Development of a Cell Size Relaxed Scheme for the Direct Simulation Monte Carlo Method

Quanhua Sun, Hongli Liu and Jing Fan

Institute of Mechanics, Chinese Academy of Sciences, Beijing, 100190 China

Abstract. The conventional direct simulation Monte Carlo (DSMC) method has a strong restriction on the cell size because simulated particles are selected randomly within the cell for collisions. Cells with size larger than the molecular mean free path are generally not allowed in correct DSMC simulations. However, the cell-size induced numerical error can be controlled if the gradients of flow properties are properly involved during collisions. In this study, a large cell DSMC scheme is proposed to relax the cell size restriction. The scheme is applied to simulate several test problems and promising results are obtained even when the cell size is greater than 10 mean free paths of gas molecules. However, it is still necessary, of course, that the cell size be small with respect to the flow field structures that must be resolved.

Keywords: direct simulation Monte Carlo method, cell size, collision scheme.
PACS: 47.45.-n

INTRODUCTION

The direct simulation Monte Carlo (DSMC) method is probably the most successful approach for simulating non-equilibrium gas flows [1]. It employs many representative particles to mimic the behavior of real gas molecules, and particle collisions and motions are decoupled using models. The conventional models require the cell size to be less than one mean free path of gas molecules. This means that a large number of cells are needed to satisfy the requirement for cases when the molecular mean free path is relatively small.

The restriction on the cell size comes with the particle collision model where particles are randomly selected within a same cell to form collision pairs regardless of their relative locations. It is found that the cell size should be less than one molecular mean free path and is recommended to be smaller than one third of the mean free path [2]. Effects of finite cell size have been studied in the literature [3,4]. It was shown that the simulated viscosity could have an error about 10% when the cells are one mean free path wide [3]. To reduce the cell size induced error, Bird proposed a subcell technique in which collision particles are selected within a same subcell that is a fine cell divided from a simulated cell [5]. Similarly, particles can be selected within a given distance using the near-partner selection technique [6]. Recently Bird [7] proposed a new selection rule that requires a particle to select the nearest particle as a possible collision partner whereas the last collided partner should be avoided. In general, if the average distance between collision partners is less than one tenth of the mean free path, the results from [3] indicates that the viscosity error is smaller than 0.7%, which should be satisfactory for many situations.

It seems that the cell size can be very large in DSMC with a proper collision-pair selection technique. However, the number of simulated particles in a cell should increase accordingly to restrict the separation distance among particles, which greatly increases the computational cost. Recall that the conventional DSMC scheme does not take into account the effects of the separation distance of collision pairs, which is really the source of the numerical error due to the cell size. If the effects of the separation distance are properly considered in particle collisions, a DSMC simulation may predict correctly the flow field using large cells. A scheme of this kind has been proposed by Usami and Nakayama using their intermolecular collision scheme [8]. However, their scheme does not conserve momentum and energy, which is critical for some applications.

In this paper, we propose a cell size relaxed scheme that allows the cell size to be much larger than the mean free path of gas molecules. Because the cell size is relatively large, the scheme is also called a large cell DSMC scheme (LCDSMC). The scheme considers the gradients of flow properties in a cell during particle collisions, which is

CP1084, *Rarefied Gas Dynamics: 26th International Symposium*, edited by T. Abe

similar to the intermolecular collision scheme of Usami and Nakayama. However, general conservation laws are enforced in this scheme. The scheme is introduced in the next section followed by several examples, and some concluding remarks are given in the final section.

CELL SIZE RELAXED DSMC SCHEME

The cell size relaxed DSMC scheme consists of two steps based on the conventional DSMC method. In the first step, the instantaneous cell-averaged flow properties are evaluated at every time step, and the cell-averaged properties are then interpolated at particle's locations using the least-squares method to get point-based properties. In the second step, the point-based properties are included in a particle collision model to obtain the post-collision velocity for collision particles. The details of the scheme are described below starting with the basic idea.

