits. The enslaving limit ($\omega\Delta t \gg 1$) yields

$$Q_{LB}(\omega\Delta t) = 1 - e^{-\omega\Delta t} \longrightarrow 1 \qquad (\omega_{LB}\Delta t \sim \mathcal{O}(1))$$

that is $f_{t+\Delta t} = f^{(eq)}_t$. In view of the relation (8), this is equivalent to state $f_{t+\Delta t} = f^{(eq)}_{t+\Delta t}$. The opposite situation ($\omega\Delta t \ll 1$) yields

$$Q_{LB}(\omega\Delta t) = 1 - e^{-\omega\Delta t} \longrightarrow 0 \qquad (\omega_{LB}\Delta t \to 0).$$

Thus, the two limits, *full-enslaving* and *free-flow*, are recovered by the LBGK, provided that the relaxation frequency is turned from bare ω to ω_{LB}. The question remains: what happens in between? A restrictive tenet is that lattice BGK cannot work properly because the intermediate regime involves all-order tensors, through the powers D^n, which cannot be reproduced correctly in the discrete lattice because of lack of symmetry. On a more optimistic vein, one could counter-argue that since *both* extreme limits are correctly recovered, there might be hope that even in between the LB method could continue to provide a reasonable agreement with continuum kinetic theory.

In order to analyze this point, we introduce the *fine-scale* Knudsen number Kn, defined as

$$Kn = \lambda/\delta, \tag{14}$$

where $\lambda = v/\omega$ is the kinetic mean-free path and δ is the smallest macroscopic length.

Let us consider the most critical situation $\delta = \Delta x = v\Delta t$, *i.e.* the macroscopic fields show appreciable variation on the scale of a single lattice unit/length. Under these specific conditions, we obtain

$$\omega\Delta t = 1/Kn \tag{15}$$

from which it follows that

$$P(\omega\Delta t) = P(Kn) = e^{-1/Kn}, \tag{16}$$

$$Q(\omega\Delta t, D\Delta t) = Q(Kn, D\Delta t) = \frac{e^{D\Delta t} - e^{-1/Kn}}{1 + KnD\Delta t}, \tag{17}$$

$$Q_{LB}(\omega\Delta t, D\Delta t) = Q_{LB}(Kn, D\Delta t) = 1 - e^{-1/Kn}. \tag{18}$$

Our Knudsen-number–dependent approach is consistent with the fact that the full enslaving limit is recovered at $Kn \to 0$, which is equivalent to use a LBGK approach (13) with $\omega_{LB}\Delta t = (1 - e^{-\omega\Delta t}) \sim \mathcal{O}(1)$. Starting from this Chapman-Enskog limit ($Kn \to 0$), it is then

