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Microflow Simulations via the Lattice Boltzmann Method

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Abstract. The exact solution to the hierarchy of nonlinear lattice Boltzmann kinetic equations, for the stationary planar Couette flow for any Knudsen number was presented by S. Ansumali et al. [Phys. Rev. Lett., 98 (2007), 124502]. In this paper, simulation results at a non-vanishing value of the Knudsen number are compared with the closed-form solutions for the higher-order moments. The order of convergence to the exact solution is also studied. The lattice Boltzmann simulations are in excellent agreement with the exact solution.

AMS subject classifications: 52B10, 65D18, 68U05, 68U07 **Key words**: Microflows, lattice Boltzmann method.

1 Introduction

Engineering interest in microelectromechanical systems (MEMS) has experienced explosive growth during the last two decades [1]. These kind of devices typically have characteristic size ranging from a few micron to a few millimeters, often with high aspect ratios. Often one is interested in gaseous flows through micro-devices such as micro-pumps, micro-turbines, and micro-valves [1]. It is well understood that for gaseous flows at those length-scales hydrodynamic framework starts to breakdown. A computational approach that recently emerged as a potential candidate for such gaseous micro-flow simulations is the lattice Boltzmann method (LB).

This computational tool has been also used to study many other microfluidic flow problems involving multiphase flows [3–7]. In all these studies, the role of proper wall boundary conditions has been shown to be essential. In this paper, the ability of the method to capture numerically, non-trivial micro-flow phenomena for single component gaseous flows, by using the diffusive boundary condition [8] is studied in detail.

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2 Lattice Boltzmann approach for microflows

The capability of the lattice Boltzmann method to simulate micro-flows stems from its kinetic theory origin. The lattice Boltzmann method is a special velocity-time-space discretization of the continuous Boltzmann BGK equation.

Even though the solution of the discrete Boltzmann BGK equation in the bulk flow is quite standard, for the implementation of the wall boundary condition several approaches exist [2, 5, 8]. The most commonly used ones are the bounce back and the kinetic diffusive boundary condition. In this paper we focus on the study of the numerical discretization of the diffusive boundary condition as presented in [8, 9]. One of the most attractive features of this boundary condition is the non-trivial micro-flow effects that can be captured without the need of tuning any parameters. For simplicity the nine-velocities, two-dimension lattice BGK model (D2Q9) will be considered. The micro-Couette flow is the selected micro-flow setup case. Analytical solutions for that problem is reported in [10, 11]. For that, the moment system of the Boltzmann BGK equation [12], combined with the properties of the D2Q9 square lattice discretization are analyzed. We consider the popular nine-velocity model, the so-called D2Q9 lattice, for which the discrete velocities are: $c_0 = (0,0)$, $c_i = (\pm 1,0)$ and $(0,\pm 1)$, for i=1-4, and $c_i = (\pm 1,\pm 1)$, for i=5-8 (see [14]). The discrete lattice Bhatnagar-Gross-Krook (BGK) equation reads:

$$\partial_t f_i + c_{i\alpha} \partial_\alpha f_i = -\frac{1}{\tau} \left(f_i - f_i^{eq} \right), \tag{2.1}$$

where τ is the relaxation parameter, and f_i^{eq} the values of populations at equilibrium. The equilibrium distribution functions neglecting terms of the order $\mathcal{O}(u^3)$ and higher can be expressed as:

$$f_i^{eq} = w_i \left(\rho + \frac{j_\alpha c_{i\alpha}}{c_s^2} + \frac{j_\alpha j_\beta}{2\rho c_s^4} (c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta}) \right), \tag{2.2}$$

where c_s is the speed of sound, $c_s = \sqrt{(k_B T_0)/m} = \sqrt{1/3}$. For the D2Q9 model, the corresponding weights w_i are:

$$w = \frac{1}{36} \begin{bmatrix} 16 & 4 & 4 & 4 & 4 & 1 & 1 & 1 & 1 \end{bmatrix}.$$
 (2.3)

In the hydrodynamic limit, this model recovers the Navier-Stokes equations with the kinematic viscosity $v = \tau c_s^2$. By considering the moments of the lattice-BGK equation, a moment system can be created and closed form solutions for specific flow setups can be obtained.

3 Moment system

Since the D2Q9 lattice is described by a set of nine distribution functions f_i , a ninemoment system will be formulated. For the isothermal D2Q9 model, the conserved fields