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LATTICE-BOLTZMANN SIMULATIONS OF FLUID FLOWS AT FINITE KNUDSEN NUMBERS

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ABSTRACT

The lattice-Boltzmann method is a possible alternative to standard computational fluid dynamics (CFD) or direct simulation Monte Carlo (DSMC) simulations of fluid flows in continuum, slip and transition regimes. We evaluate the accuracy of the lattice-Boltzmann (LB) method for the simulation of microchannel fluid flows at finite Knudsen numbers. A novel modeling of the adaptive Knudsen number as a function of fluid density is proposed in the lattice-Boltzmann model. Specific boundary conditions are used to represent the slippage at the wall and for the simulation of open flows. We compare our simulation results with DSMC data.

Keywords: DSMC, equilibrium boundary conditions, finite Knudsen number, lattice-Boltzmann, relaxation time correction

NOMENCLATURE

NOTE: In this article, we are using two unit systems: SI units and lattice-Boltzmann (abbreviated LB) units. In the nomenclature section, if a quantity is defined using both SI and LB units system, we indicate the SI units.

\begin{align*}
P & \text{[Pa]} \quad \text{pressure} \\
W & \text{[-]} \quad \text{weight coefficient} \\
c_s & \text{[m/s]} \quad \text{speed of sound} \\
\varepsilon & \text{[-]} \quad \text{discrete velocity vector} \\
f & \text{[-]} \quad \text{distribution function} \\
k_B & \text{[m^2 kg/s^2]} \quad \text{Boltzmann constant} \\
\dot{\psi} & \text{[kg/s]} \quad \text{mass flow rate} \\
t & \text{[tu]} \quad \text{time} \\
u & \text{[m/s]} \quad \text{velocity vector} \\
x & \text{[lu]} \quad \text{lattice site position} \\
\lambda & \text{[m]} \quad \text{mean free path} \\
\nu & \text{[m^2/s]} \quad \text{kinematic viscosity} \\
\pi & \text{[-]} \quad \text{constant 3.14} \\
\rho & \text{[kg/m^3]} \quad \text{density} \\
\sigma & \text{[m]} \quad \text{particle hard shell diameter} \\
\tau & \text{[-]} \quad \text{relaxation time}
\end{align*}

Subscripts and Superscripts

\begin{align*}
c & \text{copied quantity} \\
\text{calc} & \text{calculated quantity} \\
d & \text{desired (imposed) quantity} \\
i & \text{discrete direction} \\
eq & \text{equilibrium distribution} \\
\text{ref} & \text{reference quantity} \\
* & \text{quantity in SI units}
\end{align*}

1 INTRODUCTION

Direct simulation Monte-Carlo (DSMC) is standard method to simulate finite Knudsen number fluid flows, but its drawback is the large computational time required for each simulation. In this situation,
alternative numerical methods are required for simulation of finite Knudsen number flows at lower computational cost, but still maintaining reasonable accuracy. Due to its particulate nature and local dynamics, the lattice-Boltzmann (LB) method is a reliable candidate for the simulation of finite Knudsen number flows. Different models have been proposed in the literature to enhance the accuracy of the standard LB method for simulation of the finite Knudsen number flows: different slip boundary conditions at the walls, local relaxation time [1, 2] or higher order LB models [3]. Examples of slip boundary conditions for finite Knudsen number flows are the diffusive reflection boundary conditions with local accommodation coefficients [4] or the virtual wall collision mechanism [5]. However, these LB models do not represent accurately the heat transfer between the fluid and walls or temperature variation in the fluid. To simulate high Knudsen number thermal flows, we propose a coupled fluid flow and thermal solver, with the temperature field resolved using a passive-scalar approach. The first step of this thermal coupling approach is to develop a LB solver for fluid flow at high Knudsen numbers with boundary conditions that can be easily coupled with the temperature field solver. In this respect, the walls are represented using the equilibrium boundary conditions proposed by Ansumali and Karlin [6], which can be defined in both fluid flow and thermal solvers. Moreover, different boundary conditions to impose a mass flow rate at the inlet of a channel are evaluated and a model to account for the variation of the Knudsen number along the channel length is introduced.

