Kinetic Force Method with Quasiparticle Pairs for Numerical Modeling 3D Rarefied Gas Flows

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Abstract. In the paper a new way of Kinetic Force Method application for modeling rarefied gas flows is suggested. This way is founded on a kinetic equation for auxiliary two-particle distribution function of quasiparticle pairs. One-particle distribution function satisfying the classical Boltzmann equation can be obtained from the auxiliary distribution function by a simple integration. The using of quasiparticle pairs guarantees energy and momentum conservation in the course of the rarefied gas flows modeling automatically. Comparison of the results obtained by Kinetic Force Method and DSMC method is carried out on the examples of numerical simulations of the homogeneous relaxation and the vacuum pump micro flows.

Keywords: kinetic equation, two-particle distribution function, quasiparticle pairs.
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INTRODUCTION

In papers [1,2], the Boltzmann collision integral was rewritten in a divergence form. It allows considering a distribution function of molecules as a density of quasiparticles, which are moving under influence of the sum of external force and "kinetic force" along smooth trajectories in the phase space. Replacement of real molecules by quasiparticles has opened new opportunities for numerical simulations. In the present time the first variants of the algorithms of Kinetic Force Method have been developed and the principal correctness of the approach has been shown in [3,4].

In our paper we propose the way of application of Kinetic Force Method that uses an auxiliary two-particle distribution function. In our second paper [5] presented to the RGD27 conference, a kinetic equation for two-particle distribution function of molecules with the linear scattering operator and the chaos projector instead of the collision integral is presented. This equation allows using quasiparticle pairs instead of single quasiparticles for numerical simulations of gas flows. The using of quasiparticle pairs instead of single quasiparticles guarantees energy and momentum conservation in the course of the rarefied gas flow modeling automatically without special corrections.

Before discussing the numerical modeling we point out the main ideas on which the algorithm of Kinetic Force Method for quasiparticle pairs is based [5]. Let us begin from the homogeneous relaxation problem of velocity distribution function in a rarefied gas. An auxiliary two-particle distribution function $F(\boldsymbol{v},\boldsymbol{u})$ of pairs of quasiparticles $(\boldsymbol{v}_i,\ \boldsymbol{u}_i)\ \ i=1...N$ in the velocity space is obtained by filtering an actual distribution $\tilde{F}(\boldsymbol{v},\boldsymbol{u},t)$ of *N* pairs of quasiparticles

$$\tilde{F}(\boldsymbol{v},\boldsymbol{u},t)=\frac{1}{N}\sum_{i=1}^{N}\delta(\boldsymbol{v}-\boldsymbol{v}_i(t))\,\delta(\boldsymbol{u}-\boldsymbol{u}_i(t)) \tag{1}$$

by the small scales reduction transformation:

$$F(\boldsymbol{v},\boldsymbol{u}) = \hat{G}_{\tau}\tilde{F}(\boldsymbol{v},\boldsymbol{u}) = \frac{1}{\left(2\pi\overline{\kappa}\right)^{3}}\frac{1}{N}\sum_{i=1}^{N} e^{-\frac{\left[\boldsymbol{v}-\overline{\boldsymbol{v}}_{i}\right]^{2}+\left[\boldsymbol{u}-\overline{\boldsymbol{u}}_{i}\right]^{2}}{2\overline{\kappa}}}, \tag{2}$$

where

$$\overline{\kappa} = \left(1-e^{-2\tau}\right)\kappa_{s}, \qquad \overline{\boldsymbol{v}}_{i} = e^{-\tau}\boldsymbol{v}_{i} + \left(1-e^{-\tau}\right)\boldsymbol{v}_{s}, \quad \overline{\boldsymbol{u}}_{i} = e^{-\tau}\boldsymbol{u}_{i} + \left(1-e^{-\tau}\right)\boldsymbol{u}_{s},$$
$$\kappa_{s} = \frac{1}{3}\left(\left\langle \boldsymbol{v}^{2}\right\rangle_{0} - \left\langle \boldsymbol{v}\right\rangle_{0}\cdot\left\langle \boldsymbol{v}\right\rangle_{0}\right), \qquad \boldsymbol{v}_{s} = \boldsymbol{u}_{s} = \left\langle \boldsymbol{v}\right\rangle_{0}.$$

