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Improvements to the low-variance deviational simulation Monte Carlo method

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Abstract: Recently Homolle and Hadjiconstantinou presented a new particle simulation method, i. e. LVDSMC method[1] which incorporates the variance reduction idea thus attaining significant computational efficiency for low speed flows. In the present paper two improvements of this LVDSMC method are proposed. Firstly, additional auxiliary particles different from deviational particles used in the original LVDSMC are suggested to be introduced and the numerical error caused by the accumulation of the net number of deviational particles created can be restrained through employing such auxiliary particles, which is especially crucial in treating problems in and near free molecular regime. Secondly, an alternative principle used to determine the increment of the velocity parameter in the increment of the underlying Maxwell Boltzmann distribution in LVDSMC collision process is proposed to make easier the calculation of the momentum and energy fluxes across the surface of the boundary.

Key words: DSMC; LVDSMC; deviational particle; auxiliary particle
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0 Introduction

For micro scale low speed gas flow problems especially those in MEMS/NEMS applications, the Navier-Stokes equation is no longer valid and the Boltzmann equation is an appropriate one to treat them. Although the linearized Boltzmann equation can be used in place of the Boltzmann equation for low speed gas flow problems, it remains a formidable task to solve the former for its high dimensionality and huge time consumption to treat its collision integral. DSMC[2] method is a reliable method to treat gas flow problems but is very time consuming to treat low speed problem for the small information to noise ratio. A method of variance reduction, embedded in the finite difference method, was proposed to solve Boltzmann equation in[3], in which the collision integral is written as the sum of a linear term and a quadratic term (small in case of slow motion) and only the former is taken into consideration for low speed problems. Although the method of variance reduction shows significant computational efficiency compared to traditional Monte Carlo method used to treat the collision integral in solving Boltzmann equation, it retains the disadvantages of the finite difference method compared to particle methods like DSMC method.

Recently, T. M. M. Homolle and N. G. Hadjiconstantinou[1] proposed a new particle method-LVDSMC method which incorporates the idea of the variance reduction method and retains the algorithmic structure of DSMC method. By simulating only the deviation from equilibrium, it achieved a significant computational efficiency for low speed problemscompared to DSMC method and at the same time enjoys many advantages of particle method like DSMC

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method. Based on LVDSMC method, two natural improvements are proposed in this paper. First, a new kind of computational particles is proposed in section 1 to be employed to overcome the accumulation of numerical error caused by the net number of deviational particles in and near free molecular flows. Then, the procedure used to determine $\Delta \boldsymbol{U}_{MB}$ in LVDSMC collision process is proposed in section 2 to be altered a little to make easier the calculation of the momentum and energy fluxes at the boundary.

1 A new kind of computational particles used to avoid the accumulation of statistical error

During the simulation process of LVDSMC method, there are three cases where new deviational particles will be introduced into computational domain. Firstly, deviational particles are created inside cells according to $\{\Delta t[\overline{K_1}-\overline{K_2}]f^d-\Delta f^{MB}\}$ in the collision process. Here and throughout the whole paper the notations of[4] are used. Secondly, deviational particles are created at the interfaces between two neighboring cells according to $(\boldsymbol{c}\cdot\boldsymbol{n})[f^{MB(l)}(\boldsymbol{c})-f^{MB(r)}(\boldsymbol{c})]$ in the advection process. Thirdly, deviational particles are created at the interfaces between boundary and its adjacent cells according to $(\boldsymbol{c}\cdot\boldsymbol{n})[f^{MB(\mathrm{bdary})}(\boldsymbol{c})-f^{MB(\mathrm{cell})}(\boldsymbol{c})]$, $(\boldsymbol{c}\cdot\boldsymbol{n})>0$ in the advection process in the case $\boldsymbol{U}_{\mathrm{bdary}}\cdot\boldsymbol{n}=0$, where $\boldsymbol{U}_{\mathrm{bdary}}$ is the velocity of the boundary and $f^{MB(\mathrm{bdary})}(\boldsymbol{c})$ is the equivalent underlying distribution function of the boundary and $f^{MB(\mathrm{cell})}(\boldsymbol{c})$ is the underlying distribution function of its adjacent cell and $\boldsymbol{n}$ is the inner normal vector of the boundary. There are two cases where existing deviational particles will be removed from computational domain. In the collision process existing deviational particles are deleted with a probability proportional to $v(\omega)\Delta t$ and in the advection process existing deviational particles are deleted with equal numbers of positive deviational particles and negative deviational particles among those deviational particles arriving at a same part of the boundary during a same time step.