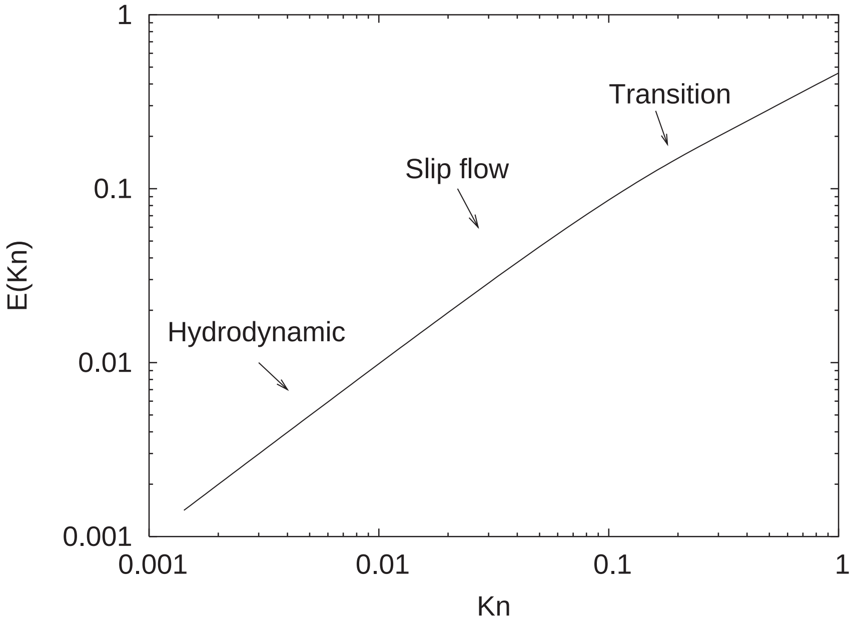

Fig. 1 – Plot of the percentage error E, as defined in (20), as a function of the Knudsen number up to the transition regime. Note that the error between the exact Boltzmann solution and the discrete form reaches a maximum of about ten percent at the top of the slip-flow regime ($Kn \sim 0.1$).

interesting to see whether the LB approach can be extended to the *slip flow* and *transition* regimes (up to $Kn \sim \mathcal{O}(1)$). In these regimes, the macroscopic fields fluctuate, in the most pessimistic case, on the same scale of the kinetic fields. Therefore, we may consistently assume that $Df/f \sim v/\delta$, and make the identification

$$D\Delta t \sim Kn. \tag{19}$$

This is the zeroth order approximation relating $D\Delta t$ to Kn. More rigorously, one should consider a full series in Kn. However, to any practical purpose, this series can be truncated at the $\mathcal{O}(Kn)$ without hampering the results up to $Kn \sim \mathcal{O}(1)$. In this approximation, the propagators become

$$Q(Kn) = \frac{e^{Kn} - e^{-1/Kn}}{1 + Kn^2},$$

$$Q_{LB}(Kn) = 1 - e^{-1/Kn},$$

where $Q(Kn)$ and $Q_{LB}(Kn)$ represent the exact physical co-propagator effects and the lattice ones, in the range $Kn < 1$, respectively. The relative departure:

$$E(Kn) = \frac{Q(Kn) - Q_{LB}(Kn)}{Q(Kn)} \tag{20}$$

is a quantitative measure of the spurious lattice-induced effects on the co-propagator. From fig. 1, where we report $E(Kn)$ as a function of Kn, it is recognized that, up to $Kn \sim 0.1$, *i.e.* in the slip-flow regime, the lattice Boltzmann approach does not differ from the exact solution for more than to within a ten percent. Only as Kn exceeds 0.1, and the transition regime is entered, significant error build-up is observed.

It is important to emphasize that the above figures apply to the worst-case scenario, in which macroscopic fields vary on the scale of a *single* lattice spacing (an extreme beyond-Chapman-Enskog situation). One may soften this assumption and assume that macroscopic fields exhibit significant variations on scales larger that a single grid spacing Δx, say

$$\delta = h\Delta x, \qquad h \geq 1, \tag{21}$$

$h = 1$ reproducing the previous worst-case scenario. This means that the Knudsen number is reduced by a factor h, $Kn \to Kn/h$, leading to a corresponding reduction in the error $E(Kn)$. In addition, we observe that $E(Kn)$ measures the error of the propagator, whereas physical observables result from the summation of discrete populations f_i over the discrete speeds (see eqs. (1)) and, consequently, $E(kn)$ as defined in (20) may well represent a pessimistic bound. In any event, the point of the present analysis is not to state the case for the accuracy of LB in the non-hydrodynamic regime, but only to point out that, even at finite-Knudsen numbers, discreteness effects remain within fairly tolerable limits, at least for semi-quantitative purposes. Whether or not LB should be used instead of more accurate, and much more expensive, methods, such as Direct Simulation Monte Carlo, remains to be decided on a case-by-case basis.

Summarizing, a non-perturbative analysis of the Boltzmann equation in BGK form, indicates that the LB method may continue to provide semi-quantitative agreement beyond the limits of the Chapman-Enskog theoretical framework. This could be of interest for the interpretation of lattice Boltzmann simulations in the finite-Knudsen regime, including kinetic modeling of fluid turbulence [27]. Clearly, in order to realize the bulk properties highlighted by the present analysis, proper kinetic boundary conditions [18,20] must be used in actual LB simulations of finite-Knudsen flows.

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