The one-particle distribution function $f(\boldsymbol{v},t)$ can be obtained from auxiliary two-particle distribution function $F(\boldsymbol{v},\boldsymbol{u})$ by integration:

$$f\left(\boldsymbol{v},t\right) = \frac{1}{2}\int d\boldsymbol{u}\left[F\left(\boldsymbol{v},\boldsymbol{u},t\right)+F\left(\boldsymbol{u},\boldsymbol{v},t\right)\right] = \frac{1}{\left(2\pi\overline{\kappa}\right)^{\frac{3}{2}}}\frac{1}{2N}\sum_{i=1}^{N}\left(e^{-\frac{\left[\boldsymbol{v}-\overline{\boldsymbol{v}}_{i}\right]^{2}}{2\overline{\kappa}}} + e^{-\frac{\left[\boldsymbol{v}-\overline{\boldsymbol{u}}_{i}\right]^{2}}{2\overline{\kappa}}}\right). \tag{3}$$

For recalculation the quasiparticles pairs velocities in the time step we use the rotation matrix with angular velocity $\boldsymbol{\Omega}(\boldsymbol{v},\boldsymbol{u})$:

$$\begin{aligned}
\boldsymbol{v}_{i}\left(t+dt\right) &= \boldsymbol{v}_{i}(t) + \frac{1}{2}\left[\left(1-\cos(\Omega_{i}dt)\right)\frac{\boldsymbol{\Omega}_{i}\times\boldsymbol{\Omega}_{i}\times}{\Omega_{i}^{2}} + \sin(\Omega_{i}dt)\,\frac{\boldsymbol{\Omega}_{i}\times}{\Omega_{i}}\right]\left[\boldsymbol{v}_{i}(t)-\boldsymbol{u}_{i}(t)\right],\\
\boldsymbol{u}_{i}\left(t+dt\right) &= \boldsymbol{u}_{i}(t) - \frac{1}{2}\left[\left(1-\cos(\Omega_{i}dt)\right)\frac{\boldsymbol{\Omega}_{i}\times\boldsymbol{\Omega}_{i}\times}{\Omega_{i}^{2}} + \sin(\Omega_{i}dt)\,\frac{\boldsymbol{\Omega}_{i}\times}{\Omega_{i}}\right]\left[\boldsymbol{v}_{i}(t)-\boldsymbol{u}_{i}(t)\right],
\end{aligned} \tag{4}$$

where the vector of angular velocity $\boldsymbol{\Omega}(\boldsymbol{v},\boldsymbol{u})$ is obtained by using the angular velocity operator $\hat{\boldsymbol{\Omega}}$ as follows [5]:

$$\boldsymbol{\Omega}\left(\boldsymbol{v},\boldsymbol{u}\right) = \left[F\left(\boldsymbol{v},\boldsymbol{u}\right)\right]^{-1}\hat{\boldsymbol{\Omega}}\,f\left(\boldsymbol{v}\right)f\left(\boldsymbol{u}\right) \cong \frac{\hat{\boldsymbol{\Omega}}\,f\left(\boldsymbol{v}\right)f\left(\boldsymbol{u}\right)}{f\left(\boldsymbol{v}\right)f\left(\boldsymbol{u}\right)}$$
$$= \int d\phi\, d\Omega_{n}\,\frac{\mathbf{v}\times\mathbf{v}\times\boldsymbol{n}}{\mathrm{v}^{2}}\left|\cos\theta\right| b\left(\mathrm{v},\cos 2\theta\right)\frac{\left[f\left(\boldsymbol{v}'_{+}\right)f\left(\boldsymbol{u}'_{+}\right)-f\left(\boldsymbol{v}'_{-}\right)f\left(\boldsymbol{u}'_{-}\right)\right]}{f\left(\boldsymbol{v}\right)f\left(\boldsymbol{u}\right)}, \tag{5}$$

