

Relaxation Time Simulation Method with Internal Energy Exchange for Perfect Gas Flow at Near-Continuum Region

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Abstract

This paper presents an internal energy exchange scheme for the Relaxation Time simulation method (RTSM) which solves the BGK equation for the perfect gas flow at near-continuum region. The Larsen-Borgnakke model with discrete rotational energies is introduced to model the energy exchange between the translational and internal modes. This development improved the agreements between RTSM and DSMC with little additional computational cost. The result shows a possibility of a hybrid RTSM/DSMC code for the continuum/rarefied gas flow.

Keywords: Monte Carlo method; near-continuum flow; RTSM; DSMC

1. Introduction

Rarefied gas flow is an important problem in aeronautics and astronautics. In recent years, the rapid development of MEMS technique has brought us an exigent requirement for the investigation of gas flow in micro systems^[1,2]. In such flows, the Knudsen number is so high that the continuum assumption breaks down, and that the molecular based methods should be used. Bird's direct

simulation Monte Carlo (DSMC) method^[3] is the standard computational method for the high-Knudsen-number flows, where the governing equation is the Boltzmann equation. In DSMC the flow is represented by a large number of simulated particles, and the flow evolution is tracked by calculating the motion of these particles and their collisions amongst themselves and with any boundaries.

The DSMC method is suitable for gas flows with a high Knudsen number. However, in micro flows the gas can be dense despite a high Knudsen number due to the small characteristic length^[4]. The frequent collisions between gas molecules bring a high cost at the computation of DSMC. Pullin^[5] proposed a particle simulation method called the Equilibrium Particle Simulation Method (EPSM) as the infinite collision rate of DSMC for a given cell network and number of simulator particles. In EPSM, as in DSMC, the flow is simulated by tracking the motion and interactions of the representative particles. However, no collisions between particles are calculated and the effect of collisions is simulated by redistributing the total momentum and energy of all the particles in each cell at each time step amongst all the particles in the cell. Chen et al.^[6] used the EPSM to combine with DSMC to handle flows in the transition regime between rarefied gas flow and fully continuum flows. Macrossan^[7-9] developed this method based on the BGK equation and proposed a new method called the Relaxation Time Simulation Method (RTSM). In RTSM, not all the particles in each cell are redistributed. The particle number for velocity distribution determined from the local relaxation time can be derived from the cell density and temperature and any desired viscosity law.

The present paper develops Macrossan's RTSM by introducing the Larsen-Borgnakke model with discrete rotational energies to model the energy exchange between the translational and internal modes. The new model is verified by a micro channel flow simulation, comparing with the DSMC method. The computational efficiencies of both the new method and the DSMC method are compared, especially in the near-continuum flow region.

2. Numerical Method

2.1 Relaxation Time simulation method

The BGK approximation simplifies the collision term on the right hand side of the Boltzmann equation by using a relaxation time that poses the greatest mathematical difficulties and needs modify. The best known model equation is called the BGK equation after Bhatnager, Gross and Krook^[10,11]. It may be written

$$\frac{\partial}{\partial t}(nf) + \mathbf{c} \cdot \frac{\partial}{\partial \mathbf{r}}(nf) + \mathbf{F} \cdot \frac{\partial}{\partial \mathbf{c}}(nf) = n\tau^{-1}(f_0 - f), \quad (1)$$

where the τ is the local relaxation time, n is the number density of molecules, f_0 is the local Maxwellian distribution.

Based on this relaxation time BGK approximation the collision term can be approximated as

$$\left[\frac{\partial nf}{\partial t} \right]_{coll} = \frac{n}{\tau}(f_0 - f). \quad (2)$$

The exact solution of Eq. (2) is

$$f(t) = (f(0) - f_0) \exp(-t/\tau) + f_0, \quad (3)$$

where $f(0) = f(t=0)$ is the particle velocity distribution established by the convection phase of the simulation before the effect of collision is simulated. That is to say, the distribution function relaxes towards equilibrium with a time interval of τ for all velocities. Therefore, after a time interval of collision $t = \Delta t$, the distribution function can be expressed as

$$f(\Delta t) = \exp(-\Delta t/\tau)f(0) + (1 - \exp(-\Delta t/\tau))f_0. \quad (4)$$

The Eq.(4) indicates that after collisions of a time interval Δt , the final distribution of molecular velocities is a mixture of the initial distribution in the cell and a statistical approximation of the final equilibrium distribution.

The relaxation time τ is a little different from the collision time. The Chapman-Enskog viscosity for the relaxation time approximation is $\mu = \rho RT\tau$ ^[12]. Therefore, the relaxation time is determined by

$$\tau = \frac{\mu}{nkT}, \quad (5)$$

where k is the Boltzmann constant, m is the molecular mass, and n is the number density.

