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Direct Simulation Method Based on BGK Equation

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Abstract. A new particle simulation method is presented here based on the BGK equation, which is a good approximation to the Boltzmann equation near equilibrium. The main idea of this method is to track down the evolution of the distribution function due to intermolecular collisions along enormous molecular trajectories which are selected randomly when molecules reflect from boundary as in the DSMC method. The simple algorithmic structure of the DSMC method is employed but, besides position and velocity, each simulated molecule will carry two additional variables: one records the value of the distribution function and another records the number of real molecules represented by the related simulated molecule. The former is updated according to the Lagrangian description of the BGK equation and the latter is updated according to the former, after which the transitional macro-quantities defined for each cell are updated according to a special scheme which can make them evolve smoothly and finally converge to their solutions. This new method achieves its efficiency by avoiding generating random fractions during the intermolecular collision process and using the increments of molecular variables to update those transitional macro-quantities, which makes the new method have the feature that the total computational time will not increase with the decrease of the magnitude of the deviation from equilibrium. The proposed method is validated by comparison with the DSMC method as criterion.

Keywords: micro gas flows, BGK equation, particle simulation method, DSMC method.
PACS: 47.61.Fg, 47.15.gm, 47.45.Ab.

INTRODUCTION

In rarefied gas flows and flows in MEMS devices, the characteristic scales will be the same order as the molecular mean free path, making the Navier-Stokes equation invalid. These kinds of problems can be simulated by the DSMC method [1]. As a large number of random fractions are used, the results of DSMC simulations contain statistic noise, which makes the DSMC method time-consuming and almost intractable to very low velocity problems although it is very successful in the simulation of high velocity problems. To overcome the difficulty encountered by the DSMC method in low-velocity cases, many particle simulation methods including [2-8] among others had been proposed independently making modifications to the standard DSMC method and obtaining improvements of efficiency for low velocity cases. Some [4, 5, 8] of them are based on the BGK equation [9].

Here, a new particle simulation method [10] based on the BGK equation is presented and will be referred to as DS-BGK method. As mentioned in the abstract, this new method retains the basic algorithmic structure of the DMSC method and so can have some advantages like simplicity, numerical stability and convenience for complex configurations. Some calculation results will be used to show the validity and the efficiency of the DS-BGK method.

DIRECT SIMULATION METHOD BASED ON BGK EQUATION

In the absence of external body force, the BGK equation can be written as a Lagrangian description:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + c_j \frac{\partial f}{\partial x_j} = \upsilon(f_{eq} - f) \tag{1}$$

In this paper, only single component gas will be considered and m is the molecular mass. The simulation process is divided into a series of time steps Δt. The computational domain is divided into a number of cells and V_m denotes the volume of cell m (used as a subscript). We estimate that the values of the time step and cell size used in the DS-BGK method should be the same as in the DSMC method. In order to ensure the simulation process is stable and avoid a time-averaging process for smooth results, the DS-BGK method will employ an enormous

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number of simulated molecules but can still be efficient. In addition to its position and velocity, each simulated molecule l carries two additional variables: N_l which means the number of real molecules represented by the simulated molecule l and is used to construct a representative sample $[\vec{x}_l, \vec{c}_l, N_l]_{all}$ of f^{tr}, F_l which equals the representative value $f^{tr}(t, \vec{x}_l, \vec{c}_l)$. The updating algorithm should satisfy the *compatibility condition* that the representative sample and the representative value are always related to the same distribution function and should make f^{tr} converge to the solution of the BGK equation. The initial value of F_l equals $f(0, \vec{x}_l, \vec{c}_l)$ when the initial values of $\vec{x}_l, \vec{c}_l$ are determined. The initial values of N_l for different simulated molecules are the same but will be changed to be different from each other in the following simulation process, through which the evolution of the distribution function due to intermolecular collisions is recorded for this new particle simulation method. During the simulation process, each simulated molecule will move uniformly and in a straight line until reflecting from the boundary and getting a new velocity randomly as in the DSMC method. F_l is updated along the straightforward trajectory according to Lagrangian description of BGK equation and N_l is updated to make N_l / F_l constant when molecule moving inside the computational domain, which is based on the extrapolation of the acceptance-rejection method that if $[\vec{x}_l, \vec{c}_l, N_l]_{all}$ is a representative sample of f_1, $[\vec{x}_l, \vec{c}_l, N_l (f_2 / f_1)_l]_{all}$ can be used as a representative sample of f_2 and so satisfies the above *compatibility condition*.