Basic Idea

In a real gas collisions occur when molecules are within a short distance that is represented by the collision cross section. In DSMC, one simulated particle usually represents a large number of real gas molecules. When the number of simulated particles is small, it is impossible for a particle to find its collision partner within the physical collision distance, which makes two particles at different locations as collision partners.

In the conventional DSMC method, collision partners are selected randomly within the same cell (or subcell) regardless of their locations. Because the flow properties at selected particles' locations may be different, the particles will experience different interactions with partners from a near location to a far location. This means that the uncoupling between the locations and collisions of particles is an approximation in the conventional DSMC method, although the accuracy of the DSMC method is guaranteed by the restriction on the cell size.

Now the question is how to include the effects of spatial locations of particles in collisions if the cell size and hence the distance between two particles is large. It is clear that collisions change the represented position of a particle in its velocity distribution function. Namely, the relative position in the distribution function is important. In order to identify the relative position for different distribution functions, a scaling variable is required. Usami and Nakayama [8] assumed that velocity distribution functions in all flow field follow local Maxwellian distributions and the velocity of one molecule in a collision pair is modified using mean flow velocity and temperature before and after the substantial collision calculation. Their scaling variable is the velocity normalized by the mean velocity and temperature. For general non-Maxwelliam distribution, the scaling variable should use the moments of the function. A simple choice is to normalize the velocity using the function's first moment, mean flow velocity, and the second moment, temperature. Hence the scaling variable can be expressed as $(\mathbf{V}-\mathbf{U})/\sqrt{2kT}$, where $\mathbf{V}$ is the particle velocity, $\mathbf{U}$ is the flow velocity, T is the flow temperature, and k is the Boltzmann constant. This expression, however, is not necessary related to Maxwellian distributions. Higher-order moments of the velocity distribution may be included in the scaling variable, which could greatly increase the complexity of the expression. The temperature components can also be used if the difference in the components is important. Because only a very limited number of moments are included in the normalized velocity, the scaling variable is approximate especially when the two distributions share few same features.

After the velocity scaling variable is set, non-dimensional velocities of collision particles are calculated using the scaling variable. Collisions are calculated in non-dimensional velocity space to determine the non-dimensional post-collision velocity, from which the appropriate post collision velocity at each particle's location can be determined. Thus each 'non-dimensional' collision represents two different 'real collisions', where one 'real collision' occurs at the location of one particle of the pair and each particle experiences exactly one 'real collision'.

Therefore, a large cell DSMC scheme should have a non-dimensional velocity that involves mean flow properties and a related collision scheme.

Evaluation of Flow Properties

Unlike the conventional collision scheme, the LCDSMC scheme requires that the flow field information is available during the simulation for particle collisions. A predetermined approach was used by Usami and Nakayama who employed an iterative procedure by running several cycles of DSMC simulations [8]. This approach is time consuming since iterations are required to reach an unchanged flow field. Another approach is to evaluate the flow properties at every time step [10]. In that approach, the statistical scatter is reduced by including the previous history using an under-relaxation factor that controls the effective sampling size. The approach predicted satisfactory results

[10] and has been employed in other research work. Hence this approach is adopted in the current LCDSMC scheme to evaluate the cell-averaged flow properties.

The cell-averaged flow properties are then interpolated at particles' locations. This can be achieved using the least-squares method [11]. For instance, the value v_i at particle location $\mathbf{r}_i$ can be calculated using the first order approximation as

$$v_i = v_c + (\mathbf{r}_i - \mathbf{r}_c)\cdot(\nabla v)_c \tag{1}$$

where v_c is the value at the cell center, and $(\nabla v)_c$ is calculated using the least-squares method. For better numerical accuracy, high-order approximations can be used by involving more cells. Other techniques such as numerical limiters can also be applied to improve the estimation at particle locations.