In the following section we introduce the lattice-Boltzmann model. The LB simulation results are compared against DSMC data for microchannel flow at low and intermediate Knudsen numbers. For the sake of simplicity, only a two dimensional solver has been implemented, but the implementation and parallelization of the LB solver for three-dimensional geometries is straightforward. The purpose of the fluid flow simulations at low Knudsen number is to validate the implementation of specific boundary conditions and models in the LB solver. Finally, simulations of the fluid flow at Knudsen numbers around 2 are performed to evaluate the limits and accuracy of our LB solver.

2 LATTICE-BOLTZMANN MODEL

The Lattice-Boltzmann (LB) method is a powerful tool for simulating weakly compressible fluid flows [7, 8]. It considers solving the discretized Boltzmann equation

\[ f_i(x + e_i, t + 1) - f_i(x, t) = \frac{1}{\tau} \left[ f_i(x, t) - f_i^{eq}(x, t) \right], \]

where \( f \) represents the distribution function for the velocity component \( i \) at position \( x \) and time \( t \). In the LB method, the physical domain is divided in square (in 2D) or cubic (in 3D) voxels with the lattice constant \( \Delta x \), and the time is discretized with the timestep \( \Delta t \). On each lattice site, the velocity vector is discretized into a finite set of directions \( e_i, i = 1 \ldots N \). In this article, we consider only the two-dimensional D2Q9 lattice, i.e. \( N = 9 \) velocities for the two-dimensional domain. All physical quantities in this section are assumed in LB units, unless a different unit system is explicitly stated. The left hand side of Eq. (1) represents the propagation (streaming) of the fluid motion. The right hand side of Eq. (1) is a simple formulation of the collision operator using a single relaxation time with the time constant \( \tau \). This formulation of the collision part is called the Bhatnagar-Gross-Krook (BGK) scheme [9], and it assumes that the equilibrium distribution function is given by [10]

\[ f_i^{eq}(x, t) = W_i \rho |1 + \frac{e_i \cdot u^{eq}_i}{c_s^2} + \frac{(e_i \cdot u^{eq}_i)^2}{2 c_s^4} - \frac{|u^{eq}_i|^2}{2 c_s^2}|, \]

where the weights \( W_i \) for the D2Q9 lattice site are given by

\[ W_i = \begin{pmatrix} 4 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 9 & 9 & 9 & 9 & 36 & 1 & 36 & 1 & 36 \end{pmatrix}. \]

The density and bulk velocity in absence of any external acceleration acting in the fluid are given as

\[ \rho = \sum_i f_i(x, t), \]

\[ u = \sum_i f_i(x, t) \cdot e_i. \]

In absence of any external force, the equilibrium velocity \( u^{eq} \) equals the bulk velocity \( u \). The speed of sound in LB is a lattice-dependent quantity, which takes the value [7]

\[ c_s = \frac{1}{\sqrt{3}}, \]

which can be employed in the equation of state for pressure as

\[ P = c_s^2 \rho. \]

The kinematic viscosity (\( \nu \)) of the fluid is represented in the LB model by the relaxation time \( \tau \) according to

\[ \nu = c_s^2 \left( \tau - \frac{1}{2} \right). \]

As the speed of sound is a fixed value in LB units (Eq. (6)), the relaxation time as function of kinematic viscosity is given as

\[ \tau = 3\nu + 0.5. \]

The computational domain is extended with two layers of halo lattice sites in all directions. The halo
sites are needed to implement some of the boundary conditions, e.g. free-slip, periodic, bounce-back, equilibrium at wall. The collision operator is applied only to the fluid lattice sites, while the streaming is applied in all sites (including the halo).

2.1 Finite Knudsen flow simulation

The Knudsen number can be defined using the quantities in LB units as

\[ Kn = \frac{\nu}{c_s N}, \]  \hspace{1cm} (10)

where the kinematic viscosity \( \nu \) is defined by Eq. (8), \( N \) is the number of lattice sites representing the characteristic length (channel height, in this case) and the speed of sound \( c_s \) is defined by Eq. (6). In our simulations, the Knudsen number is introduced in the model through the relaxation time, using Eqs. (8) and (10):

\[ \tau = \frac{Kn N}{c_s} + 0.5. \]  \hspace{1cm} (11)