According to equation (1), F_l is updated along the trajectory of the simulated molecule l:

$$\frac{dF_l}{dt} = \upsilon (f_{eq} - F_l) \tag{2}$$

f_{eq} should be updated after each Δt according to $\vec{x}_l, \vec{c}_l, N_l$ of those simulated molecules staying inside the same cell. Unfortunately, this scheme for updating f_{eq}, which is demanded by the BGK equation, cannot control statistical noise because the average number of simulated molecules staying inside each cell is still small although it is much larger than that used in the DSMC method.

Adoption of A Transitional Maxwell Distribution Function

As $n_{eq}, \vec{u}_{eq}, T_{eq}$ calculated by molecular transient information (including $\vec{x}_l$, $\vec{c}_l$ and N_l) after each time step contain large statistical noise, three transitional variables $n_{eq}^{tr}, \vec{u}_{eq}^{tr}, T_{eq}^{tr}$ are assigned to each cell to construct a transitional Maxwell distribution function $f_{eq}^{tr} = n_{eq}^{tr} (\frac{m}{2\pi k T_{eq}^{tr}})^{3/2} \exp(\frac{-m(\vec{c} - \vec{u}_{eq}^{tr})^2}{2kT_{eq}^{tr}})$ and those transitional variables can be taken as tentative values of their physical variables. $n_{eq}^{tr}, \vec{u}_{eq}^{tr}, T_{eq}^{tr}$ equal $n_{eq}, \vec{u}_{eq}, T_{eq}$ at the initial state of the simulation process and are updated after each time step according to a special principle (see Eq. (4)). As f_{eq}^{tr} is used in Eq. (2) in place of f_{eq}, it is desirable to prove that $n_{eq}^{tr}, \vec{u}_{eq}^{tr}, T_{eq}^{tr}$ equal $n_{eq}, \vec{u}_{eq}, T_{eq}$ after convergence, which will be discussed at the end of this section.

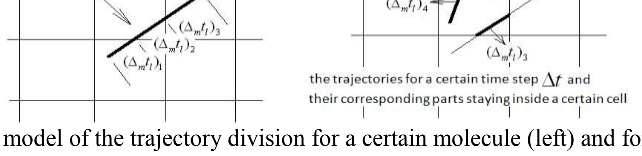

FIGURE 1. A schematic model of the trajectory division for a certain molecule (left) and for a certain cell (right)

The trajectory of each simulated molecule is always straightforward and during a given time step, the trajectory of each simulated molecule is a short segment and may be divided into several parts (each part stays inside a cell, see Fig. 1 left). After employing f_{eq}^{tr}, ΔF_l is calculated for each of those parts and for a certain part (staying inside the cell m and taking moving-time $\Delta_m t_l$ of the simulated molecule l), $f_{eq,m}^{tr}$ is constant and the formulation of $\Delta_m F_l$ can be written as follows after integration of equation (2) where f_{eq} should be replaced by f_{eq}^{tr} :

$$F_l^{new} - f_{eq,m}^{tr} = (F_l^{old} - f_{eq,m}^{tr})\exp(-\upsilon\Delta_m t_l), \Delta_m F_l = F_l^{new} - F_l^{old}, \Delta_m t_l \le \Delta t \tag{3}$$

After updating F_l for each part (see Fig. 1 left), N_l is updated correspondingly to make N_l / F_l constant.

