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DSMC and R13 modeling of the adiabatic surface

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ABSTRACT

Adiabatic wall boundary conditions for rarefied gas flows are described with the isotropic scattering model. An appropriate sampling technique for the direct simulation Monte Carlo (DSMC) method is presented, and the corresponding macroscopic boundary equations for the regularized 13-moment system (R13) are obtained. DSMC simulation of a lid driven cavity shows slip at the wall, which, as a viscous effect, creates heat that enters the gas while there is no heat flux in the wall. Analysis with the macroscopic equations and their boundary conditions reveals that this heat flux is due to viscous slip heating, and is the product of slip velocity and shear stress at the adiabatic surface. DSMC simulations of the driven cavity with adiabatic walls are compared to R13 simulations, which both show this non-linear effect in good agreement for Kn < 0.3.

1. Introduction

Significant reduction in size of electro mechanical systems extends the demands for modeling and interpreting the flow behavior of gasses to micro scales. As the mean free path λ, i. e., the average distance that a molecule travels between collisions becomes comparable with the flow length scale, L, the theoretical assumption in the conventional constitutive relations, i.e., the laws of Navier–-Stokes and Fourier, lose their validity. The Knudsen number, which is the ratio of the mean free path to the characteristic length of the flow domain, $\mathrm{Kn} = \frac{\lambda}{L}$, is the main indicator of the degree of rarefaction in gases.

The Boltzmann equation describes the behavior of a gas flow at every degree of rarefaction [1]. However, due to the six dimensional phase space and the complexity associated with the molecular collision term, solving the Boltzmann equation is challenging, and numerically expensive. Some researchers propose to solve kinetic model equations using deterministic numerical schemes [2,3]. These model equations have the same main characteristics as the Boltzmann equation, but avoid some of the complexity arising due to the collision term.

Another method to approximate the Boltzmann equation, is to derive a set of macroscopic transport equations which can describe the flow behavior to various degrees of accuracy. The Grad moment method [4] extends the set of conventional hydrodynamic variables, such as, density, temperature, and velocity, by introducing stress, heat flux, and other higher moments. However, due to the hyperbolic nature, the Grad moment equations exhibit un-physical subshocks [5,6].

The regularized 13 moments (R13) equations are derived by combining elements of the Grad and Chapman-Enskog methods, utilizing the concept of order of magnitude in the Knudsen number [7,8]. The R13 equations are stable [9], accurate up to the third order in terms of Knudsen number, and benefit from a complete set of boundary conditions [10,11].

Alternatively, the Boltzmann equation can be solved by stochastic schemes, commonly known as direct simulation Monte Carlo (DSMC). The DSMC method, first proposed by Bird [12], is a particle based microscopic method that converges to the solution of Boltzmann equation in the limit of infinite simulating particles [13]. In this method, simulating particles represent a cloud of gas molecules that travel and collide with each other and solid surfaces. The macroscopic properties of the gas, such as temperature, shear stress or heat flux are obtained by taking the appropriate average of microscopic properties of simulating particles.

According to Maxwell's original paper [14], when the surface is microscopically rough *and* the incident molecules are performing multiple scattering, *or* are momentarily trapped *or* absorbed on the surface, we can expect the surface to behave as a diffusive reflector. However, it is well known from experiments on molecular beams that diffusive reflection typically does *not* occur. Instead, beams are reflected in plumes that center on the reflection direction [1,15]. To

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at least have some elements of the plume, Maxwell amended his model by the possibility for specular reflection.

As listed in [12], the diffusive reflection law should be critically reviewed when one or more of the following factors are present:

- The ratio of the molecular weight of the gas to the surface molecules is small in comparison with unity.
- Or the translational energy of the molecules relative to the surface is larger than several electron volts.
- A smooth metal surface that has been outgassed through exposure to high vacuum and high temperature.

In the current study, we model a rarefied gas of light atoms enclosed in a cavity with heavy surface molecules. In the collision, the (light) gas particle has little change of absolute kinetic energy, while its collision angle depends on the detailed microscopic geometry of collision with the (heavy) surface atom.

The conventional assumptions for the diffuse surface cannot be employed here. At such a surface, particles thermalize with the wall, and leave in a Maxwell distribution– that is accompanied by marked exchanged between gas particle and the wall. The Maxwell model would allow the description of non-diffusive collisions only by accounting for more specular reflections. However, specular reflection are not expected, since the surface is never flat-on the microscopic level. Moreover, specularly reflecting walls exchange neither energy nor momentum, hence there is no shear force on the gas.