$$\boldsymbol{v}'_{\pm} = \boldsymbol{v} + \frac{\left[\left(1-\cos\phi\right)\hat{n}^{2} \pm \sin\phi\,\hat{n}\right]\mathbf{v}}{2}, \quad \boldsymbol{u}'_{\pm} = \boldsymbol{u} - \frac{\left[\left(1-\cos\phi\right)\hat{n}^{2} \pm \sin\phi\,\hat{n}\right]\mathbf{v}}{2}.$$

RESULTS OF SIMULATIONS

To illustrate the Kinetic Force Method for quasiparticle pairs we have considered two kinds of problems. One of them is the problem of homogeneous relaxation of Maxwell's molecules to the equilibrium. The differential cross section for Maxwell's molecules ($\sigma \mathrm{v} = \nu = const$) is taken to be isotropic: $\frac{d\sigma}{d\Omega} = \frac{\sigma}{4\pi}$, where v is a relative velocity of molecules. As well known, the exact time dependence of the distribution function moments can be obtained from the Boltzmann equation for Maxwell's molecules exactly. It gives us an opportunity to compare the exact moments with the moments calculated in the course of modeling and thus to check up the abilities of the Method. In this problem for convenience, we use the system of units, in which the mean free time between collisions and number density are equal to unity: $\tau = n^{-1}\nu^{-1} = 1,\ n = 1$. The initial velocity distribution function is taken to be:

$$f\left(\boldsymbol{v}_x\right) = \frac{1}{2\delta}\exp\left(-\frac{\left|\boldsymbol{v}_x\right|}{\delta}\right),\ f\left(\boldsymbol{v}_y\right) = \frac{1}{2\delta}\exp\left(-\frac{\left|\boldsymbol{v}_y\right|}{\delta}\right),\ f\left(\boldsymbol{v}_z\right) = \frac{1}{2\delta}\exp\left(-\frac{\left|\boldsymbol{v}_z\right|}{\delta}\right), \tag{6}$$

where $\delta = 0.5$, $\overline{\kappa} = 0.01$.

The graph of initial distribution function $f(\boldsymbol{v}_x)$ (6) and the graph of the actual distribution function of quasiparticles filtered according to (2) in the initial moment are presented in figure 1(*a*). Coincidence in details of the graphs depends on the choice of smoothing parameter $\overline{\kappa}$: evidently, for the better coincidence we need to take the smaller value of this parameter and to increase the whole quantity of particles simultaneously. In our numerical example we use 10000 pairs of quasiparticles.