During the current Δt and for each cell m (see Fig. 1 right), some molecules will run inside this cell and their $\Delta_m N_l$ can be obtained easily according to $\Delta_m F_l$. Obviously, $\Delta_m N_l$ is the number increment of real molecules of class $\vec{c}_l$ associated with intermolecular collisions inside cell m during the current time step. If we make a summation $\sum'$ over all those simulated molecules, then, $\sum' \Delta_m N_l$ means the number increment of real molecules of all existing classes associated with intermolecular collisions inside the same cell m during the same time step and is expected (*note: usually not*) to equal zero as required by the conservation principle for the intermolecular collision process. So, if $\sum' \Delta_m N_l$ is positive, we should decrease $n_{eq,m}^{tr}$ and then $\sum' \Delta_m N_l$ will decrease at the next time step according to equation (2), and vice versa. It is an auto-regulation algorithm which can ensure that $\sum' \Delta_m N_l$ fluctuates near zero. Similarly, $\sum \Delta_m N_l m\vec{c}_l$ and $\sum \Delta_m N_l m\vec{c}_l^{\,2} / 2$ are related respectively to momentum increment and kinetic energy increment of real molecules of all existing classes associated with intermolecular collisions occurring inside the same cell and during the same time step and can be used to update $\vec{u}_{eq,m}^{\,tr}$ and $T_{eq,m}^{tr}$. Now, the algorithms for updating $n_{eq}^{tr}, \vec{u}_{eq}^{\,tr}, T_{eq}^{tr}$ of cell m are:

$$\begin{aligned}
n_{eq,m}^{tr,new} &= \frac{n_{eq,m}^{tr,old} V_m - \sum \Delta_m N_l}{V_m} \\
\vec{u}_{eq,m}^{\,tr,new} &= \frac{n_{eq,m}^{tr,old} V_m \vec{u}_{eq,m}^{\,tr,old} - \sum \Delta_m N_l \vec{c}_l}{n_{eq,m}^{tr,new} V_m} \\
T_{eq,m}^{tr,new} &= \frac{[n_{eq,m}^{tr,old} V_m (3kT_{eq,m}^{tr,old} / 2 + m(\vec{u}_{eq,m}^{\,tr,old})^2 / 2) - \sum \Delta_m N_l m\vec{c}_l^{\,2} / 2] - n_{eq,m}^{tr,new} V_m m(\vec{u}_{eq,m}^{\,tr,new})^2 / 2}{n_{eq,m}^{tr,new} V_m 3k / 2}
\end{aligned} \tag{4}$$

Here, it should be pointed out that as a random fraction is used in the molecular reflection process on the boundary and so any possible representative trajectory can be selected according to its probability (see next section) during the simulation process, we can expect that the feature of all existing classes can represent the feature of all possible classes and so the summation over all existing classes in the DS-BGK method can be taken as equivalent to the integration over all possible classes in the description of a kinetic equation. It is obvious that those updating algorithms of equation (4) have the function of auto-regulation which can make $\sum' \Delta_m N_l$, $\sum \Delta_m N_l \vec{c}_l$ and $\sum \Delta_m N_l m\vec{c}_l^{\,2} / 2$ converge to zero and then the following equation is satisfied because the summation over all existing classes can be taken as equivalent to the integration over all possible classes as discussed above:

$$\int_{-\infty}^{\infty} \upsilon(f_{eq}^{tr} - f)\psi_k(\vec{c})d\vec{c} = 0 \tag{5}$$

where $\psi_1 = 1, (\psi_2, \psi_3, \psi_4) = \vec{c}, \psi_5 = \vec{c}^{\,2}$. As $\int_{-\infty}^{\infty} \upsilon(f_{eq} - f)\psi_k(\vec{c})d\vec{c} = 0$ is always satisfied by the original BGK equation, it is easy to prove that $n_{eq}^{tr}, \vec{u}_{eq}^{\,tr}, T_{eq}^{tr}$ equal $n_{eq}, \vec{u}_{eq}, T_{eq}$ after convergence where equation (5) is satisfied. For closed problem, equation (4) has another function in that it ensures an important definite condition:

