Particle-in-Cell method for solving the Boltzmann equation

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Abstract. A method of the numerical solution of the Boltzmann equation, which belongs to the family of deterministic particle-in-cell methods, and results of its application are described. Such a method is based on the possibility of presenting the collision integral of the Boltzmann equation in divergent form.

INTRODUCTION

The Boltzmann equation for a single-particle distribution function $f = f(t, \overrightarrow{r}, \overrightarrow{v})$, which describes the rarefied gas dynamics, has the form

$$L(f) \equiv \frac{\partial f}{\partial t} + \overrightarrow{v} \frac{\partial (f)}{\partial \overrightarrow{r}} = St(f), \tag{1}$$

with the right-hand side containing a nonlinear integral operator, which is the collision integral

$$St(f) = \int_{R^3} d^3 v_1 \int_{S^2} d^2 n (f' f'_1 - f f_1) |\overrightarrow{V}| \sigma(V, cos(\theta)), \tag{2}$$

where

$$f = f(t, \overrightarrow{r}, \overrightarrow{v}), \qquad f_1 = f(t, \overrightarrow{r}, \overrightarrow{v_1}), \qquad f' = f(t, \overrightarrow{r}, \overrightarrow{v}'), f'_1 = f(t, \overrightarrow{r}, \overrightarrow{v_1}'),$$

$$\overrightarrow{v}' = \frac{\overrightarrow{v} + \overrightarrow{v_1}}{2} + \frac{|\overrightarrow{V}|}{2} \overrightarrow{n}, \qquad \overrightarrow{v_1}' = \frac{\overrightarrow{v} + \overrightarrow{v_1}}{2} - \frac{|\overrightarrow{V}|}{2} \overrightarrow{n}, \tag{3}$$

$\overrightarrow{V} = \overrightarrow{v} - \overrightarrow{v_1}$, $\overrightarrow{n}$ is the unit vector (collision parameter) defining the direction of the relative velocity after the collision, and $\sigma = \sigma(V, cos(\theta))$ is the differential scattering cross section (θ is the angle between the relative particle velocity vectors before and after the collision).

There are several differential and integral forms of presentation of the Boltzmann equation. It seems of interest to use its divergent form to construct conservative numerical methods of rarefied gas dynamics, in particular, the particle-in-cell (PIC) method of the nonlinear Boltzmann equation. One of the first publications in this field available for the authors was the paper [1]. In that paper, a force field whose effect is equivalent to the collision integral in the Boltzmann equation was introduced to derive a kinetic equation in divergent form. Somewhat later, the divergent form of the Boltzmann equation was used in [2, 3] to solve problems of semiconductor physics. Two new independent approaches to presenting the Boltzmann collision integral in divergent form have been recently developed in [4, 5, 6, 7]. Based on results obtained in [6, 7], a new method called the Kinetic Force Method for numerical simulation of rarefied gas problems was proposed in [8].

PARTICLE-IN-CELL METHOD FOR SOLVING THE BOLTZMANN EQUATION

In accordance with [1], Eq. (1) can be written in the form

$$L(f) \equiv \frac{\partial f}{\partial t} + \frac{\partial (\overrightarrow{v} f)}{\partial \overrightarrow{r}} + \frac{\partial (\overrightarrow{Q})}{\partial \overrightarrow{v}} = 0, \tag{4}$$

$$\frac{\partial \overrightarrow{Q}}{\partial \overrightarrow{v}} = -St(f), \tag{5}$$

where $\overrightarrow{Q}(t, \overrightarrow{r}, \overrightarrow{v}) = \overrightarrow{F}(t, \overrightarrow{r}, \overrightarrow{v}) f(t, \overrightarrow{r}, \overrightarrow{v})/m$ is the vector flux of molecules in the velocity space. Being written in such a manner, the Boltzmann equation has the form of a differential conservation law and describes a compressible flux of molecules in the phase space under the action of the vector field with the physical space component $\overrightarrow{v}$ and the velocity space component $\overrightarrow{F}/m$. The time evolution of the distribution function $f(t, \overrightarrow{r}, \overrightarrow{v})$ can be interpreted as a result of two additive processes: transfer in the actual space and transfer in the space of velocities, which is caused by changes in velocities induced by the collective force $\overrightarrow{F}$. To find this force, we have to solve Eq. (5). At fixed boundary conditions, this equation admits numerous solutions that differ from each other by the vortex component. For this reason, versatile divergent presentations of the collision integral are possible. As in [1], we assume that the flux $\overrightarrow{Q}$ is vortex-free. Then, it can be presented as a gradient of a certain scalar field Φ:

$$\overrightarrow{Q} = -\frac{\partial \Phi}{\partial \overrightarrow{v}} \tag{6}$$