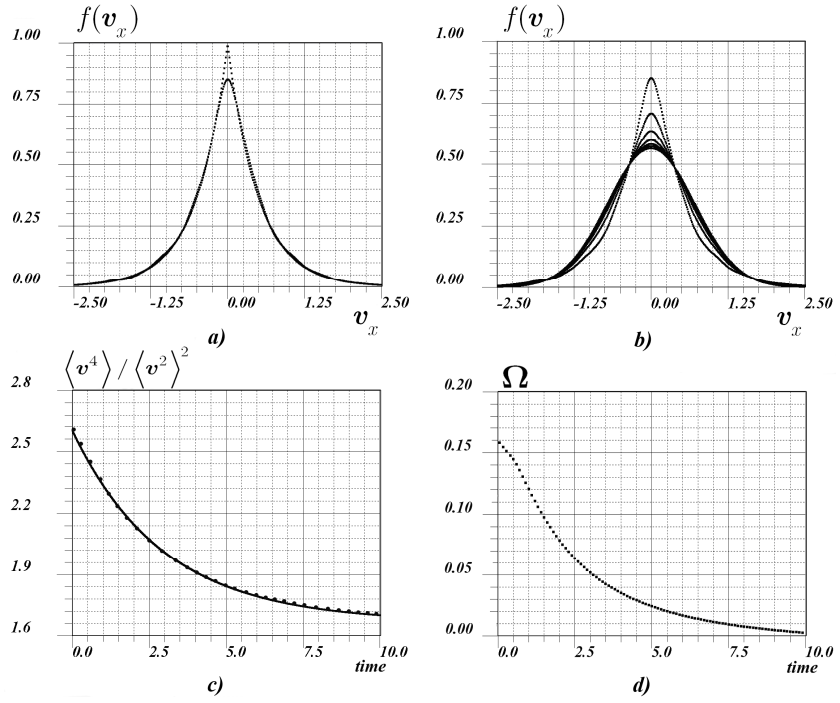

FIGURE 1. (*a*) The exact initial distribution function $f(\boldsymbol{v}_x)$ (dotted line) and reconstructed one (solid line).

(*b*) The velocity distribution function at the different time moments: *t* = 0.0, 2.0, 4.0, …
(*c*) The exact fourth dimensionless moment of the distribution function of Maxwell's molecules (firm line) and simulated one (dots). (*d*) The magnitude of the mean angular velocity.

The evolution of the distribution function $f(\boldsymbol{v}_x)$ to Maxwell's distribution function is presented in figure 1(*b*). Due to the smoothness of quasiparticles trajectories we choose the comparative large time step. In this example it is equal to 0.1.

Figure 1(*c*) shows the comparison of the exact fourth dimensionless moment $\left\langle \boldsymbol{v}^4 \right\rangle / \left\langle \boldsymbol{v}^2 \right\rangle^2$ of the distribution function of Maxwell's molecules and its values calculated by Kinetic Force Method in the course of relaxation. One can see satisfactory coincidence of exact and simulated moments and an absence of fluctuations.

The graph of the averaged angular velocity is presented in figure 1(*d*). The angular velocity is monotonously decreasing in the relaxation process. As it should be, in the equilibrium state the angular velocity is equal to zero. It means that kinetic force and accelerations of quasiparticles decrease on time and turn to zero in the equilibrium.

In the second example of the homogeneous relaxation we considered a mixture of gases of Maxwell's molecules having the different temperatures in the initial moment: $RT_1 = 0.2,\ RT_2 = 2.0$. We generated quasiparticles in the initial moment in accordance with the following distribution:

$$f(\boldsymbol{v}) = \frac{5}{9} f_1\left(\boldsymbol{v}\right) + \frac{4}{9} f_2\left(\boldsymbol{v}\right), \tag{7}$$

$$f_1\left(\boldsymbol{v}\right) = \frac{1}{\left(2\pi R T_1\right)^{\frac{3}{2}}} \exp\left(-\frac{\boldsymbol{v}^2}{2RT_1}\right),\ \ f_2\left(\boldsymbol{v}\right) = \frac{1}{\left(2\pi R T_2\right)^{\frac{3}{2}}} \exp\left(-\frac{\boldsymbol{v}^2}{2RT_2}\right). \tag{8}$$

Figure 2 illustrates the comparison of the results calculated by Kinetic Force Method and by DSMC for this problem. Figures 2(*a*) and 2(*b*) present a dimensionless fourth moment $\left\langle \boldsymbol{v}^4 \right\rangle / \left\langle \boldsymbol{v}^2 \right\rangle^2$ obtained by these two methods. Figures 3(*a*) and 3(*b*) present the evolution of the distribution function $f\left(\boldsymbol{v}_x\right)$ to equilibrium in this example. The equilibrium distribution function is the Maxwellian with $RT_1 = 1.0$. Both Methods give actually the same results.