$$\sum_{Domain}^{converge} N_l = \overset{eq(5)}{=} \sum_{Domain}^{converge} V_m n_{eq,m}^{tr} = \frac{1}{2}\left(\sum_{Domain}^{converge} N_l + \sum_{Domain}^{converge} V_m n_{eq,m}^{tr}\right) \overset{eq(4)}{=} \frac{1}{2}\left(\sum_{Domain}^{initial} N_l + \sum_{Domain}^{initial} V_m n_{eq,m}^{tr}\right) = \sum_{Domain} N_{real} \tag{6}$$

which means the total number represented by simulated molecules equals that of real molecules after convergence.

Until now, only the updating schemes of $\vec{x}_l, \vec{c}_l, F_l, N_l$ and $n_{eq}^{tr}, \vec{u}_{eq}^{tr}, T_{eq}^{tr}$ for the process occurring inside the computational domain have been introduced. In addition, $\vec{c}_l$ and F_l will change after molecular reflection from the boundary (see next section).

Boundary Conditions

In this section, the subscript l is omitted for velocity variables. The selecting principle of the reflecting velocity $\vec{c}_r$ is the same as in the DSMC method. $\vec{c}_i$ is the incoming velocities, the subscript $2,3$ is for the tangential velocity component and the subscript 1 is for the velocity component along the normal direction pointed into the flow domain which means that $c_{r,1}$ is positive and $c_{i,1}$ is negative. In the DS-BGK method, F_l is changed to the value of the distribution function f_B at the boundary after molecule reflecting from boundary. So, f_B should be recorded and updated after each time step so that the new value of F_l can be calculated according to f_B after $\vec{c}_r$ being determined. Although F_l will be changed, N_l remains unchanged after reflection, which is consistent with the mass conservation principle of the reflection process and also satisfies the above *compatibility condition*.

For different type of boundary conditions, $f_B(c_{r,1} > 0)$ has different forms. For CL boundary condition [11]:

$$\begin{aligned} f_{B,CL} = a\frac{1}{\sqrt{\pi\alpha_\tau}}\exp\left[-\frac{(\tilde{c}_{r,2}-\sqrt{1-\alpha_\tau}\,\tilde{c}_{i,2})^2}{\alpha_\tau}\right]\cdot\frac{1}{\sqrt{\pi\alpha_\tau}}\exp\left[-\frac{(\tilde{c}_{r,3}-\sqrt{1-\alpha_\tau}\,\tilde{c}_{i,3})^2}{\alpha_\tau}\right]\cdot \\ \frac{1}{\pi\alpha_n}\exp\left[-\frac{\tilde{c}_{r,1}^2+(1-\alpha_n)\tilde{c}_{i,1}^2}{\alpha_n}\right]\int_0^{2\pi}\exp\left[\frac{2\sqrt{1-\alpha_n}\,\tilde{c}_{r,1}\left|\tilde{c}_{i,1}\right|}{\alpha_n}\cos\theta\right]d\theta \end{aligned} \tag{7}$$

where $\tilde{c}_{r,j} = c_{r,j}/\sqrt{2kT_{wall}/m}, \tilde{c}_{i,j} = c_{i,j}/\sqrt{2kT_{wall}/m}, (j=1,2,3)$, α_τ, α_n are the accommodation coefficients of the kinetic energy of the tangential velocity component and the normal velocity component, respectively. The factor a can be determined by the mass conservation principle which demands that the number N_i of the incoming molecules equals the number N_r of the reflecting molecules. N_i can be estimated by f_{eq}^{tr} of the adjacent cell of the boundary concerned and its formulation can be written as following:

$$N_i = n_{eq}^{tr}\sqrt{\frac{kT_{eq}^{tr}}{2\pi m}}\left\{\exp\left[-\left(\frac{-u_{eq,1}^{tr}}{\sqrt{2kT_{eq}^{tr}/m}}\right)^2\right]+\sqrt{\pi}\,\frac{-u_{eq,1}^{tr}}{\sqrt{2kT_{eq}^{tr}/m}}\left[1+erf\left(\frac{-u_{eq,1}^{tr}}{\sqrt{2kT_{eq}^{tr}/m}}\right)\right]\right\} \tag{8}$$