Conservative Collision Scheme

Collisions are calculated in non-dimensional velocity space to determine the non-dimensional post-collision velocity. The variable hard sphere (VHS) model [1] is used for the current study. We use subscript 1 and 2 to identify the two colliding particles and superscript ' to denote the post-collision velocity. Following the VHS model, the post-collision values for the scaling variable can be expressed as:

$$\left(\frac{\mathbf{V}_1-\mathbf{U}_1}{\sqrt{2kT_1}}\right)' = \frac{1}{2}\left(\frac{\mathbf{V}_1-\mathbf{U}_1}{\sqrt{2kT_1}}+\frac{\mathbf{V}_2-\mathbf{U}_2}{\sqrt{2kT_2}}\right)+\frac{1}{2}\left|\frac{\mathbf{V}_1-\mathbf{U}_1}{\sqrt{2kT_1}}-\frac{\mathbf{V}_2-\mathbf{U}_2}{\sqrt{2kT_2}}\right|\mathbf{e}(\theta,\phi) \tag{2}$$

$$\left(\frac{\mathbf{V}_2-\mathbf{U}_2}{\sqrt{2kT_2}}\right)' = \frac{1}{2}\left(\frac{\mathbf{V}_1-\mathbf{U}_1}{\sqrt{2kT_1}}+\frac{\mathbf{V}_2-\mathbf{U}_2}{\sqrt{2kT_2}}\right)-\frac{1}{2}\left|\frac{\mathbf{V}_1-\mathbf{U}_1}{\sqrt{2kT_1}}-\frac{\mathbf{V}_2-\mathbf{U}_2}{\sqrt{2kT_2}}\right|\mathbf{e}(\theta,\phi) \tag{3}$$

where $\mathbf{e}$ is a unit vector having an arbitrary phase angle θ and an arbitrary azimuth angle ϕ. Then the post-collision velocities of the pair can be derived as:

$$\mathbf{V}_1' = \mathbf{V}_1 - \frac{\sqrt{T_1}}{2}g(\mathbf{e}(\theta_0,\phi_0)-\mathbf{e}(\theta,\phi)),\quad \mathbf{V}_2' = \mathbf{V}_2 + \frac{\sqrt{T_2}}{2}g(\mathbf{e}(\theta_0,\phi_0)-\mathbf{e}(\theta,\phi)) \tag{4}$$

where g is calculated as:

$$\frac{\mathbf{V}_1-\mathbf{U}_1}{\sqrt{2kT_1}}-\frac{\mathbf{V}_2-\mathbf{U}_2}{\sqrt{2kT_2}} = \left|\frac{\mathbf{V}_1-\mathbf{U}_1}{\sqrt{2kT_1}}-\frac{\mathbf{V}_2-\mathbf{U}_2}{\sqrt{2kT_2}}\right|\mathbf{e}(\theta_0,\phi_0) = \frac{g}{\sqrt{2k}}\cdot\mathbf{e}(\theta_0,\phi_0) \tag{5}$$

It is noticed that the momentum and energy are not conserved in each collision with the modified collision model. Conservation of momentum and energy is only satisfied statistically because angles θ and ϕ are sampled from a spherical distribution. We adopt an approach [9] proposed by Pareschi and Trazzi to adjust the post-collision velocities so that the total momentum and energy can be conserved. In this study, the following adjustment is applied to all particles in a cell instead of two particles in a collision pair.

Assume that we have n particles whose i-th particle has a pre-collision velocity V_i and post-collision velocity V_i'. The modified velocity V_i'' of the i-th particle can be expressed as:

$$\mathbf{V}_i'' = \frac{\mathbf{V}_i' - \boldsymbol{\lambda}}{\tau} \tag{6}$$

where parameters $\boldsymbol{\lambda}$ and τ are determined using the conservation laws:

$$\sum_{i=1}^{n}\frac{\mathbf{V}_i'-\boldsymbol{\lambda}}{\tau} = \sum_{i=1}^{n}\mathbf{V}_i,\quad \sum_{i=1}^{n}\left(\frac{\mathbf{V}_i'-\boldsymbol{\lambda}}{\tau}\right)^2 = \sum_{i=1}^{n}\mathbf{V}_i^2 \tag{7}$$

which gives:

$$\tau^2 = \frac{n\sum_{i=1}^{n}\mathbf{V}_i'^2-\left(\sum_{i=1}^{n}\mathbf{V}_i'\right)^2}{n\sum_{i=1}^{n}\mathbf{V}_i^2-\left(\sum_{i=1}^{n}\mathbf{V}_i\right)^2},\quad \boldsymbol{\lambda} = \frac{\sum_{i=1}^{n}\mathbf{V}_i'-\tau\sum_{i=1}^{n}\mathbf{V}_i}{n} \tag{8}$$

