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Communications in Nonlinear Science and Numerical Simulation 12 (2007) 1277–1282

Communications in
Nonlinear Science and
Numerical Simulation

www.elsevier.com/locate/cnsns

Relaxation time simulation method with internal energy exchange for perfect gas flow at near-continuum conditions

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Received 23 September 2005; accepted 6 January 2006
Available online 20 March 2006

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 discrete rotational energies are introduced to model the relaxation of internal energy modes. This development improved the agreements between RTSM and DSMC with little additional computational cost. The result shows a possibility of an improved hybrid RTSM/DSMC code for the continuum/rarefied gas flow.

PACS: 05.10.Ln; 47.45.–n; 47.70.Nd

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

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1. Introduction

Rarefied gas flow is an important problem in aeronautics and astronautics. In resent years, the rapid development of MEMS technique has brought us an exigent requirement for the investigation of gas flow in microsystems [1,2]. In such flows, the Knudsen-number is so high that the continuum assumption breaks down, and 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 [4].

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doi:10.1016/j.cnsns.2006.01.012

The DSMC method is suitable for gas flows with a high-Knudsen-number. However, in microflows the gas can be dense despite a high-Knudsen-number due to the small characteristic length [5]. The frequent collisions between gas molecules bring a high cost at the computation of DSMC. Pullin [6] proposed 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. Macrossan [7] and Chen et al. [8] used EPSM in combination with DSMC to handle flows in the transition regime between rarefied gas flow and fully continuum flows. Macrossan [9–11] 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 RTSM by introducing a model with discrete rotational energies to model the energy exchange between the translational and internal modes. A microchannel flow simulation, comparing with the DSMC method, verifies the new model. 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 greatest mathematical difficulties for any solution of the Boltzmann equation lie in the collision term on the right hand side. One approach is to simplify the problem by modeling the collision term. The best known model equation is the Bhatnager, Gross and Krook [12,13] (or BGK) equation. It may be written

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

where the τ is the local relaxation time, n is the number density of molecules, f_0 is the local Maxwellian distribution, which would be established in the collision rate were sufficiently large. In other words the collision term bas been approximated as

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

and this provides an approximation of the change in f brought about in any DSMC cell during the collision stage of the calculation. The exact solution of Eq. (2) is

$$f(t) = (f(0) - f_0)\exp(-t/\tau) - f_0, \tag{3}$$

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 constant of τ for all velocities. After a time interval $t = \Delta t$, the distribution function can be expressed as

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

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

The Chapman–Enskog viscosity for the relaxation time approximation is $\mu = \rho RT\tau$ [14]. Therefore, in RTSM, the relaxation time in each cell is determined by

$$\tau = \frac{\mu}{nkT}, \tag{5}$$

where k is the Boltzmann constant, m is the molecular mass, and n is the number density, and T is the kinetic temperature in the cell.

2.2. Discrete internal energy model

The discrete internal energy model deals with internal and translational energies exchange for inelastic inter-particles collisions. In this model, the equilibrium distribution function for the internal energy of a molecule maybe written as

$$f_{\varepsilon_\mathrm{i}} \propto \varepsilon_\mathrm{i}^{\zeta/2-1}\exp(-\varepsilon_\mathrm{i}/(kt)), \tag{6}$$

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 as inelastic. Therefore, when the 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

$$P_\mathrm{R} = P_\mathrm{V}\cdot\frac{1}{Z_\mathrm{R}} = \left[1-\exp\left(-\frac{nkT\Delta t}{\mu(T)}\right)\right]\cdot\frac{1}{Z_\mathrm{R}(T)}, \tag{7}$$

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 of the translational one:

$$P_\mathrm{R} = 1-\exp\left(-\frac{4}{\pi Z_\mathrm{R}(T)}\cdot\frac{nkT\Delta t}{\mu(T)}\right). \tag{8}$$

Eq. (8) shows it is not necessary that any particle that 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 Junction 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 $R_\mathrm{f} > P_\mathrm{V}$, the particles will be selected to undergo translational relaxation. The number of particles given new velocities is $N_\mathrm{t} = P_\mathrm{V}\cdot N_\mathrm{p}$ where the total number of particles number in one cell is N_p. A similar process is performed for the rotational relaxation, and the number of particles that are given a new rotational energy is $N_\mathrm{r} \approx P_\mathrm{R}\cdot N_\mathrm{p}$. 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 redistributed energy can be calculated as

$$T_\mathrm{c} = \frac{2E_\mathrm{tot}/k}{3N_\mathrm{t}+2N_\mathrm{r}}. \tag{9}$$

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 plays the same role as the sampled temperature in one cell for Pullin's EPSM [6].

