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A Finite-Difference Lattice Boltzmann Approach for Gas Microflows

G. P. Ghiroldi and L. Gibelli*

Dipartimento di Scienze e Tecnologie Aerospaziali, Via la Masa 34, Politecnico di Milano, 20156 Milano, Italy.

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Abstract. Finite-difference Lattice Boltzmann (LB) models are proposed for simulating gas flows in devices with microscale geometries. The models employ the roots of half-range Gauss-Hermite polynomials as discrete velocities. Unlike the standard LB velocity-space discretizations based on the roots of full-range Hermite polynomials, using the nodes of a quadrature defined in the half-space permits a consistent treatment of kinetic boundary conditions. The possibilities of the proposed LB models are illustrated by studying the one-dimensional Couette flow and the two-dimensional square driven cavity flow. Numerical and analytical results show an improved accuracy in finite Knudsen flows as compared with standard LB models.

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Key words: Lattice Boltzmann models, half-range Hermite polynomials, kinetic boundary conditions.

1 Introduction

The outgrowing development of microelectromechanical systems (MEMS) has spurred interest in studying gas flows in devices with microscale geometries. These flows, which are referred to as gas microflows, are usually distinguished by relatively large Knudsen numbers and small Mach numbers. Because of the large Knudsen numbers, the conventional hydrodynamic approach breaks down and a description based on the Boltzmann equation is required [1]. Numerical evidence from full solutions of the Boltzmann equation suggests that accurate results for isothermal flows can also be determined by simpler kinetic model equations such as the one proposed by Bathnagar, Gross and Krook and, independently, by Welander (BGKW) [1]. Therefore it is a common practice to model

*Corresponding author. *Email addresses:* `gian.ghiroldi@mail.polimi.it` (G. P. Ghiroldi), `livio.gibelli@polimi.it` (L. Gibelli)

isothermal gas microflows by the BGKW kinetic model equation and, due to the small Mach numbers, to linearize it around the equilibrium state [2]. Numerous studies on gas microflows based on the numerical solution of the linearized BGKW kinetic model equation [3–5] and/or the linearized Boltzmann equation [6] have been reported over the years. Recently, the Lattice Boltzmann (LB) method has attracted considerable interest as an alternative tool for studying gas flows in microfluidic devices [7–14]. Although it was evolved from lattice-gas cellular automaton models for mimicking the Navier-Stokes hydrodynamics, the LB method can potentially describe gas microflows since it can be viewed as the discrete ordinate method to solve the linearized BGKW kinetic model equation [15,16]. Within the framework of single relaxation time modeling, several high-order LB models have been developed in the attempt to adequately reproduce the non equilibrium effects of finite Knudsen flows, such as the velocity slip at the solid walls and the nonlinear stress-strain relationship within the Knudsen layer [17,18]. Some models have been derived by using a local mean free path in order to account for the presence of solid surfaces [7]. Although this approach has been shown to be effective in many applications, it is phenomenological in nature and, as such, not perfectly general. Composite models have also been developed which result from the superposition of discrete velocities determined from odd and even quadrature formula [9]. However, the most common strategy is using a greater number of discrete velocities determined from a full-range Gauss-Hermite quadrature [8, 11, 12], possibly adopting a multiscale approach to contain the increase in the computational cost [10]. However, more discrete velocities do not guarantee an improved accuracy because of the quadrature error in dealing with the boundary conditions [13]. As a matter of fact, abscissae of the full-range Gauss-Hermite quadrature schemes are derived to obtain accurate evaluation of the moments of the distribution function defined over the entire velocity space. In contrast, they provide only an approximately estimate of the half-range integrals that enter in the formulation of kinetic boundary conditions [19].

The present work aims at showing that the capability of standard finite-difference LB models to describe finite Knudsen gas flows can be improved by using weights and nodes as given by the half-range Gauss-Hermite quadrature [20]. This velocity space discretization permits to explicitly account for the discontinuity of the distribution function at the solid walls and therefore leads to a faster convergence rate of the numerical solution. In kinetic theory applications, the importance of a consistent treatment of boundary conditions has been recognized as early as the sixties of the past century [21] and the half-range discrete ordinate method has been widely used since then [22–26]. However to the authors' knowledge, no previous works have explicitly shown that the quadrature based on half-range Hermite polynomials can easily address the issue of boundary conditions for the LB simulations of gas microflows [13]. As a matter of fact, although it is well known that finite-difference LB models can be developed from different quadrature formula [27], most of the high-order LB models applied to simulate gas flows in microchannels use the roots of full-range Hermite polynomials as discrete velocities [7–13]. In Ref. [19] it was observed that an improved accuracy in dealing with boundary conditions can be achieved