Further improvement of the numerical accuracy can be obtained if a minor modification is applied to the normalized pre-collision velocity. The idea is to enlarge the difference of flow properties involved in the scaling variable because the aforementioned conservation enforcement may smooth the flow field. Namely,

$$\mathbf{U}_1^m = \mathbf{U}_1 + c_u(\mathbf{U}_1-\mathbf{U}_2),\quad \mathbf{U}_2^m = \mathbf{U}_2 - c_u(\mathbf{U}_1-\mathbf{U}_2) \tag{9}$$

$$T_1^m = T_1\cdot(T_1/T_2)^{c_T},\quad T_2^m = T_2\cdot(T_2/T_1)^{c_T} \tag{10}$$

where c_u and c_T are the enlargement factors. This modification is based on numerical observation and the value of enlargement factors should be determined by numerical tests.

NUMERICAL TESTS

The large cell DSMC scheme has been applied to simulate several flows that are used to illustrate the validity of the scheme. There are two purposes for the numerical tests. One is to check the basic idea of the collision scheme. For this purpose, the flow properties at particles' locations can be interpolated from predetermined flow properties. Another purpose of the tests is to evaluate the overall performance of the scheme.

Planar Couette Flow

The planar Couette flows considered here include the velocity Couette flow where one plate is at rest and the other moves at 300m/s, and the thermal Couette flow where one plate is kept at 273K and the other at 373K. The plates are separated by 1m and their accommodation coefficients are set to 1. Between the plates is argon gas that is modeled using the VHS molecular model.

The cell size induced error for the velocity Couette flow has been investigated by Alexander and his collaborators [3]. They showed that the error can be illustrated using a normalized transverse momentum flux $(F-F^K)/F^K$, where F^K is the kinetic flux when the cell size approaches zero. Theoretically, the normalized flux can be predicted using the Green-Kubo theory when the cell size is smaller than 4 mean free paths and approaches to the free-molecular limit when the cell size is larger. These analytic expressions are given as

$$\frac{F-F^K}{F^K}=\frac{16}{45\pi}\frac{L^2}{\lambda^2}, \text{ and } \frac{F^*-F^K}{F^K}=\frac{24}{15\pi}\frac{L}{\lambda}-1 \tag{11}$$

where F^* is the free-molecular result, L is the cell size, and λ is the mean free path.

Figure 1 (a) shows the simulated numerical error expressed as the normalized transverse momentum flux when the flow Knudsen number is 0.01. A total number of 100,000 particles are simulated and the time step is about 0.2 mean collision time for all the cases. The numerical error due to the finite time step should be less than 0.5% following the analysis of Hadjiconstantinou [4]. The statistical error in the simulation results is estimated to be about 0.01 for the normalized flux based on the sampling size [10]. The plot shows that the conventional DSMC results can be roughly predicted by the Green-Kubo theory for small-cell cases and the free-molecular results for large-cell cases. The figure also shows the LCDSMC results where the flow information used in the collision scheme is interpolated from a conventional DSMC simulation when the cell size is 0.1λ. It is shown that the numerical errors from LCDSMC are decreased by nearly one order of magnitude as compared with those from the conventional DSMC method. Further improvement can be obtained after applying the enlargement factors. The values of the factors are: $C_u=0.055$ and $C_T=0.02$, which gives best results for the current thermal Couette flow and velocity Couette flow. Figure 1 (b) shows the simulated numerical error in the normalized thermal flux whose expression is similar to the normalized momentum flux. Again, LCDSMC can reduce the cell-size induced error significantly and the enlargement factors can further improve the simulation accuracy. Similar results are obtained when the flows are in other Knudsen numbers (e.g., Kn=0.1,1.0). For the Couette flows, good results are also obtained when the instantaneous values of the flow properties are used in the collisions.