3. Results and discussion

The present algorithm was performed in FORTRAN based on the standard DSMC code [3] in UNIX system. To verify the new models, a 2D gas flow in a microchannel is simulated and the results are compared with the standard DSMC method. The physical model is shown in Fig. 1. The channel is 5 μm long and 1 μm wide. The incoming gas Knudsen-number is 0.1. The freesteam velocity u_∞ is 200 m/s and the temperature T_∞ is 300 K. The channel walls are isothermal and the temperature is 300 K. Fully diffuse reflection is used to calculate the collisions between the molecules and the walls. 50 × 20 cells and 4 × 4 subcells in each cell are used. The time step is set that a molecule with a characteristic speed $\sqrt{8kT/\pi m}+u$ will move a quarter of a cell size

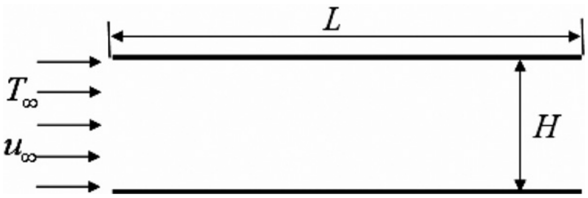

Fig. 1. Channel flow with freesteam coming gas.

in one step. Over 10^5 simulated particles are used 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 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.

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-pre-

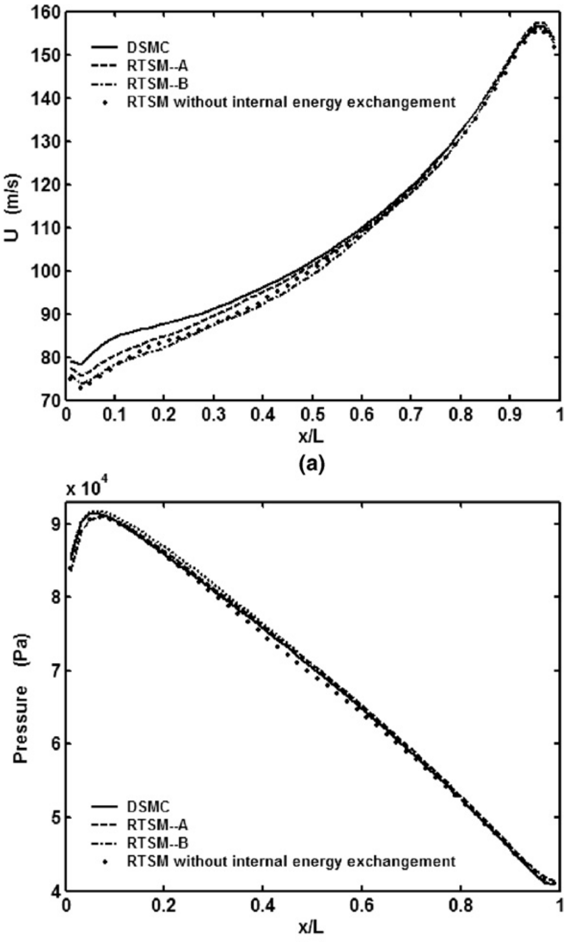

Fig. 2. Velocity and pressure along the midline of the channel: (a) velocities comparisons; (b) pressure comparisons.

(a) DSMC

(b) RTSM

Fig. 3. Temperature contours: (a) the standard DSMC; (b) the RTSM in scheme A.

dicted, which was ascribed to the fact that the Prandtl number for the BGK equation has the unrealistic value of unity. Recently, a few new models were reported to modified the BGK equation by changing the equilibrium distribution [15,16], which were expected to give a realistic Prandtl number and improve the heat transfer modeling. These new models will be introduced into our future work.

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 relaxation scheme. Discrete rotational energies were used to model the energy exchange between the translational and internal modes. Although the Prandtl number in the RTSM is still overestimated, the present results show a possibility of an improved hybrid RTSM/DSMC code for the continuum/rarefied gas flow.

Acknowledgement

The present work was supported by the National Natural Science Foundation of China (Grant No. 59995550-2) and National Key Basic Research and Development Program of China (Grant No. 1999033106).

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