On the other hand, the Knudsen number defined using quantities in SI units is given by

\[ Kn = \frac{\lambda^*}{H^*} = \frac{k_B T^*}{\sqrt{2\pi}(\sigma^*)^2 P^* H^*}, \]  \hspace{1cm} (12)

where \( \lambda^* \) is the mean free path, \( H^* \) is a characteristic length, \( k_B \) is the Boltzmann constant and \( \sigma^* \) is the particle hard shell diameter. In this formula, the superscript * indicates that the physical quantities are considered in SI units. Considering the isothermal fluid flow lattice-Boltzmann, one observes that the right hand side of the Eq. (12) is constant except for the pressure. Based on this observation and using the ideal gas equation of state assumed in the LB model (Eq. (7)), we consider that \( Kn \rho^* = \text{constant} \). Furthermore, replacing in this constant relation the definition of the Knudsen number in LB units (Eq. (10)) and the relation between the relaxation time and viscosity (Eq. (8)), we found the following correction for the relaxation time:

\[ \tau = 0.5 + \frac{(\tau_{\text{ref}} - 0.5) \rho_{\text{ref}}}{\rho}. \]  \hspace{1cm} (13)

For the testcase considered in this project, density at the outlet is imposed and the Knudsen number at the outlet is known. Therefore, we choose the reference values for density \( \rho_{\text{ref}} \) and relaxation time \( \tau_{\text{ref}} \) as the values at the outlet.

2.2 Boundary conditions

The walls are represented in our model using the boundary conditions proposed by Ansumali and Karlin [6]. Such boundary conditions are implemented by imposing on the halo lattice sites an equilibrium distribution with zero value of the normal component of velocity and the tangential velocity is the opposite tangential velocity in the neighboring fluid lattice site. With this approach, the wall is positioned at the half distance between halo and neighboring fluid lattice site. Moreover, the distributions going to the fluid nodes (unknown distributions) are re-scaled such that mass coming from the fluid nodes is conserved. According to Toschi and Succi [5], this boundary condition is significantly improving the accuracy and stability of the LB simulations at high Knudsen numbers with respect to the bounce-back boundary condition. Bounce-back boundary conditions are standard LB conditions to represent the walls, which are implemented by reversing the direction of the distribution function in the lattice sites situated next to the wall.

To represent open flows, i.e. to impose a desired density, velocity, or mass flow, two types of boundary conditions are implemented:

- Zou-He boundary conditions (abbreviated BC-ZH), documented in [11, 12], are derived assuming that the bounce-back condition holds in the direction normal to the boundary. These boundary conditions are applied on the fluid lattice sites closest to the inlet/outlet (not in the halo lattice) after the streaming step.

- equilibrium boundary conditions following the approach of Ansumali and Karlin [6] (abbreviated BC-AK). They are applied on the halo sites, before streaming, by imposing the equilibrium distributions calculated using the desired quantity and values copied from the closest lattice site in the fluid domain. For instance, if we impose a density \( \rho_d \) at the inlet using these conditions, one copies the velocity from the neighboring fluid site \( u_c \) and calculate the equilibrium distribution on the halo site \( f_i^* (\rho, u_i) \). If the mass flow rate \( \dot{m} \) is imposed with this condition, the density is copied from the neighboring fluid site \( \rho_e \) and velocity is calculated from the mass flow rate \( u_{\text{calc}} = \dot{m} / \rho_e \).

3 SIMULATION RESULTS

The simulation results for finite Knudsen flows obtained using the LB code are compared to DSMC simulations. For comparison, we consider a two dimensional hydrogen gas flow through a parallel plate channel of 150mm×7mm (see Figure 1). For this testcase, the mass flow rate is imposed at the inlet and the pressure at the outlet. In the LB model, the pressure is proportional to density (Eq. (7)) and the density will be imposed at the outlet. We compare LB and DSMC results for two Knudsen numbers measured at the outlet: low Knudsen number simulations (\( Kn \approx 0.07 \)) to validate the implementation of the LB model, and intermediate Knudsen number simulations (\( Kn \approx 1.7 \)) to evaluate the limits and accuracy of our LB model. In this section, both SI and LB unit system are used. The quantities of DSMC simulations are given in SI units. The LB simulations are performed using
quantities in LB units, but the simulation results are converted in SI units for comparison with the DSMC data. The unit system of quantity is explicitly stated for each particular situation.