2.2 Larsen-Borgnakke model

The Larsen-Borgnakke model is a phenomenological model to deal with internal and translational energies exchange for inelastic inter-particles collisions^[3]. In this model the distribution function for the internal energy of a molecule may be written as

$$f_{\varepsilon_i} \propto \varepsilon_i^{\zeta/2-1} \exp(-\varepsilon_i/(kT)), \quad (6)$$

where ε_i is the internal energy of a molecule, and ζ is the internal degrees of freedom. In fact, not all collisions are regarded inelastic. Therefore when the Larsen-Borgnakke model is introduced into the RTSM method, the crucial part is the determination of the probability of the inelastic parts. We have tried two methods to determine the rotation relaxation fraction. Scheme A is to select a certain part from the molecules with translational energy redistribution. The fraction of molecules for the rotational energy relaxation P_R is then

$$P_R = P_V \cdot \frac{1}{Z_R} = \left[1 - \exp\left(-\frac{nkT\Delta t}{\mu(T)}\right) \right] \cdot \frac{1}{Z_R(T)}, \quad (7)$$

where P_V is the probability for the translational energy relaxation, Z_R is the rotational relaxation number which is a function of local temperature. This scheme is consistent with the standard DSMC of Bird^[3].

The second scheme *B* is to use a rotational relaxation probability independent with the translational one:

$$P_R = 1 - \exp\left(-\frac{4}{\pi Z_R(T)} \cdot \frac{nkT\Delta t}{\mu(T)}\right) \quad (8)$$

Eq. (8) shows it is not necessary that any particle which undergoes rotational relaxation also undergo translational relaxation at the same time.

2.3 Redistribution procedures

In each time step of the RTSM simulation, the number density n , temperature T in each cell are sampled. After the local viscosity μ and the rotational relaxation number Z_R , which are function of local temperature in cells, are calculated, the probabilities for translational relaxation and rotational relaxation can be obtained from Eqs. (5-8). For the translational energy relaxation, if a random number $R_f > P_V$, the particles will be selected to undergo translational relaxation. The relaxed particle number N_t is about $P_V \cdot N_p$ with N_p is the total particles number in one cell. Similar process is performed for the rotational relaxation, and the rotational relaxation number is $N_r \approx P_R \cdot N_p$. Both the translational energy and rotational energy, which need redistribution, form a thermal energy pool with a total energy E_{tot} . Thus the characteristic temperature of the re-distributed energy can be calculated as

$$T_c = \frac{2E_{tot} / k}{3N_t + 2N_r} \quad (9)$$

All the rescaling procedures for either the translational redistribution or the rotational redistribution will be based on this characteristic temperature. It is clear that this temperature equals to the sampled temperature in one cell for Pullin's EDSM^[5].

3. Results and Discussion

The present algorithm was performed in FORTRAN based on the standard DSMC code^[3] in UNIX system. The INDEX technique of DSMC is introduced to avoid tracking each particle so that little additional memory is required. To verify the new models, a 2D gas flow in a micro channel is simulated and the results are compared with the standard DSMC method. The physical model is shown in Fig. 1.

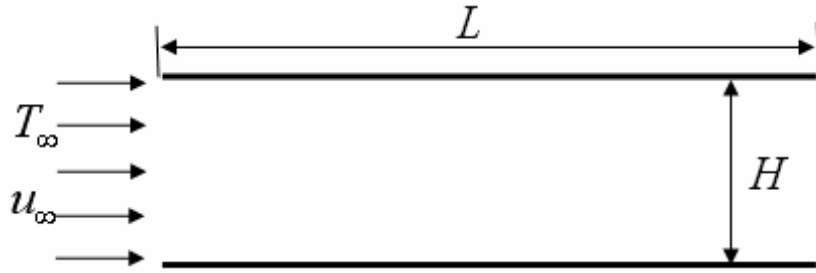
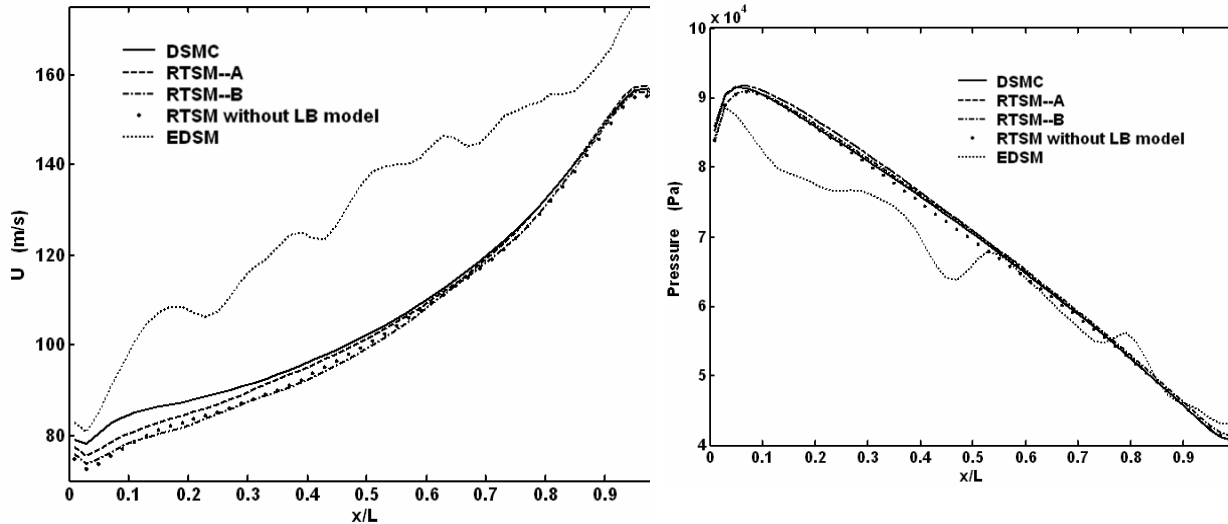