As defined and discussed in[4], the mass conservation equation of the collision process is:

$$\int_{-\infty}^{+\infty}\{\Delta t[\overline{K_1}-\overline{K_2}]f^d-\Delta f^{MB}\}\mathrm{d}\boldsymbol{c}=0 \qquad (1)$$

In the case $\boldsymbol{U}_{MB}\cdot\boldsymbol{n}=0$ ($\boldsymbol{U}_{MB}$ is the velocity parameter of $f^{MB(\mathrm{cell})}$), the mass conservation equation of the advection process at boundary leads to a new equation related to the process of creating deviational particles at boundary:

$$\int_{(\boldsymbol{c}\cdot\boldsymbol{n})>0}(\boldsymbol{c}\cdot\boldsymbol{n})[f^{MB(\mathrm{bdary})}(\boldsymbol{c})-f^{MB(\mathrm{cell})}(\boldsymbol{c})]\mathrm{d}\boldsymbol{c}=0 \qquad (2)$$

Although the condition $\boldsymbol{U}_{MB}\cdot\boldsymbol{n}=0$ is very severe, it is a convenient choice to meet this condition in LVDSMC simulation process, which will be discussed in section 1.2. Eq. (1) and (2) demand that the net numbers of deviational particles created during a time step is zero:

$$n^{(1)}_{\mathrm{net,\,creat}}=n^{(2)}_{\mathrm{net,\,creat}}=\sum_{i=1}^{j}\mathrm{sgn}(i)=0 \qquad (3)$$

where j is the number of deviational particles created according to the integral kernel of Eq. (1) or (2) during a time step and $\mathrm{sgn}(i)$ equals 1 if the deviational particles i is positive and equals -1 if negative. The existence of numerical error usually makes the net number $n^{(1)}_{\mathrm{net,\,creat}}$ and $n^{(2)}_{\mathrm{net,\,creat}}$ not zero and deviational particles corresponding to the net number may remain inside the computational domain and their persistent movements lead to the accumulation of numerical error which is remarkable especially for problems in and near free molecular regime (see the numerical example at the end of this paragraph).

The authors suggest here to employ new kind of computational particles (named auxiliary particles) to counteract the net number of deviational particles created during each time step. The idea of introducing auxiliary particles is that if $n^{(1)}_{\mathrm{net,\,creat}}$ (or $n^{(2)}_{\mathrm{net,\,creat}}$) not equals zero, a number (the absolute value of $n^{(1)}_{\mathrm{net,\,creat}}$, or of $n^{(2)}_{\mathrm{net,\,creat}}$) of auxiliary particles are created according to the same principle as deviational particles. And $\mathrm{sgn}(i)$ of auxiliary particles is assigned to 1 if $n^{(1)}_{\mathrm{net,\,creat}}$ (or $n^{(2)}_{\mathrm{net,\,creat}}$) is smaller than zero or to -1 if bigger than zero. It is stipulated that the movements of auxiliary particles do not contrib-

ute to the transportations of mass, momentum and energy and auxiliary particles are not used to calculate integrals[4] like $\int F(\boldsymbol{c}_1) f^d(\boldsymbol{c}_1) d\boldsymbol{c}_1$ in the collision process. Auxiliary particles are used only to alter the net number of computational particles arriving at a part of the boundary during a time step now including deviational particles and auxiliary particles. It is important that auxiliary particles are created according to the same principle as deviational particles so that they can move along with deviational particles and may arrive at a same part of the boundary during a same time step as those deviational particles created during the same time step.