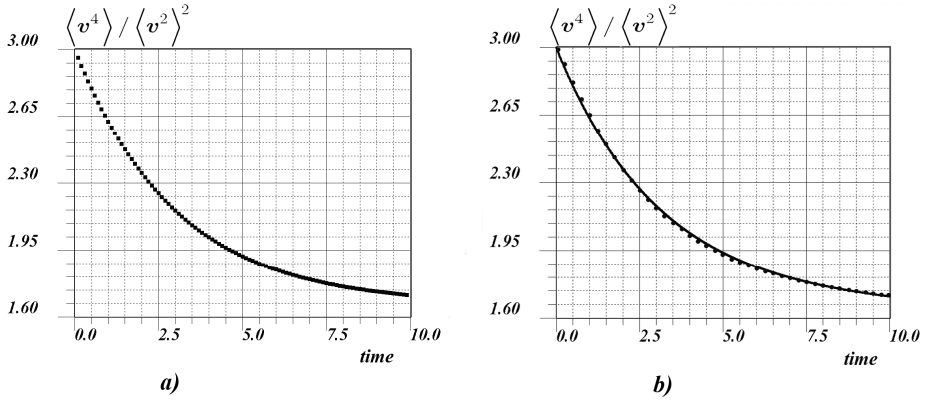

FIGURE 2. The exact dimensionless fourth moment for two temperatures mixture of Maxwell's molecules: (*a*) is obtained by DSMC method; (*b*) is obtained by Kinetic Force Method. In figure 2(*b*) firm line illustrates the exact dimensionless fourth moment and dots illustrate the simulated one.

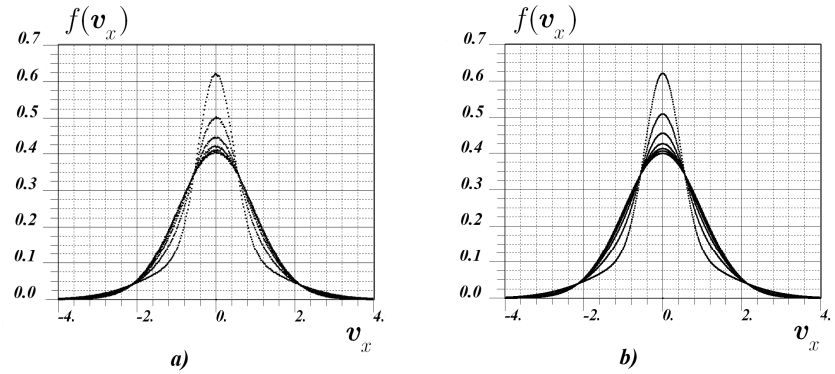

FIGURE 3. The velocity distribution function for two temperatures mixture of Maxwell's molecules at the different times: t = 0.0, 2.0, 4.0, …: (*a*) is obtained by DSMC; (*b*) is obtained by Kinetic Force Method.

Let's go on to the consideration of a non homogeneous problem. As an example we have chosen micro flow in a vacuum pump. The scheme of the vacuum pump is presented in Figure 4. The vacuum pump consists of two horizontal plates disposed one above another on the distance h. Down plate is moving with the speed u in the right direction.

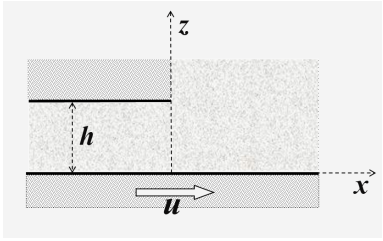

FIGURE 4. The scheme of the vacuum pump.

This problem has a practical importance. Recently, it was found experimentally that the friction between a partly polished diamond coating and a metal surface was drastically reduced as a relative speed of sliding surfaces was increased [6]. It seems that diamond coating floats in the air above metal surface. This phenomenon shows the possibility of new air lubrication systems. Also in [6] the floating mechanism was simulated by using the DSMC method.

