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Semiclassical Lattice Boltzmann Simulations of Rarefied Circular Pipe Flows

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Abstract. Computations of microscopic circular pipe flow in a rarefied quantum gas are presented using a semiclassical axisymmetric lattice Boltzmann method. The method is first derived by directly projecting the Uehling-Uhlenbeck Boltzmann-BGK equations in two-dimensional rectangular coordinates onto the tensor Hermite polynomials using moment expansion method and then the forcing strategy of Halliday et al. [Phys. Rev. E., 64 (2001), 011208] is adopted by adding forcing terms into the resulting microdynamic evolution equation. The determination of the forcing terms is dictated by yielding the emergent macroscopic equations toward a particular target form. The correct macroscopic equations of the incompressible axisymmetric viscous flows are recovered through the Chapman-Enskog expansion. The velocity profiles and the mass flow rates of pipe flows with several Knudsen numbers covering different flow regimes are presented. It is found the Knudsen minimum can be captured in all three statistics studied. The results also indicate distinct characteristics of the effects of quantum statistics.

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1 Introduction

Over the past two decades, significant advances in the development of the lattice Boltzmann methods (LBMs) [1–4] based on classical Boltzmann equations with the relaxation time approximation of Bhatnagar, Gross and Krook (BGK) [5] have been achieved. The

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lattice Boltzmann methods have demonstrated its ability to simulate hydrodynamic systems, magnetohydrodynamic systems, multi-phase and multi-component fluids, multi-component flow through porous media, and complex fluid systems, see [6]. The lattice Boltzmann equations (LBE) can also be directly derived in *a priori* manner from the continuous Boltzmann equations [7, 8]. Most of the classical LBMs are accurate up to the second order, i.e., Navier-Stokes hydrodynamics and have not been extended beyond the level of the Navier-Stokes hydrodynamics. A systematical method [9, 10] was proposed for kinetic theory representation of hydrodynamics beyond the Navier-Stokes equations using Grad's moment expansion method [11].

However, most of the existing lattice Boltzmann methods, despite their great success, are limited to hydrodynamics of classical particles. Recent development in nanoscale transport requires carriers of particles of arbitrary statistics [12]. The generalization of the successful LBMs for classical gas to that for particles of arbitrary statistics is thus desirable. Specifically, a semiclassical Boltzmann equation, which is analogous to the classical Boltzmann equation, for transport phenomenon in quantum gases has been developed by Uehling and Uhlenbeck (UUB) [13]. Also, to avoid the mathematical complexity of the collision term, BGK-type relaxation time models to capture the essential properties of carrier scattering mechanisms can be similarly devised for the Uehling-Uhlenbeck Boltzmann equation for various carriers and have been widely used in carrier transports [14]. Recently, a new semiclassical lattice Boltzmann method for the Uehling-Uhlenbeck Boltzmann-BGK (UUB-BGK) equations based on Grad's moment expansion method by projecting the UUB-BGK equations onto Hermite polynomial basis has been presented [15] for D2Q9 lattice model. Hydrodynamics based on moments up to second and third order expansions are presented. Simulations of flow over a circular cylinder at low Reynolds numbers have been tested and have been found in good agreement with previous available results.

One of the most common and important classes of fluid dynamical problems is the axisymmetric flow in which the flow symmetry with respect to an axis can be identified. Classical axisymmetric lattice Boltzmann method was first proposed by Halliday et al. [16] using a forcing strategy. By introducing source terms, the macroscopic equations for the axisymmetric flows can be recovered through Chapman-Enskog expansion. The method of Halliday et al. has been successfully applied to a number of axisymmetric flow problems [17–25]. Recently, an interesting lattice Boltzmann model for axisymmetric flows based on Boltzmann-BGK equation in cylindrical coordinates has been proposed [26].

The objective of this work is to present the simulation of circular pipe flow in rarefied gases of arbitrary statistics using a semiclassical axisymmetric lattice Boltzmann method. The rarefied circular pipe flows considered here covers the Knudsen $(\lambda \gg D)$, slip $(\lambda \sim D)$ and Poiseuille $(\lambda \ll D)$ regions, where λ is the mean free path and D is the pipe diameter. The size-variation effects in transport phenomena occur whenever the mean free path λ of the elementary carriers becomes comparable in magnitude to the characteristic dimensions of the system under study. When inter-particle collisions become relatively more