In order to show the accumulation process of numerical error caused by the net number and the effect of using auxiliary particles, the Couette flow problem in free molecular regime is simulated by LVDSMC method. The upper plate is stationary and the velocity of the lower plate is 10m/s and the temperature of the two plates is $T = 300$K. The distance between the two plates is 10 nm and diffuse reflection boundary condition is used. The number density of gas (Argon) is $n = 2\times10^{25}$ and the molecular mass is $m = 66.3\times10^{-27}$g. The theoretical shear stresses subjected by the upper plate and lower plates are[5]:

$$\tau^{\text{upper}} = -\tau^{\text{lower}} = m(U_1 - U_2)n\sqrt{\frac{kT}{2\pi m}} = 1322.2\text{Pa} \tag{4}$$

In LVDSMC simulation of this problem, the initial underlying f^{MB} for each cell is:

$$f^{MB}(\boldsymbol{c}) = n\left(\frac{m}{2\pi kT}\right)^{3/2}\exp\left[-\frac{m(\boldsymbol{c})^2}{2kT}\right] \tag{5}$$

which remains unchanged for no collision between molecules in free molecular problems and equals to the equivalent underlying distribution function of the upper plate throughout the simulation process. During each time step, deviational particles are created only according to the difference between $f^{MB(\text{bdary})}(\boldsymbol{c})$ of the lower plate and $F^{MB(\text{cell})}(\boldsymbol{c})$ of its neighboring cell. The recorded data of the simulation process by original LVDSMC method indicates that:

$$\begin{aligned}
\sum_{l=1}^{400}(n^{+}_{1,\text{creat}})_l &= 765153\\
\sum_{l=1}^{400}(n^{-}_{1,\text{creat}})_l &= 763636\\
n^{+}_{400,\text{existing}} &= 4656\\
n^{-}_{400,\text{existing}} &= 3139\\
\sum_{l=1}^{400}(n^{+}_{1,\text{creat}})_l - \sum_{l=1}^{400}(n^{-}_{1,\text{creat}})_l &= n^{+}_{400,\text{existing}} - n^{-}_{400,\text{existing}}
\end{aligned} \tag{6}$$

where $(n^{+}_{1,\text{creat}})_l$ (or $(n^{-}_{1,\text{creat}})_1$) is the number of positive (or negative) deviational particles created at the lower plate during time step l and $n^{+}_{400,\text{existing}}$ (or $n^{-}_{400,\text{existing}}$) is the number of positive (or negative) deviational particles remained inside the computational domain after 400 time steps. It is noted that small relative error (only about 0.2 percents) between $\sum_{l=1}^{400}(n^{+}_{1,\text{creat}})_l$ and $\sum_{l=1}^{400}(n^{-}_{1,\text{creat}})_l$ leads to big relative error between $n^{+}_{400,\text{existing}}$ and $n^{-}_{400,\text{existing}}$, which will increase with time step. The net number of $n^{+}_{l,\text{existing}} - n^{-}_{l,\text{existing}}$ can not be cancelled during simulation process of original LVDSMC method and those deviational particles corresponding to $n^{+}_{l,\text{existing}} - n^{-}_{l,\text{existing}}$ will come and go incessantly between the two plates, which results in additional transportations to the two plates. Figure 1 shows that the statistical solutions of the two shear stresses by original LVDSMC method deviate from their analytical values of Eq. (4) and are bigger than the analytical values because $n^{+}_{l,\text{existing}}$ is bigger than $n^{-}_{l,\text{existing}}$ after about 400 time steps. The sampling process usually needs to last enough time steps to get smooth solutions, which makes the deviation from correct values more remarkable. But after introducing the suggested auxiliary particles, the LVDSMC simulation results of the shear stresses acting on the two plates agree well with analytical values (see Fig. 2).

For problems near the free molecular regime, the accumulation of net number is also obvious because only few of deviational particles corresponding to the net number can be deleted with probability proportional to $v(\omega)\Delta t$ in collision process.