The problem is formulated as follows. In the initial moment there is no air in the channel between the plates. Air molecules, which are coming into channel have the following parameters: a mean free path is estimated as $\lambda = 6.5 \cdot 10^{-8} m$, temperature $T = 273K$, number density $n_0 = 2.68 \cdot 10^{25} m^{-3}$. We choose the differential cross section of molecules as the cross section of solid spheres. The down plate moves rightward with the speed $u = 10\ m/s$. We assume that the Knudsen number $Kn = \lambda / h = 0.1$.

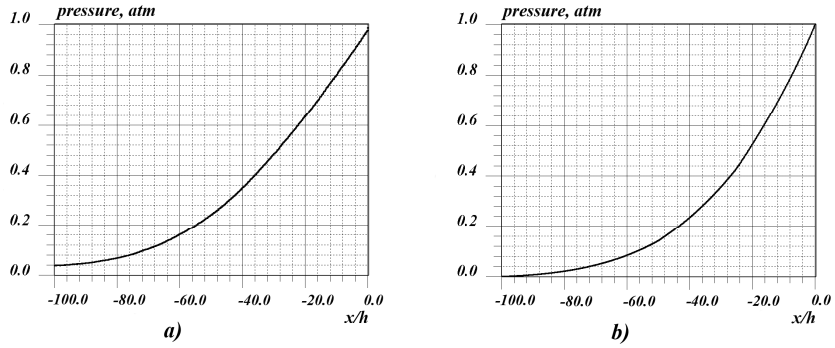

FIGURE 5. The averaged over the height pressure along the channel: *(a)* is obtained by DSMC Method; (*b*) is obtained by Kinetic Force Method.

Kinetic Force is averaged over the height of the channel, but the moving of quasiparticles is three-dimensional. Molecules are reflected by the plates according the diffuse reflection model.

Figures 5(*a*) and 5(*b*) present the results of numerical simulations of the air pressure in the vacuum pump obtained by DSMC Method and by Kinetic Force Method. Figures 6(*a*) and 6(*b*) present the number density distribution along the pump calculated by these methods. These results are coinciding well enough. Calculations show that temperature is almost uniform in the cannel and pressure is proportional to the number density.

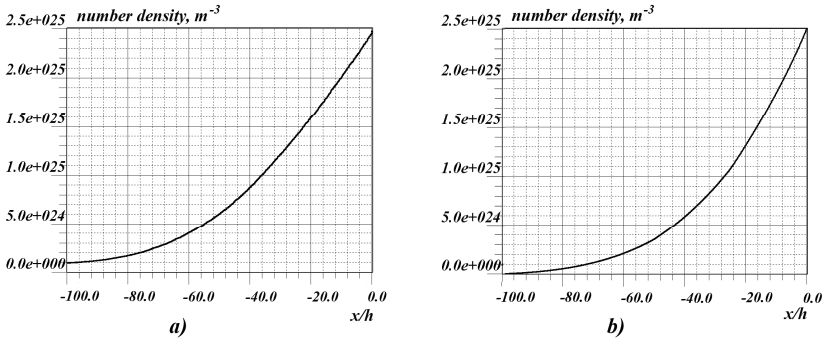

FIGURE 6. The averaged over the height number density along the channel:
(*a*) is obtained by DSMC Method; (*b*) is obtained by Kinetic Force Method.

CONCLUSIONS

We have performed simulations of rarefied gas flows by both DSMC and Kinetic Force Method. The DSMC method has been dominant numerical method for obtaining solutions of the Boltzmann equation for the last 40 years. Kinetic Force Method is a new one. Our algorithm is one of the first attempts of applying the idea of representation the Boltzmann collision integral in a divergence form and substituting real molecules by quasiparticles for numerical simulations. Of course, considerable resources of improvement the effectiveness of our method are still available. We hope that Kinetic Force Method will give good results in the nearest future.

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