According to Eq. (7), N_r can be calculated:

$$N_r = \int_{c_{r,1}>0} f_{B,CL}\,c_{r,1}\,d\vec{c}_r = a(2kT_{wall}/m)^2 \tag{9}$$

If N_r equals N_i, then the factor a is determined and $f_{B,CL}$ is known for any reflecting velocity $\vec{c}_r$. F_l will be updated to the value of $f_{B,CL}$ at $\vec{c}_r$ after reflection from boundary. If the boundary is not static, the relative velocities should be used in the above equations to get the new value of F_l.

If we let $\alpha_\tau = \alpha_n = 1$, we will get Maxwell boundary condition. For specular reflection boundary condition, there is no need to update the value of f_B at the boundary because F_l remains unchanged after reflection from boundary.

Calculation of Flux of Molecular Quantity on the Boundary Surface

As in the DSMC method, it is convenient for the DS-BGK method to calculate the flux $\Gamma(Q)$ of any quantity $Q(\vec{c})$ in unit time and across unit area of the boundary surface:

$$\Gamma(Q) = \frac{1}{\Delta t \Delta S} \sum_{l} N_l [Q_i(\vec{c}) - Q_r(\vec{c})]_l \tag{10}$$

where the summation is over all those simulated molecules reflecting from a given area ΔS during the time step Δt and $Q_r(\vec{c}), Q_i(\vec{c})$ are the reflecting quantity and incoming quantity, respectively.

Summary of the Algorithmic Structure

In summary, the algorithm of the DS-BGK method proceeds as follows:

1. Initialization. Generate many cells and simulated molecules and assign them with initial values.
2. Each simulated molecule moves uniformly and in a straight line before encountering boundary. During each Δt, the trajectory may be divided into several parts (see Fig. 1 left), then F_l and N_l are updated according to equation (3) for each part. After each Δt, f_{eq}^{tr} of each cell (see Fig. 1 right) is updated according to equation (4). When encountering boundary, $\vec{c}_r$ is selected randomly and then F_l is updated as described above.
3. After convergence, $n_{eq}^{tr}, \vec{u}_{eq}^{tr}, T_{eq}^{tr}$ can be used to output the final results.

SIMULATION RESULTS OF THE DS-BGK METHOD

Comparison of the DS-BGK Method with the DSMC Method

Here, the DS-BGK method is verified by comparison with the DSMC method in a 2-D driven cavity gas flow. The Maxwell boundary condition and cell size and time step used in the DS-BGK method is the same as in the DSMC method and. The parameter υ of the BGK equation is determined by μ_{BGK}, so the momentum exchange should be simulated correctly by the DS-BGK method, which will be verified by the comparison of velocity distributions. Here, the DS-BGK method uses about 2000 molecules in each cell. As we can see, for Kn=0.063, the agreement of the DS-BGK method with the DSMC method is very good; for Kn=6.3 in the transitional regime, the agreement is still good overall although the difference between the two results is obvious in some regions.

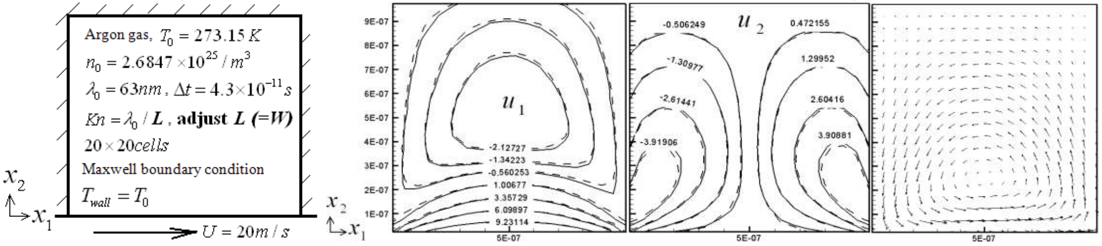

FIGURE 2. Velocity distributions by the DS-BGK method (dashed line) and the DSMC method (solid line), Kn=0.063.