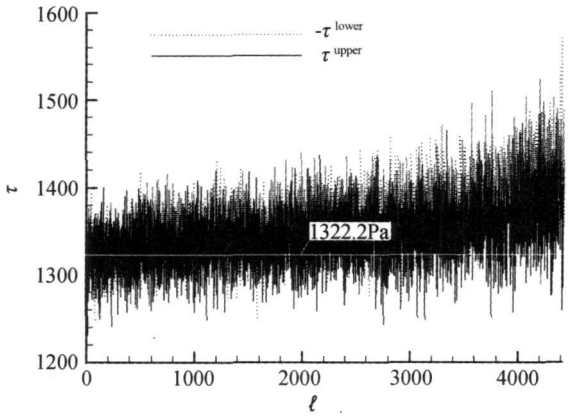

Fig. 1　The shear stresses acting on the two plates calculated by the original LVDSMC method (free molecular Couette flow, Argon, n= 2× 10^{25}, U= 10m/ s, T= 300K)

图 1　原始 LVDSMC 方法给出的作用在上下平板的切应力(自由领域的 Couette 流, 氩气, n= 2× 10^{25}, U= 10m/ s, T= 300K)

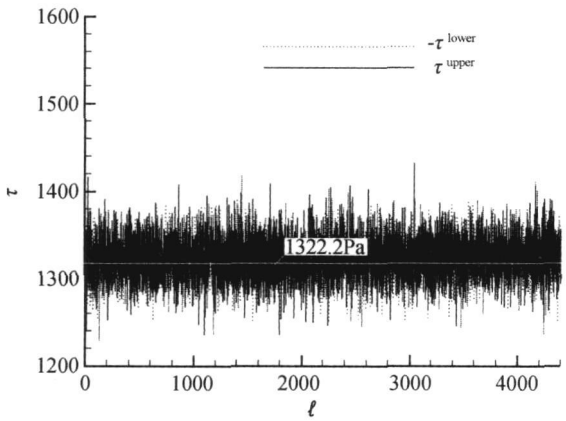

Fig. 2　The shear stresses acting on the two plates calculated by the LVDSMC method after employing auxiliary particles (free molecular Couette flow, Argon, n= 2× 10^{25}, U= 10m/ s, T= 300K)

图 2　采用辅助粒子后 LVDSMC 方法给出的作用在上下平板的切应力(自由领域的 Couette 流, 氩气, n= 2× 10^{25}, U= 10m/ s, T= 300K)

2　An alternation used in the procedure to determine ΔU_{MB}

In the advection process, the movement corresponding to f^{MB} can be neglected if f^{MB} is independent of space. When considering a cell k in the cases where f^{MB} is dependent of space, the movement corresponding to f^{MB} of all cells can be divided into two parts: part Ⅰ is of the case in which the underlying distributions of all cells are the same as $f^{MB(k)}$ and part Ⅱ is of the case in which the underlying distribution of any cell h equals $f^{MB(h)} - f^{MB(k)}$. Then, part Ⅰ can be neglected for its independence of space and only part Ⅱ needs to be taken into consideration. The method proposed in Ref. [4] to deal with the movement corresponding to f^{MB} deals in fact with only part Ⅱ and only takes into consideration the neighboring cells of cell k instead of all cells. When cell k is adjacent to the boundary, the boundary can be considered as a neighboring cell in the case $\boldsymbol{U}_{\text{bdary}} \cdot \boldsymbol{n} = 0$. The effect of part Ⅱ can be implemented by distributing deviational particles at the surface of cell k and then moving them for a randomly chosen fraction of a time step.

As discussed above, the advection process of LVDSMC contains three parts: first, the movements of the existing deviational particles lasting for a time step; second, the movements of newly created deviational particles lasting for a randomly chosen fraction of a time step; third, the movement corresponding to part Ⅰ of each cell. The movement corresponding to part Ⅰ is neglected in LVDSMC method because it does not contribute to the change of distribution function. But, it must be taken into consideration when calculating the fluxes of any quantity of interest across the boundary. In fact, compared to the movements of existing deviational particles and newly created deviational particles, the movement corresponding to part Ⅰ contributes most to the normal pressure of the boundary. Taken the calculation sample described in section 1. 1 again, the fluxes of normal momentum across the surfaces of the two plates carried by the movements of deviational particles, denoted by $p^{\text{upper}}_{\text{particle}}$ and $p^{\text{lower}}_{\text{particle}}$, are shown in figure 3. The calculation result shows that $p^{\text{upper}}_{\text{particle}}$ and $p^{\text{lower}}_{\text{particle}}$ fluctuate around zero and their absolute values are much smaller than the actual flux of normal momentum $nkT \approx 8.28 \times 10^4$ pa, which is about the flux carried by the movement corresponding to part Ⅰ (see Eq. (8)). After cognizing the contribution of part Ⅰ to fluxes across the surface of the boundary, it is desirable to know how to calculate fluxes contributed by part Ⅰ and how to simplify the calculation of those fluxes.