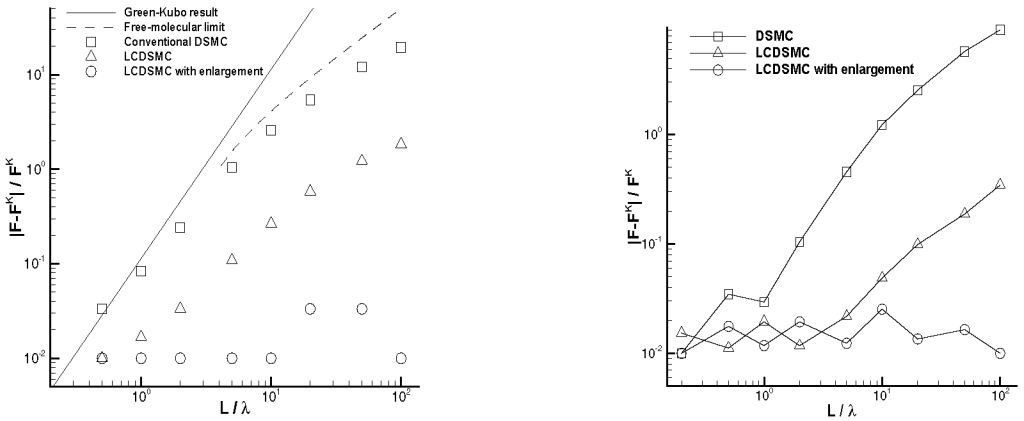

FIGURE 1. Normalized flux as a function of the cell size when Kn=0.01. (a) Transverse momentum flux in velocity Couette flows, (b) Thermal flux in thermal Couette flows.

Flow over an Inclined Flat Plate

The vortex flow behind an inclined flat plate is a classical problem and has been simulated by Usami and Mizuguchi to evaluate their scheme. As a comparison, we revisit this problem to evaluate our LCDSMC scheme.

The test problem is illustrated in Fig. 2(a) where the plate length is 60λ (λ is the undisturbed mean free path) and the computational domain is 580λ by 580λ. The simulated gas is argon whose inflow Mach number is 0.7 and the Reynolds number is about 50. The inflow gas has a temperature of 288 K, a pressure of 0.9 Torr, and an angle of attack of 45 degree. Although the computational domain is limited because of numerical cost, it can still verify the scheme because the comparison is based on the same grid, computational domain, and boundary conditions.

As in reference 8, we plot the vector field in a uniform length to show the difference of the simulation results. In addition, streamlines are plotted when needed. Figure 2 (b) shows the results from the reference case that is calculated using the conventional DSMC scheme. These reference results are obtained using a cell size of 1λ and 5 by 5 sub-cells are employed in a cell. The effective cell size is then about 0.2λ. Two vortexes are clearly identified behind the flat plate in Fig. 2(b) although only one vortex was mentioned in reference 8. When the cell size is increased to 10λ, the flow field calculated by conventional DSMC as shown in Fig. 2(c) is unphysically smoothed and no vortex is observed.

The results using the LCDSMC scheme are shown in Figs. 2(d) to 2(f). The enlargement factors $C_u = 0.055$ and $C_T = 0.02$. This is important since these are the same values of enlargement factors found for the Couette flows, which suggests at least the same values might be used for all cases. In Fig. 2(d) the mean flow properties is interpolated from the reference results so that the effects of the flow evaluation can be separated. The cell size used in Fig. 2(d) is 10λ while the results agree very well with those in Fig. 2(b) when the effective cell size is 0.2λ. This clearly shows that cell size larger than the molecular mean free path can be used in LCDSMC simulations.