Then, Eq. (5) reduces to the Poisson equation

$$\frac{\partial}{\partial \overrightarrow{v}} \cdot \frac{\partial \Phi}{\partial \overrightarrow{v}} = St(t, \overrightarrow{r}, \overrightarrow{v}), \tag{7}$$

Equation (7) is solved in the space of velocities with fixed values of time at fixed points of the physical space. Correspondingly, we skip writing the dependences of the functions on the variables t and $\overrightarrow{r}$, which have the meaning of parameters in this context. The solution of Eq. (7), which satisfies the natural boundary condition $\Phi(\overrightarrow{v}) \longrightarrow 0$ as $|\overrightarrow{v}| \longrightarrow \infty$, has the form

$$\Phi(\overrightarrow{v}) = \frac{1}{4\pi} \int\limits_{R^3} \frac{St(\overrightarrow{v}')}{|\overrightarrow{v} - \overrightarrow{v}'|} d^3 v'. \tag{8}$$

Correspondingly, we obtain

$$\overrightarrow{Q}(\overrightarrow{v}) = \frac{\partial \Phi}{\partial \overrightarrow{v}} = -\frac{1}{4\pi} \int\limits_{R^3} \frac{St(\overrightarrow{v}')(\overrightarrow{v} - \overrightarrow{v}')}{|\overrightarrow{v} - \overrightarrow{v}'|^3} d^3 v' \tag{9}$$

The formulation of Eq. (4) with the flux determined by Eq. (9) does not imply a particular form of the collision term; therefore, we can speak about the divergent form of kinetic equation extending it to the model kinetic equations as well. The Boltzmann equation written in divergent form is similar in many aspects to the Vlasov kinetic equation, which describes the collisionless plasma, or to the collisionless stellar dynamics (CSD) equation [9], which describes the motion of starts in galaxies. These collisionless kinetic equations can be written in the form $Df/Dt = 0$, where D/Dt is the Lagrangian derivative in the phase space. The phase density remains unchanged along the trajectories, i.e., the phase density is a Lagrangian invariant. In the Boltzmann equation (1), the flux divergence is not equal to zero because of collisions (the collision integral is not equal to zero); therefore, it cannot be presented in the analogous form. Equation (4) describes a compressible phase medium. The equations of characteristics include an equation for the change in the phase density along the trajectories. Despite this difference between the Boltzmann equation and collisionless kinetic equations, it is possible to use the particle-in-cell numerical method successfully applied to model processes in the collisionless plasma and stellar systems [10, 11]. In contrast to the PIC method in plasma physics or collisionless stellar dynamics, particles in cells of the *phase* space should be considered here. Let us present the distribution function as a sum of the form

$$f(t, \overrightarrow{r}, \overrightarrow{v}) = \sum_{p=1}^{N} n_p K(\overrightarrow{r}, \overrightarrow{v}, \overrightarrow{R}_p(t), \overrightarrow{V}_p(t)), \tag{10}$$

where $\overrightarrow{R}_p(t)$ and $\overrightarrow{V}_p(t)$ are three-dimensional vector functions of time. Following the ideology of PIC methods, the individual terms of this sum can be interpreted as particles whose shape, size, and location are determined by a function K called the particle kernel; the constants n_p define the particle weight. In addition to the requirement to satisfy the conservation law, which, in the case of kernel normalization

$$\int\limits_{R^3 \times R^3} K d^3 r d^3 v = 1, \tag{11}$$

has the form

$$\int\limits_{R^3 \times R^3} f(t, \overrightarrow{r}, \overrightarrow{v})d^3rd^3v = \sum_{p=0}^{N} n_p, \tag{12}$$

the function K is subjected to additional requirements: non-negativity and symmetry of some kind. One can see that the expansion (10) satisfies Eq. (4) if the following conditions having the form of a dynamic system in the phase space ("particle motion equations") are met:

$$\frac{d\overrightarrow{R}_p}{dt} = \overrightarrow{V}_p, \quad \frac{d\overrightarrow{V}_p}{dt} = \frac{1}{m}\overrightarrow{F}_p(t, \overrightarrow{R}_p, \overrightarrow{V}_p). \tag{13}$$