All DSMC calculations are done with G.A. Bird’s DS2V code v4.5.06 [13, 14]. At the inlet we adopt a ‘flow entry’ boundary condition. It requires a number density and average inlet velocity. At the exit we specify a number density and a static gas temperature. This temperature is fixed at 295 K in all our runs. The gas-wall interaction is modeled by the Cercignani-Lampis-Lord scattering kernel. This kernel contains several parameters, called accommodation coefficients. When these coefficients are all set to unity, one retrieves the fully diffuse scattering kernel of Maxwell. We expect this kernel to reproduce the bounce-back boundary condition of the LB model at the larger scale. The desired mass flow rate at the desired static outlet pressure is realized by tuning the two parameters at the flow entry together with the number density at the outlet. This iterative procedure was done manually.

In order to convert the quantities and dimensions considered in the DSMC simulations from SI to LB units, we choose the number of lattice sites on the channel height, the density at the outlet and calculate the relaxation time $\tau$ from the Knudsen number measured at the outlet of the DSMC simulations (see Eq. (11)). By fixing these quantities, one can determine the space, time and mass unity, which are further employed to convert the SI to LB units and vice-versa. Following this approach, the parallel plate channel is represented by 450 × 21 lattice sites and the relaxation time and density are calculated/chose for each testcase. In the following simulations, maximum $10^5$ iterations of the LB solver, i.e. about 15 minutes of single core computation time, are required to obtain the steady-state solution for both density and velocity fields.

### 3.1 Simulation of fluid flow at low Knudsen number

We consider DSMC simulations with the inlet mass flow rate $\dot{m} = 31.8 \cdot 10^{-6}$ kg/s and the outlet pressure $P = 20$ Pa. In the LB model, the density imposed at the outlet is chosen as 0.1 and the inlet mass flow rate determined from unit conversion is 0.0155. The relaxation time for Knudsen number 0.076 at the outlet is calculated as $\tau = 3.26$.

The fluid flow results are presented in Figures 2 and 3. We compare the DSMC data (solid lines) against the LB simulations in two situations: dashed lines are results obtained by correcting the fluid flow relaxation time with density (Eq. (13)) and the dotted lines are the results obtained for constant fluid flow relaxation time ($\tau$ = constant).

![Figure 1. Parallel plate channel](image1)

In order to convert the quantities and dimensions considered in the DSMC simulations from SI to LB units, we choose the number of lattice sites on the channel height, the density at the outlet and calculate the relaxation time $\tau$ from the Knudsen number measured at the outlet of the DSMC simulations (see Eq. (11)). By fixing these quantities, one can determine the space, time and mass unity, which are further employed to convert the SI to LB units and vice-versa. Following this approach, the parallel plate channel is represented by 450 × 21 lattice sites and the relaxation time and density are calculated/chose for each testcase. In the following simulations, maximum $10^5$ iterations of the LB solver, i.e. about 15 minutes of single core computation time, are required to obtain the steady-state solution for both density and velocity fields.

![Figure 2. Comparison of density (a), velocity (b) and mass flow rate (c) along the channel at low Knudsen number (Kn = 0.076)].(image2)
Figure 3. Density (left) and velocity (right) profiles obtained from cross-sections on the channel height at three positions along the channel: inlet, middle, and outlet.
the channel height. In Fig. 3, we present a cross-section of density and velocity on the channel height at three positions along the channel: at the inlet, in the middle of channel length and at the outlet. One observes that although the mass flow rate is similar in both LB simulations (Fig. 2(c)), a dramatic improvement of the density (Fig. 2(a)) and velocity profiles (Fig. 2(b)) in respect with the DSMC simulations is obtained by using the correction Eq. (13). The improvement is obvious when looking at the density profile at the inlet (Figs. 2(a) and 3(b)). Therefore, we apply the correction Eq. (13) in the following LB simulations of the finite Knudsen flows.