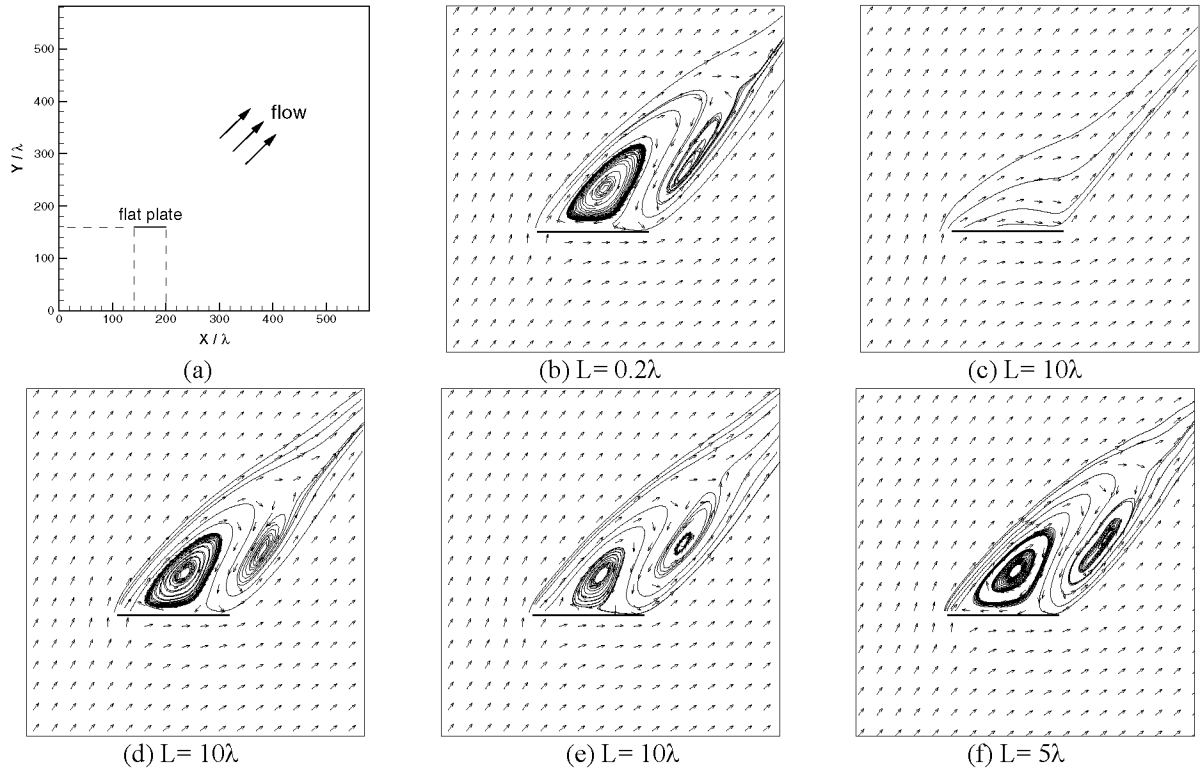

FIGURE 2. Steady flow over an inclined flat plate using DSMC simulations. (a) Schematics of the problem, (b) Reference case (L≈0.2λ), (c) DSMC (L=10λ), (d) LCDSMC(L=10λ) with enlargement factors ($C_u = 0.055$ and $C_T = 0.02$) using reference values for collisions, (e) LCDSMC(L=10λ) with enlargement factors ($C_u = 0.055$ and $C_T = 0.02$) using instantaneous values for collisions, (f) LCDSMC(L=5λ) with enlargement factors ($C_u = 0.055$ and $C_T = 0.02$) using instantaneous values for collisions.

Further evaluation of the LCDSMC scheme is given to the technique calculating the cell-averaged flow properties. Figs. 2(e) and 2(f) show the results when the instantaneous flow field is used in particle collisions where the cell size is 10λ and 5λ, respectively. These results are similar to those in the reference case. However, the size of the major vortex in Fig 2(e) becomes smaller. This is because the first-order interpolation of the flow field values is based on the large cell results instead of the reference data that use much more cells. When the cell size is halved, the results (Fig. 2(f)) get better. It is basically a grid resolution problem. This reminds us that the cell size even for the LCDSMC scheme should not be larger than the size of the flow structures such as shock waves. For instance, models may be needed in LCDSMC simulations to include effects of vortexes whose size is smaller than the cell size in turbulent flows.