Numerical PIC methods imply the use of an Eulerian grid in the phase space. The force field $\overrightarrow{F}(t, \overrightarrow{r}, \overrightarrow{v})$ is calculated at the nodes of this grid, with subsequent interpolation of the field to the phase space points where the particles are located. The number of the Eulerian grid nodes in the phase space is substantially smaller than the number of particles N in most cases.

To calculate the force in the computational grid nodes, one has to calculate the values of the distribution function in these nodes. This is made by the "particle-to-cell" interpolation otherwise called the distribution of particle attributes [10]. In our case, the number of molecules (or the fraction of molecules, depending on normalization) associated with the p-th particle, equal to the weight n_p in expansion (10), is distributed among the nodes.

Let us indicate nodes of the computational grid in the phase space by the pair of indices (I, α): I ensures indexation of the nodes in the physical space (which is three-dimensional in the general case), and α provides indexation in the three-dimensional velocity space. First, we use the nearest grid point method (NGP [10]) and assign the weight n_p of a particle to the node (I, α). Otherwise, using the particle-in-cell (PIC), cloud-in-cell (CIC) or other methods of interpolation, we distribute this weight among the nodes in the physical space so that

$$\sum_{I}\Delta n_{I,\alpha} = n_p \tag{14}$$

After that, with a fixed index I, each fraction $\Delta n_{I,\alpha}$ is distributed among the nodes of the velocity grid $(I, \alpha), (I, \alpha + 1), (I, \alpha - 1)$, etc., depending on the interpolation method used. *After this procedure, not only the conservation law (12) should be valid, but also the momentum and energy should be conserved.* Note that this requirement cannot be satisfied in the traditional PIC methods used in plasma physics [12], because they deal with the physical rather than phase space. In our computations, we used the interpolation proposed in [13] for conservative correction of collision integral calculations (note that the interpolation with such properties for correcting collision integral calculations was first proposed in [14]). With such a distribution, the momentum and energy are conserved. Finally, to obtain the phase density in the computational grid nodes, we divide the distributed fractions of particles by the phase cell volume.

After the particle-to-grid interpolation procedure, we calculate the collision integral in the computational grid nodes. Two approaches are used for collision integral calculations: based on the adaptive Monte Carlo method [15] of estimating multidimensional integrals with the function values at points between the nodes being found by means of trilinear interpolation and the regular method used in [13]. The next stage of computations by the proposed method is calculating expression (8) whose grid approximation in the velocity space has the form

$$\Phi_\alpha = \frac{1}{4\pi}\sum_{\alpha'} \frac{St_{\alpha'}}{h_v\sqrt{(\alpha_x - \alpha'_x)^2 + (\alpha_y - \alpha'_y)^2 + (\alpha_z - \alpha'_z)^2}}. \tag{15}$$

Expression (15) has the form of a convolute, and the convolute theorem can be used for its calculation. Then, the calculation of the sum of sequence (15) reduces to obtaining a discrete Fourier image of the sequence

$$\hat{\Phi}_\beta = \sqrt{LMN}\hat{St}_\beta \hat{G}_\beta, \tag{16}$$

where L, M, N are the dimensions of the regular grid in the velocity space, $\hat{St}_\beta$ is the Fourier image of the grid approximation of the collision integral, and $\hat{G}_\beta$ is the Fourier image of the sequence $G_\beta = 1/\sqrt{\beta_x^2 + \beta_y^2 + \beta_z^2}$, and to applying the inverse Fourier transform to $\hat{\Phi}_\beta$. The grid approximation of the vector field $\overrightarrow{F}(t, \overrightarrow{r}, \overrightarrow{v})$ is found by using finite differences. As the Fast Fourier Transform is highly efficient, the time needed to calculate the force field is negligibly small, as compared to the time needed to calculate the collision integral. Therefore, force field