3.2 Simulation of fluid flow at intermediate Knudsen number

We consider the DSMC simulations with the inlet mass flow rate \( \dot{m}_L = 3.66 \cdot 10^{-6} \) kg/s and the outlet pressure \( P = 0.8 \) Pa. In the LB model, the density imposed at the outlet is chosen as 0.1 and the inlet mass flow rate determined from the unit conversion is 0.04. The relaxation time for Knudsen number 1.71 at the outlet is calculated as \( \tau = 62.7 \). In Figure 4, we compare the DSMC data (solid lines) against the LB simulations (dashed lines). One notices differences in the density value at the inlet of the channel when comparing the DSMC and LB simulation results. To explain these differences, one can argue that we consider isothermal LB model, while temperature variation is integrated in the DSMC model. But these differences cannot be explained by the lack of coupling with the thermal field because, in these DSMC simulations, the temperature has small variations in the range 290 \( \pm \) 295 K over the domain. Furthermore, we run LB simulations with different profiles (constant or Poiseuille) of the mass flow rate profile, but we observed a change only on the velocity profile at the inlet and not a significant change of the density value along the channel.

3.3 Discussion of the simulation results

Furthermore, we investigate the influence of the Mach number on the variation of density along the channel in the LB simulations. It is known that following the SI to LB unit conversion, the speed of sound is not accurately represented in the LB simulations. Moreover, with the LB model considered in this work, one can not choose independently Mach and Knudsen numbers. If the speed of sound is not accurately represented in the LB simulations, one can expect errors in the density profile. As a rule of thumb, the LB method is expected to be accurate for Mach numbers up to values around 0.15. Regarding the value of Mach number in the DSMC simulations, we found a maximum value \( \text{Ma} = 0.34 \) for the low Knudsen number flow (section 3.1) and \( \text{Ma} = 0.55 \) for the high Knudsen number flow (section 3.2). Looking at the LB simulation results, we found the maximum value of velocity in LB units is 0.2 (\( \text{Ma} = 0.34 \)) for the low

Knudsen number flow (section 3.1) and the maximum value of velocity in LB units is 0.4 (\( \text{Ma} = 0.7 \)) for the high Knudsen number flow (section 3.2). For this reason, we considered another DSMC simulation of fluid flow at high Knudsen number 2.04, which has the maximum Mach number \( \text{Ma} = 0.13 \). In the DSMC simulation, the inlet mass flow rate is \( \dot{m} = 0.83 \cdot 10^{-6} \) kg/s and the outlet pressure \( P = 0.8 \) Pa. The density imposed at the outlet is chosen as 0.1 and the inlet mass flow rate is determined as 0.011. The relaxation times for Knudsen number 2.04 at the outlet obtained from unit conversion are \( \tau = 75.1 \). The fluid flow relaxation time \( \tau \) corresponds to a Knudsen number at the outlet of 2.

The comparison of LB and DSMC simulation results for the fluid flow are presented in the Figure 5. In these LB simulations, we impose the mass flow rate at the inlet using different types of boundary conditions: equilibrium boundary conditions, i.e. BC-AK (dashed lines) and Zou-He boundary conditions, i.e. BC-ZH with constant (dotted lines) or Poiseuille profile (dash-dot lines). In these simulations, the maximum value of velocity is relatively small 0.16 (\( \text{Ma} = 0.27 \)) and one notices a better match of velocity and density profiles.
Nevertheless, we can not explain the dependency on the type of boundary condition used to impose the mass flow rate at the inlet: the equilibrium boundary conditions BC-AK is better matching the DSMC density profile, while the Zou-He boundary conditions BC-ZH is matching the velocity profiles. This observation can help understanding the background of large deviations observed in the density profiles of the other LB simulations, but further investigations are required.

4 CONCLUSION

We implemented and validated a lattice-Boltzmann solver for simulation of the fluid flow at finite Knudsen numbers. Equilibrium boundary conditions are considered at the wall and two different methods to impose the mass flow rate at the inlet are presented. We introduced a correction of the relaxation time with density $\tau(\rho)$, which is critical to reproduce the physics of fluid flows at finite Knudsen numbers. We found good agreement between DSMC and LB simulation results of fluid flow at small Knudsen numbers. The LB simulation results at Knudsen number around 2 shown a qualitative agreement with the DSMC results, but the density at the inlet of the channel is different. We explain this difference by comparing the Mach number in different LB simulations. As outlook, a consistent approach for coupling the momentum and thermal fields in the LB model is expected to improve the accuracy of the LB simulations of fluid flow at finite Knudsen numbers. Further investigation on the boundary conditions to impose the desired mass flow rate at the inlet is required.

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