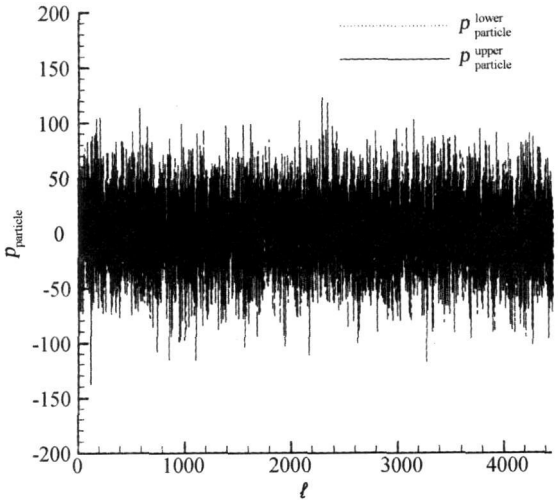

Fig. 3 The fluxes of normal momentum carried by the movement of deviational particles (free molecular Couette flow, Argon, $n = 2\times10^{25}$, $U = 10$m/s, $T = 300$K)

图 3 由偏差粒子运动实现的法向动量的输运(自由领域的 Couette 流, 氩气, $n = 2\times10^{25}$, $U = 10$m/s, $T = 300$K)

In the case $\boldsymbol{U}_{bdary}\cdot\boldsymbol{n} = 0$, the expression of the flux $\Gamma^{I}(Q)$ of $Q(\boldsymbol{c})$ in unit time across unit area of the boundary carried by the movement corresponding to part Ⅰ is:

$$\Gamma^{I}(Q) = \int_{-\infty}^{\infty} -Q(\boldsymbol{c})(\boldsymbol{c}\cdot\boldsymbol{n})f^{MB(cell)}\,d\boldsymbol{c} \qquad (7)$$

where $\boldsymbol{n}$ is the inner normal vector of the boundary and $f^{MB(cell)}$ is the underlying distribution of the cell adjacent to the boundary. Let $Q(\boldsymbol{c})$ be the momentum component mc_n normal to the boundary, the momentum component mc_τ parallel to the boundary and the translational energy $mc^2/2$, respectively, the flux $\Gamma^{I}(Q)$ will be a part of the normal pressure, the shear stress and the heat flux, respectively. The solution of $\Gamma^{I}(Q)$ is usually complicated if $\boldsymbol{U}_{MB}\cdot\boldsymbol{n}\neq0$. If $\boldsymbol{U}_{MB}\cdot\boldsymbol{n} = 0$, Eq. (7) has simple solutions for different $Q(\boldsymbol{c})$ of interest:

$$\begin{aligned}\Gamma^{I}(mc_n) &= n_{MB}kT_{MB}\\ \Gamma^{I}(mc_\tau) &= 0\\ \Gamma^{I}(mc^2/2) &= 0\end{aligned} \qquad (8)$$

where n_{MB} and T_{MB} are the number density and temperature of $f^{MB(cell)}$.

In LVDSMC collision process, the increment $\Delta\boldsymbol{U}_{MB}$ used to determine Δf^{MB} and update $\boldsymbol{U}_{MB}$ of f^{MB} is calculated[4]:

$$\Delta\boldsymbol{U}_{MB} = \frac{\Delta t}{n_{MB}}\int \omega_1 V(\omega_1) f^{d}(\boldsymbol{c}_1)\,d\boldsymbol{c}_1 \qquad (9)$$