calculations require minor computer resources. The computations were performed with the FFTW software package [16] implementing the Fast Fourier Transform. The last stage of the computational cycle of solving the Boltzmann equation by the PIC method involves numerical integration of the system of equations of motion (13). The values of $\vec{F}_p(t, \vec{R}_p, \vec{V}_p)$ are found by interpolating of the grid vector function $\vec{F}_{I,\alpha}$ at the phase space point $(\vec{R}_p, \vec{V}_p)$. The interval τ of integration of system (13) is chosen so that the length of the phase trajectories during this time remains the phase cell size. Summarizing the description of the PIC method used to solve the Boltzmann equation, we show the diagram (Fig. 1), which illustrates the algorithm of rarefied gas flow computations.
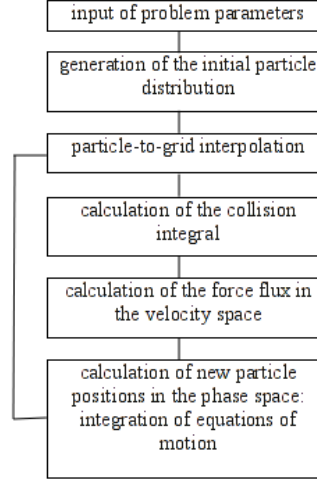

FIGURE 1. Diagram of actions in calculating rarefied gas dynamics by the PIC method

NUMERICAL EXAMPLE

The main difficulties of the PIC method described above are associated with computing the particle trajectories in the velocity space. Therefore, we chose the test problem of uniform relaxation as the first step. We computed homogeneous relaxation of a gas consisting of the Maxwell molecules with the initial distribution function corresponding to Bobylev's exact solution at $t = 0$ [17]:

$$f(t, v) = \frac{1}{(2\pi\tau)^{3/2}} \exp\left(-\frac{v^2}{2\tau}\right)\left[1 + \frac{1-\tau}{\tau}\left(\frac{v^2}{2\tau} - \frac{3}{2}\right)\right], \tau(t) = 1 - \frac{2}{5}e^{-t/6}, \quad t \geq 0. \tag{17}$$

In the case of homogeneous relaxation, the equations of the problem have the form

$$\frac{\partial f}{\partial t} + \frac{\partial(\vec{F}f)}{\partial \vec{v}} = 0, \tag{18}$$

$$\vec{F}f = -\frac{\partial \Phi}{\partial \vec{v}}, \tag{19}$$

$$\Phi(\vec{v}) = \frac{1}{4\pi}\int_{R^3}\frac{St(\vec{v}')}{|\vec{v} - \vec{v}'|}d^3v'., \tag{20}$$

$$St(f) = \int_{R^3}d^3v_1\int_{S^2}d^2n(f'f_1' - ff_1)|\vec{V}|\sigma(V, cos(\theta)), \tag{21}$$

and the equations of motion of the particles are

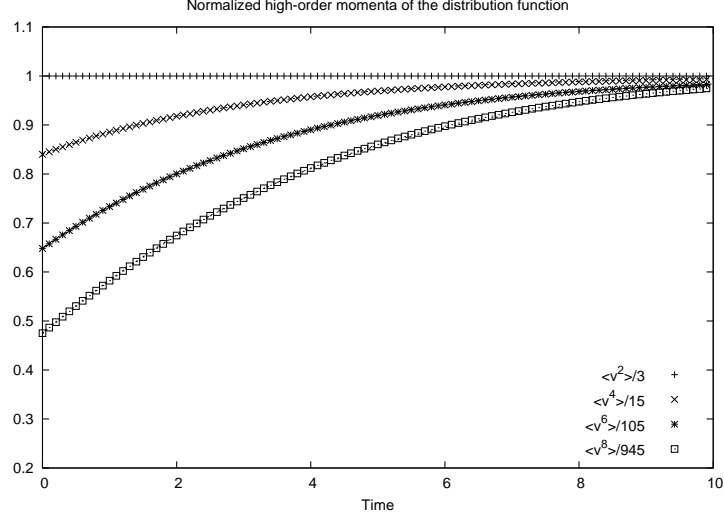$$\frac{d\vec{V}_p}{dt} = \frac{1}{m}\vec{F}_p(t, \vec{V}_p). \tag{22}$$