Fig. 1 Channel flow with freestream incoming gas

The channel is $5 \mu\text{m}$ long and $1 \mu\text{m}$ wide. The incoming gas Knudsen number is 0.1. The freestream velocity u_∞ is 200 m/s and the temperature T_∞ is 300 K. The channel walls are isothermal and the temperature is 300 K. Full diffuse model is used to calculate the collisions between the molecules and the walls. 50×20 cells and 4×4 subcells in each cell are used. In each time step, the molecules can move half of cell size with a most possible velocity $(\sqrt{8kT/\pi m} + u)$. Over 10^5 simulated particles are calculated for each method and the sample size is over 2×10^6 . The results are shown in Fig. 2.

Fig. 2 shows the results of the modified RTSMs and the standard DSMC. Different schemes for RTSM to determine the rotation relaxation probability are plotted and compared. The generally-used EPSM is also showed in the same figures. The results show that the rotational relaxation in scheme A improves the RTSM results with better agreement with the standard DSMC results, when comparing with the scheme B and non-rotational relaxation RTSM. The reason may lie in the scheme A is closer

to the method in DSMC than the scheme B. The EPSM has large deviations and fluctuations from the standard DSMC result, which even can not be improved soundly by increasing sample sizes even up to 10^8 .



(a) Velocity comparisons

(b) Pressure comparisons

Fig. 2 Velocity and pressure along the midline of the channel

Fig. 3 compares the temperature contours at same contour-levels between the DSMC and the RTSM in scheme A. Difference between the contours indicated the thermal conductivity in the RTSM was over-predicted, which was ascribed to the Prandtl number for the BGK equation was always unity instead of a real one. Recently, a few new models were reported to modified the BGK equation in

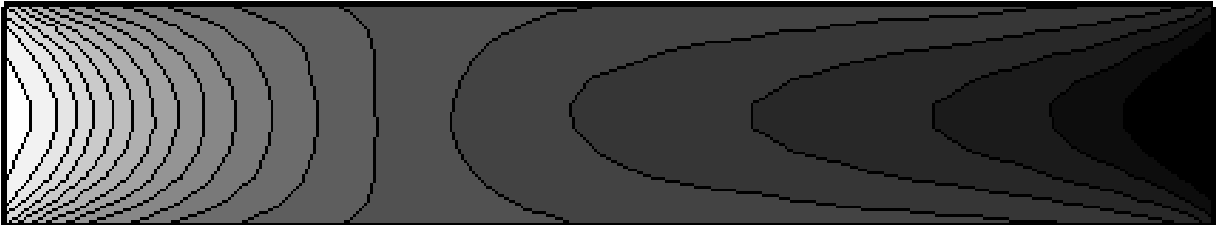


Fig. 3 (a) Temperature contours. DSMC



Fig. 3 (b) Temperature contours. RTSM, Scheme A

equilibrium distribution^[13,14], which were expected to get a Prandtl number closer to the real one and to improve the heat transfer modeling in RTSM. These new models will be introduced into our future work for the next step.

From Eq. (4), the computational cost of RTSM is mainly relative to the relaxation time τ and increases little with the gas density n , while that of DSMC is basically determined by the gas density. When the gas density is larger than a certain value, the RTSM method will be more efficient than the DSMC method. For the channel flow shown in Fig. 1, the efficiencies of both methods are on a same level for a Knudsen number of 0.05. When the Knudsen number is 0.01, the efficiency of DSMC is about 30% of that of RTSM. These comparisons show that for the near continuum flow the RTSM method is more efficient than the DSMC method and could replace DSMC in that region.

4. Conclusions

The Relaxation Time simulation method (RTSM) was modified and improved by introducing the internal energy exchange scheme. The Larsen-Borgnakke model with discrete rotational energies is introduced to model the energy exchange between the translational and internal modes. The developed RTSM agrees better with the standard DSMC with little additional computational cost. Although the Prandtl number in the RTSM is still overestimated, the present results show a possibility of a hybrid RTSM/DSMC code for the continuum/rarefied gas flow.

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