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Simulation of micro- and nano-scale flows via the lattice Boltzmann method

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Abstract

We use the lattice Boltzmann method (LBM) for analysis of high and moderate Knudsen number phenomena. Simulation results are presented for microscale Couette and Poiseuille flows. The slip velocity, nonlinear pressure drop, and mass flow rate are compared with previous numerical results and/or experimental data. The Knudsen minimum is successfully predicted for the first time within the LBM framework. These results validate the usage of the LBM based commercial, arbitrary geometry code PowerFLOW for simulating nanoscale problems.

Keywords: Lattice Boltzmann; Knudsen number; Micro-scale; Nano-scale; PowerFLOW

1. Introduction

Navier–Stokes equations (NSEs) are based upon the continuum assumption, which is valid when the characteristic length L of the system is much larger than the mean free path λ of the molecules. Therefore, the ratio of λ to L, defined as the Knudsen number $Kn = \lambda/L$, is a natural measure of applicability of the NSEs.

In many cases involving macroscopic flows, the Kn is indeed small ($Kn \leqslant 0.001$). However, there are now increasingly many applications where Kn is relatively large. As an example, in a micro-scale channel or microelectromechanical systems (MEMS), Kn can reach or exceed 0.1 depending on the characteristic length of interest, given that $\lambda = 65$ nm for air at room temperature. High Kn flow may also occur in a low pressure vacuum device or at high altitude. It is known that for $Kn > 0.001$, the continuum assumption is no longer valid and modifications to the NSEs are necessary.

The entire flow region can be categorized into several regimes based on the Kn [1]: continuum flow, $Kn \leqslant 10^{-3}$; slip flow, $10^{-3} \leqslant Kn \leqslant 10^{-1}$; transition flow, $10^{-1} \leqslant Kn \leqslant 10$; free-molecule flow, $Kn > 10$. In the above four regimes, different dynamic models can be used. Interestingly, almost all of these models are based on or can be derived from the kinetic equation, or the molecular dynamics and the direct simulation Monte Carlo (DSMC) [2]. For continuum flows, the first choice is still the NSEs with no-slip boundary conditions, although the lattice Boltzmann method (LBM) is now becoming a viable alternative. NSEs with slip boundary

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conditions have been applied to describe moderate *Kn* regime. The first-order slip boundary condition has been proposed by Maxwell [3]:

$$u = \frac{2-\sigma}{\sigma}\,\lambda\,\left.\frac{\partial u}{\partial y}\right|_w, \tag{1}$$

where σ is the so-called tangential-momentum-accommodation coefficient defined as the fraction of molecules which are reflected diffusely. It depends on the fluid–solid interface property and can be determined experimentally. It has been shown that the first-order slip boundary conditions are approximately valid for *Kn* less than 0.1 [4]. It is possible to extend the applicable *Kn* a little further by adding the second-order effects to the slip boundary conditions [4], but for $Kn > 0.1$, much more serious modifications to the NSEs must be introduced in addition to the phenomenological slip boundary conditions, since the continuum approximation breaks down completely.

Whereas Boltzmann equation (BE) is valid for all *Kn* flows, it is difficult to solve except for the free-molecule regime, mostly because of the nonlinear collision term. Numerous approximations based on BE have been developed. The Chapman–Enskog method has been widely used to simplify the BE, in which the BE is expanded as a function of the *Kn*. The first term represents the Maxwellian equilibrium distribution function f_0. The Euler equations can be derived from f_0 as the approximation of the distribution function. The first two terms in Chapman–Enskog expansion, $f_0 + Knf_1$, may be used to derive the NSEs, which represents a first-order departure from the thermal equilibrium. The so-called Burnett equations can be derived from the first three terms ($f_0 + Knf_1 + Kn^2 f_2$), which represents a second-order departure from equilibrium.

During the last few years, LBM has been introduced for solving slip flows [5,6]. Since LBM is directly derived from microscopic principles, it seems to be a natural tool for studying rarefied gas dynamics. Other advantages of LBM include low numerical diffusion, scalable performance in a parallel computing environment, coding simplicity, and robustness in dealing with complex boundary conditions. LBM has already had substantial impact on fundamental research and engineering applications involving hydrodynamics of small *Kn* flow [7–10].

In this paper, we apply LBM beyond the continuum regime, i.e., for flows involving $Kn > 0.001$. We first outline some fundamentals in LBM and high *Kn* extensions. Simulations of Couette flow will then be presented and the results are compared with those of the first-order modified Reynolds equation (MRE). Simulation results for Poiseuille flows are compared with both the previous numerical results and experimental data. We demonstrate that famous Knudsen minimum effect [11] is successfully predicted for the first time using LBM.

2. The numerical algorithm

2.1. Outline of LBM

The most common form of the lattice Boltzmann equation (LBE) is [7,12,13]:

$$f_i(\mathbf{x} + \hat{c}_i\Delta t, t + \Delta t) - f_i(\mathbf{x}, t) = C_i, \tag{2}$$

where f_i are the particle density distributions defined for a finite set of discrete particle velocity vectors $\{\hat{c}_i : i = 0, \ldots, b\}$. These particle speeds define links among nodes on a given lattice. The collision term on the right side of Eq. (2) often uses the so-called Bhatnagar–Gross–Krook (BGK) approximation [10,12–15],

$$C_i = -\frac{f_i - f_i^{eq}}{\tau}, \tag{3}$$

with a single relaxation time τ. Here, f_i^{eq} is the local equilibrium distribution function that has an appropriately prescribed functional dependence on the local hydrodynamic properties. The basic hydrodynamic quantities, such as fluid density ρ and velocity $\mathbf{u}$, are obtained through moment summations in the velocity space,

$$\rho(\mathbf{x}, t) = \sum_i f_i(\mathbf{x}, t) \quad \text{and} \quad \rho\mathbf{u}(\mathbf{x}, t) = \sum_i \hat{c}_i f_i(\mathbf{x}, t). \tag{4}$$