FIGURE 2. Homogeneous relaxation computed by the PIC method

As compared to the general case, the computational cycle lacks only the interpolation to the grid nodes of the physical space. Figure 2 shows the normalized moments $< v^{2n} >_N = < v^{2n} >/(2n+1)!!$ of the Bobylev distribution function of the 2-nd, 4-th, 6-th, and 8-th orders and their theoretical values (solid curves). The computational domain size is $[-6,6]^3$, the computational grid has $32 \times 32 \times 32$ nodes, and the time step in the computational cycle is $\tau = 0.05$.

In calculating the collision integral, we used the idea proposed in [18] with small modifications. The idea is to reject nodes with small values of the phase density in calculating the collision integral. The authors [18] estimated the error of calculating gas-dynamic moments depending on the threshold value of the phase density, assuming that the distribution is little different from the equilibrium one. We propose another criterion for node rejection. The following procedure is used:

- the nodes are sorted in decreasing order of the distribution function;
- partial sums of this decreasing sequence are found and compared with the total sum

$$\sum_{i=0}^{n} f_i v_i^{2p} / \sum_{i=0}^{N} f_i v_i^{2p} < \varepsilon, \tag{23}$$

where N is the total number of grid nodes and i is the linear index of the node.

Nodes with linear indices $i < n$ are left for collision integral calculations. Despite the apparent complexity of such an algorithm, it can be effectively implemented with the use of the Standard Template Library (STL) of the C++ language. The cost of execution of this algorithm are multiply compensated owing to a decrease in the number of nodes in calculating the collision integral. Let us give the number of remaining significant nodes on the $32 \times 32 \times 32$ computational grid (the total number of nodes is 32,768) at the initial time as a function of the values of ε and p:

Variant	ε	p	Number of nodes	Efficiency
I	0.01	0	2500	x200
II	0.01	1	3500	x70
III	0.01	2	7500	x20

Figure 3 shows the normalized moments $< v^{2n} >_N = < v^{2n} >/(2n+1)!!$ of the Bobylev distribution function of the 2-nd, 4-th,... 12-th orders and their theoretical values (solid curves), which illustrate the dependence of the model computation accuracy on the number of nodes of the computational grid in the velocity space.
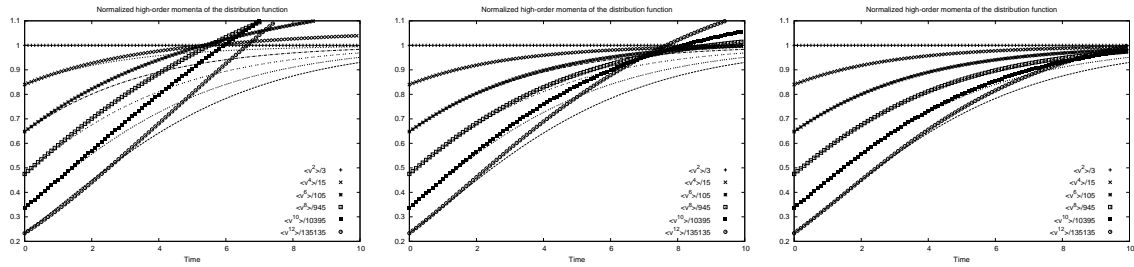
FIGURE 3. The normalized moments of Bobylev distribution function. Variant I, II,III

CONCLUSIONS

The basic conclusion of the present study is the fact that the modified PIC method used for numerical simulations of rarefied gas dynamics provides adequate results in homogeneous relaxation computations. The computations also show that the interpolation method proposed in [13] and used here does not distort the evolution of higher-order moments. Therefore, we can start solving spatially inhomogeneous problems, which are expected to reveal the capabilities of the method to the full extent.

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