which usually lead to $\boldsymbol{U}_{MB}\cdot(\boldsymbol{n})\neq0$ for numerical error. As $\Delta\boldsymbol{U}_{MB}$ (also Δn_{MB} and Δc_{MB}) can be determined by arbitrary methods different from Eq. (9), using the tangential part $\Delta\boldsymbol{U}_{MB} - (\Delta\boldsymbol{U}_{MB}\cdot\boldsymbol{n})\boldsymbol{n}$ of $\Delta\boldsymbol{U}_{MB}$ calculated by Eq. (9) in place of $\Delta\boldsymbol{U}_{MB}$ would have some advantages. In the case when the initial $\boldsymbol{U}_{MB}$ is zero or parallel to the boundary, adding $\Delta\boldsymbol{U}_{MB} - (\Delta\boldsymbol{U}_{MB}\cdot\boldsymbol{n})\boldsymbol{n}$ to $\boldsymbol{U}_{MB}$ assures $\boldsymbol{U}_{MB}\cdot\boldsymbol{n} = 0$ throughout the simulation process. If the initial $\boldsymbol{U}_{MB}$ is not zero and not parallel to the boundary, it is simple to assign $\Delta\boldsymbol{U}_{MB}$ to $-(\boldsymbol{U}_{MB}\cdot\boldsymbol{n})\boldsymbol{n}$ at any a time step, where $\boldsymbol{U}_{MB}$ is the velocity parameter at that time step. Then, using the tangential part $\Delta\boldsymbol{U}_{MB} - (\Delta\boldsymbol{U}_{MB}\cdot\boldsymbol{n})\boldsymbol{n}$ of $\Delta\boldsymbol{U}_{MB}$ calculated by Eq. (9) in place of $\Delta\boldsymbol{U}_{MB}$ can also make Eq. (8) valid during the following time steps.

For problems of complicated configuration, let $\boldsymbol{U}_{MB}$ and T_{MB} of the underlying distribution of cells adjacent to the boundary be the same as the boundary, in which the advection process at the complicated boundary related to part Ⅱ can be neglected because the $f^{MB(bdary)}(\boldsymbol{c})$ of the boundary is the same as the $f^{MB(cell)}(\boldsymbol{c})$ of its neighboring cells.

3 Conclusions

Additional computational particles (named auxiliary particles) different from deviational particles used in the original LVDSMC method are introduced to counteract the net number of deviational particles created during the simulation process, which can overcome the accumulation of numerical error in problems near free molecular regime. An alternative principle used to determine $\Delta\boldsymbol{U}_{MB}$ in LVDSMC collision process is proposed, which makes easier the calculation of the total fluxes of momentum and energy across the surface of the boundary.

References:

[1] HOMOLLE T M M, HADJICONSTANTINOU N G. Low-variance deviational simulation Monte Carlo[J].

Phys. Fluids, 2007, 19(4): 1-4.

[2] BIRD G A. Molecular gas dynamics and the direct simulation of GAS flow[M]. larendon Press, 1994.

[3] Baker L L, HADJICONSTANTINOU N G. Variance reduction for Monte Carlo solutions of the Boltzmann equation[J]. *Phys. Fluids*, 2005, 17(5): 041703(1-4).

[4] HOMOLLE T M M, HADJICONSTANTINOU N G. A low-variance deviational simulation Monte Carlo for the Boltzmann equation[J]. *J. Computational Physics*, 2007, 226: 2341-2358.

[5] SHEN C. Rarefied gas dynamics-fundamentals, simulations and micro-flows[R]. Springer, 2005.

对 LVDSMC 方法的改进

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摘　要: 最近, Homolle 和 Hadjiconstantinu 提出了新的粒子模拟方法——LVDSMC 方法[1], 该方法采用了减少方差的思想从而提高了低速流动问题中的计算效率。本文针对 LVDSMC 方法提出两点改进: 第一, 除了方法中原来已采用的偏差粒子, 在计算近自由分子流问题时建议额外地采用一些辅助粒子, 从而可以约束计算过程中原始算法在生成偏差粒子时计算误差的累积效应; 第二, 提出一个可选的用于计算潜在 Maxwell Boltzmann 分布函数中的速度参数的增量, 从而使得表面的应力及热流的计算变得简单。

关键词: DSMC; LVDSMC; 偏差粒子; 辅助粒子