Modeling particles reflecting from a surface with a defined temperature is straightforward [12]; however, in the case of an adiabatic surface, assigning a velocity to the reflecting particle from a wall with unknown temperature becomes non-trivial. Researchers have proposed various methods to implement the adiabatic boundary condition in the DSMC method. Wang et al. [16,17] introduced the inverse temperature sampling technique to heat flux on the wall. More recently, Akhlaghi et al. [18] proposed an iterative scheme to impose the heat flux boundary condition in DSMC method. In this scheme, an estimate to the wall temperature is initially made. Then, as the solution evolves in time, the wall temperature is modified according to the predicted heat flux associated with the assumed temperature. They showed that by using the Maxwell model and adjusting the wall temperature iteratively, one can make the energy flux through a surface vanish, i.e., model an adiabatic Maxwell surface. Tzeng et al. [19], proposed a microscopic method to model the adiabatic surface. In this model the normal component of the velocity is reversed, while the two other planar components are obtained by using a single random number, such that the magnitude of velocity vector remains unchanged in the collision. Although this microscopic treatment leads to zero energy transfer through the surface, the use of normal velocity reversal in this model seems not necessary true for the particles colliding with a rough wall.

In the current study the isotropic scattering kernel [20] is utilized to model the adiabatic surface in the DSMC method and R13 equations. Here, the *no energy transfer* condition is directly imposed on each particle colliding with the adiabatic surface. This method is expected to be fast and more accurate in convergence of the DSMC solution compared to the iterative schemes. The appropriate sampling technique in the DSMC method is presented, and the corresponding boundary equations for the R13 equations are derived. Then we briefly discuss the steps required to model an adiabatic Maxwell surface using the macroscopic approach, and show the agreement between the macroscopic boundary conditions obtained from the adiabatic Maxwell model, and the isotropic scattering model for the R13 equations. Using the obtained boundary conditions, the DSMC and R13 equations are utilized to model a partly adiabatic cavity in the rarefaction regime. The DSMC results show that the heat flux profile has a component normal to the adiabatic surface. This generated heat is well captured by the R13 equations, which allows us to interpret it as the viscous slip heating in the boundary of the adiabatic surface. Indeed, the heat flow into the gas is the product of shear stress and slip velocity.

The remainder of the paper is organized as follows. The solution methods utilized in this study are introduced in Section 2. In Section 3 the boundary condition to model an adiabatic surface using the isotropic scattering kernel is described, then in Section 3.3 the microscopic approach for modeling the adiabatic surface in the DSMC is introduced. The associated macroscopic boundary conditions for the R13 equations are derived in Section 3.4. The adiabatic Maxwell surface is presented in Section 3.5, and the appropriate wall temperature is introduced. Afterwards, in Section 4 the proposed boundary conditions are utilized to perform a microscopic and macroscopic modeling of the partly adiabatic lid driven cavity, and the obtained results are discussed. The paper ends with our conclusions in Section 5.

2. Governing equation and method of solution

2.1. Distribution function and Boltzmann equation

In kinetic theory a gas is described by the density distribution function $f(t, x_i, c_i)$ such that $f d\mathbf{x} d\mathbf{c}$ denotes the number of particles in the phase space element $d\mathbf{x}d\mathbf{c}$ at time t. The Boltzmann equation describes the evolution of the density distribution function in phase space ($\mathbf{x}$, $\mathbf{c}$) by accounting for the translational motion and collisions of the particles in the gas, as

$$\frac{\partial f}{\partial t} + c_k \frac{\partial f}{\partial x_k} + G_k \frac{\partial f}{\partial c_k} = \mathscr{J}(f,f), \tag{1}$$

where G_k is the external force acting on the gas. The term $\mathscr{J}(f,f)$ is the collision operator that describes the change of the distribution function due to interaction between particles.

Macroscopic quantities such as mass density ρ, velocity v_i, temperature T, shear stress σ_{ij} and heat flux q_i are moments of the distribution function, obtained by integration over velocity space $\mathbf{c}$,

$$\begin{aligned} &\rho = m\int f d\mathbf{c}, \quad v_i = \frac{m}{\rho}\int c_i f d\mathbf{c}, \quad 3RT = \frac{m}{\rho}\int C^2 f d\mathbf{c}, \\ &\sigma_{ij} = m\int C_{<i}C_{j>} f d\mathbf{c}, \quad 2q_i = m\int C_i C^2 f d\mathbf{c}. \end{aligned} \tag{2}$$

Here, m is the mass of particle, R is the specific gas constant and $C_i = c_i - v_i$ is the peculiar velocity of the gas particles.

A rarefied gas is well described by the Boltzmann equation for all Knudsen numbers. However, the Boltzmann equation is difficult to solve deterministically due to six dimensional phase space description, as well as the non-linearity in the collision term.

2.2. DSMC method (microscopic method)

The DSMC method is a statistical method, based on the kinetic theory of dilute gases, to model rarefied gas flows [12]. In this method, many independent simulating particles are used to model gaseous flows, where each particle represents a large number of real gas molecules. In the DSMC method the simulating particles are allowed to move and collide; however, the motion and collision of the particles are assumed to be decoupled. The time step is chosen as a fraction of the mean collision time to ensure pure motion in the elapsed movement time. In order to implement DSMC, the flow domain must be divided into computational cells.