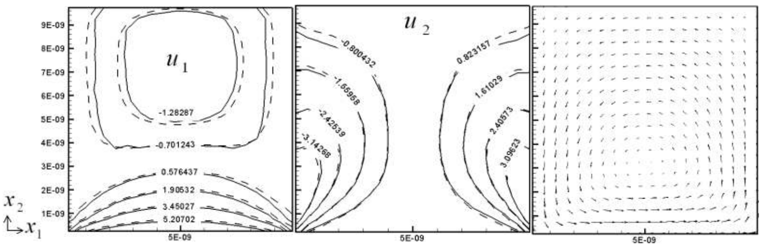

FIGURE 3. Velocity distributions by the DS-BGK method (dashed line) and the DSMC method (solid line), Kn=6.3.

Discussion about the Efficiency of the DS-BGK Method in Low-velocity Cases

With respect to efficiency, the total computational time can be taken as the key parameter. In the above simulation where U=20m/s and Kn=0.063, the total computational time used by the DS-BGK method is about 7 minutes running on one CPU of Lenovo E43A (having usual capability) but the DSMC simulation takes about 30 hours using about 67 molecules in each cell on average and sampling about 3.4×10^6 times. When U decreases to only 0.1m/s (Kn keeps unchanged), the total computational time of the DS-BGK method is still about 7 minutes. As the total computational time of the DSMC method is usually inverse proportional to the square of Mach number if the computational time used for the convergent process is negligible, it will be very time-consuming for DSMC simulation in such a low-velocity case. The explanation for the high efficiency of the DS-BGK method is that it avoids generating random fractions during the intermolecular collision process and uses the increments (instead of the transient values) of molecular variables to update the transitional macro-quantities defined for each cell, which can reduce the statistical noise due to non-continuous events of molecules moving into or out of the cell. If we decrease the average number of simulated molecules per cell used by the DS-BGK method, the relative statistical scatter, namely the ratio of statistical scatter to useful information, will increase and the time-averaging process may become necessary for getting a smooth result. But, the influence of Mach number on the relative statistical scatter is negligible as shown in Fig. 4 where the evolution of the simulation processes (shown by a certain contour of u_1) for this two test cases are given. As the transient result in Fig. 4 is smooth, the time-averaging process is avoided here.

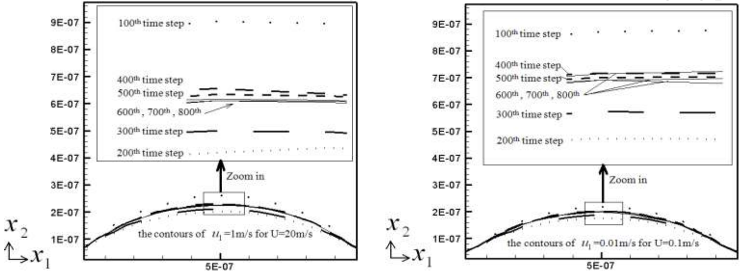

FIGURE 4. Evolution of a certain contour calculated by the DS-BGK method, Kn=0.063, U=20m/s (left) and U=0.1m/s (right).

CONCLUSIONS

A new particle simulation method based on the BGK equation is proposed here and named as DS-BGK method. It is verified by comparison with the DSMC method as criterion and efficient for low-velocity cases of gas flow problems. The physical quantity transportation process of the real molecules is represented by the movements of the simulated molecules with the help of molecular weightings in the DS-BGK method. It is therefore convenient for the DS-BGK method to employ a complicated and more realistic boundary condition, namely the CLL reflection model [12] which is a good application and extension of the CL reflection model [11].

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