CONCLUDING REMARKS

The conventional DSMC method has a strict restriction on the cell size because the error becomes obvious when the cell size is greater than one mean free path of the gas molecules. This size restriction requires a DSMC simulation to have a large number of computational cells, which makes DSMC inaccessible for many practical applications. The cell size restriction, however, can be relaxed if the flow field information can be properly involved during particle collisions.

The proposed large cell DSMC method was shown to be able to predict correct results when the cell size is larger than the molecular mean free path. In order to do this, extra operations are required during the simulation in addition to the regular DSMC operations. Thus a LCDSMC simulation takes more time than a DSMC simulation for each time step. The extra time is spent on the evaluation of cell-averaged flow properties, point-based flow properties at particles' locations, modification to enforce general conservation, and others. Our simulation showed that a LCDSMC took about twice of the time spent on a similar DSMC simulation for every time step. The LCDSMC method also required a larger number of time steps to reach a steady state because the mean flow properties are involved in the collision model. As to the number of simulated particles, it is desired to have more particles in LCDSMC thus the evaluated flow properties exhibit less statistical scatter, but it is not a necessity. Because the computational cost for LCDSMC is larger than that of DSMC when the cell size is the same, it is suggested to employ the subcell technique when the cell size is comparable to one molecular mean free path and to use the LCDSMC method otherwise.

The LCDSMC may have more applications in low Knudsen number flows because these flows cost more computational resources for DSMC to simulate. The velocity distribution functions in low Knudsen number flows deviate less from the Maxwellian distribution and the scaling of the function in LCDSMC should work better for these flows, which may indicate that relatively larger cells can be used for LCDSMC in lower Knudsen number flows. In addition, other techniques such as the time relaxed Monte Carlo method can be combined with LCDSMC, so that the numerical cost can be further reduced for a particle method to simulate low Knudsen number flows.

ACKNOWLEDGMENTS

The authors would like to thank Prof. Ching Shen and Prof. Iain Boyd for many helpful discussions. This work is supported by the National Natural Science Foundation of China (10742001 and 50836007).

REFERENCES

1. G. A. Bird, *Molecular Dynamics and the Direct Simulation of Gas Flows*, Clarendon, Oxford, 1994.
2. C. Shen, *Rarefied Gas Dynamics: Fundamentals, simulations and micro flows*, Springer, 2005.
3. F. J. Alexander, A. L. Garcia, and B. J. Alder, *Phys. Fluids* **10**, 1540,1998.
4. N. G. Hadjiconstantinou , *Phys. Fluids* **12**, 2634, 2000.
5. G. A. Bird, *Phys. Fluids* **30**, 364, 1987.
6. Q. Sun, I. D. Boyd, C. Cai, J. H. Clemmons, J. H. Hecht, *J. Spacecraft Rockets* **43**, 186, 2006.
7. G. A. Bird, "Sophisticated versus simple DSMC" in *Rarefied Gas Dynamics*, edited by M. S. Ivanov and A. K. Rebrov, 2007, pp. 815.
8. M. Usami and T. Nakayama, "Intermolecular collision scheme of DSMC taking molecular locations within a cell into account," in *Rarefied Gas Dynamics,* edited by A. D. Ketsdever and E. P. Muntz, 2003, pp. 374.
9. L. Pareschi and S. Trazzi, *International Journal for Numerical Methods in Fluids* **48**, 947, 2005.
10. Q. Sun and I. D. Boyd, *Journal of Thermophysics and Heat Transfer* **19**, 329, 2005.
11. C. L. Lawson and R. J. Hanson, *Solving Least Squares Problems,* Englewood Cliffs, New Jersey, 1974.