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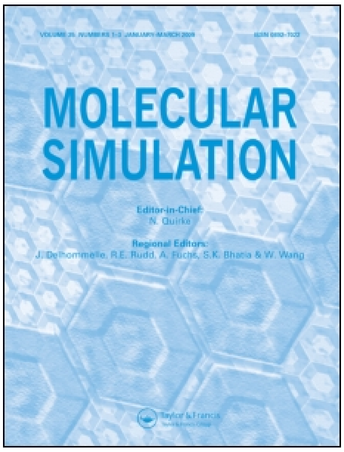

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The Treatment of Molecular Collisions in DSMC Methods

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THE TREATMENT OF MOLECULAR COLLISIONS IN DSMC METHODS

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We describe Direct Simulation Monte Carlo (DSMC) methods which model systems under low pressure with emphasis on the treatment of molecular collisions in DSMC methods. According to the treatment of molecular collisions, several variants of DSMC methods can be distinguished. This work compares some versions of DSMC methods (Bird's time counter, no time counter, Babovsky's, Nanbu's, Koura's null collision technique. Yanitskiy's, Abe's and direct (Kac's) methods).

KEY WORDS: Direct simulation Monte Carlo, Boltzmann equation, Kac equation.

1 INTRODUCTION

The flow of rarefied gases is frequently encountered is theoretical study as well as in technical practice. The development of computing hardware has enabled researchers to take into consideration the inter-molecular interactions during the collisions of molecules more exactly in the DSMC method of rarefied gas flow modelling. This leads to more complex models utilizing knowledge from statistical mechanics and quantum chemistry, which until recently have been solved only within isolated theoretical study in these fields. This article approaches the DSMC methods of rarefied gas flow modelling for the wider expert community from the field of statistical mechanics and quantum chemistry in order to enable them to utilize their knowledge in descriptions of complex macroscopic systems (e.g. the reaction of $N_2 - O_2$ at hypersonic flow around a solid body [10]).

The state of the system at the low pressure is described by the distribution functions. For a one-particle distribution function $f(\vec{c},\vec{r},t)$ the expression

$$f(\vec{c},\vec{r},t)\,d\vec{c}\;d\vec{r}\;dt$$

represents the probability that the molecule with velocity $\langle\vec{c},\vec{c}+d\vec{c}\rangle$ will be found in volume $\langle\vec{r},\vec{r}+d\vec{r}\rangle$ at the time $\langle t,t+dt\rangle$. The condition that the molecules do not interact during their motion, but only in the moment of mutual collision, must be fulfilled to describe the system by the one-particle distribution function. In some cases the N-particle distribution function, $\Phi(\mathbb{C})$, is used, where $\mathbb{C}$ is 3-dimensional vector with the members $\mathbb{C}=\{\vec{c}_1,\vec{c}_2,\ldots\vec{c}_N\}$.

Several kinetic equations for the description of the development of the system are available. These equations describe the development of the distribution function with position and time. These equations express the influence of molecular motion (convection), the effect of external force (electrostatic field, gravitation) and the collisions between molecules on the distribution function.

The main problem is to evaluate quantitatively the influence of collisions. For a collision between two molecules *i*, *j*, the molecules velocities $\vec{c}_i, \vec{c}_j$ prior to the collision will be exchanged for the velocities $\vec{c}_i, \vec{c}_j$ after the collision, thus exchange of intramolecular energy will occur. The term in the kinetic equation expressing the change of the distribution function as a consequence of such a collision must include before and after-collision states of the molecules for all possible combinations of collisions. This results in a integral collision team in the kinetic equation and also in an integral-differential kinetic equation.

Methods based on the solution of kinetic equations (linearization, moment methods) are unable to solve more sophisticated, i.e. real problems. Therefore following developments in computing technology, there were attempts at numeric modeling of an evolving system. A first, completely deterministic method was described by Alder and Wainwright in 1958 [1], however, due to its complicated nature it is slow and memory demanding. In 1963 Bird introduced a probabilistic approach into the modeling of rarefied gas flow and so created the basis for the direct simulation Monte Carlo method (DSMC) [2, 15].

At present the DSMC is the most widely used approach in research and modeling of the characteristics of rarefied gas flow, it is used to model the aerodynamics of rocket-planes and space shuttles [4, 7, 9], to determine inter-molecular potentials of molecules, to coat thin films of materials [6, 12], reactions of gas mixtures in heterogeneous systems [10], interactions of gases with the surface [11], flow in vacuum equipment [3, 5] and to determine the evaporation and condensation of substances [13].

The aim of this work is to summarize and evaluate different variants of the treatment of molecular collisions in DSMC methods and to show their advantages and restrictions from the standpoint of time requirements and rigorousness.

2 THEORETICAL

2.1 *Kinetic Equations and Division of DSMC Methods*

Several kinetic equations for the description of systems under low pressure ($Kn \simeq 1$ or $Kn > 1$) have been derived, which describe the development of such systems. From the standpoint of the linkage to the DSMC methods, the most important equations include the Boltzmann and Kac equations.

The Boltzmann equation

$$I_c(\vec{c}, \vec{r}, t) = \vec{c}\,\frac{\partial f(\vec{c}, \vec{r}, t)}{\partial \vec{r}} + \vec{a}\,\frac{\partial f(\vec{c}, \vec{r}, t)}{\partial \vec{c}} + \frac{\partial f(\vec{c}, \vec{r}, t)}{\partial t} \tag{1}$$

is a nonlinear integral-differential equation for the one-particle distribution function $f(\vec{c}, \vec{r}, t)$, where $\vec{c}$ is the velocity and $\vec{r}$ is the position vector of a molecule, $\vec{a}$ is the alteration of $\vec{c}$ when acted by an external force. The expression $I_c(\vec{c}, \vec{r}, t)$ represents a collision integral (change of the distribution function due to collisions between molecules).

The Kac equation

$$\frac{\partial \Phi_t(\mathbb{C})}{\partial t} = \frac{1}{V} \sum_{1 \leqslant i < j \leqslant N} g_{ij} \int (\Phi_t(\mathbb{C}_{ij}) - \Phi_t(\mathbb{C})) d\sigma_{ij} \tag{2}$$

is a linear integral-differential equation for the N-particle distribution function $\Phi(\mathbb{C})$, where

$$\mathbb{C} = \{\vec{c}_1, \vec{c}_2, \ldots \vec{c}_N\},$$

$$\mathbb{C}_{ij} = \{\vec{c}_1, \vec{c}_2, \ldots, \vec{c}_{i-1}, \vec{c}\,'_i, \vec{c}_{i+1}, \ldots, \vec{c}_{j-1}, \vec{c}\,'_j, \vec{c}_{j+1}, \ldots, \vec{c}_N\}$$

The Kac equation is derived from the following postulates:

1) The Probability that, of the total number of possible combinations, only the pair of molecules i, j with speeds c_i, c_j would collide, is given by the quantity W_{ij},

$$W_{ij} = \omega_{ij}/\lambda$$

where

$$\omega_{ij} = g_{ij}\sigma(g_{ij})/V$$

$$\lambda = \Sigma\omega_{ij}$$

V is the volume of a cell, $\sigma(g_{ij})$ is a cross section of a molecule pair i, j (for the hard sphere model, $\sigma = \pi d^2$ where d is diameter of molecule but in general if molecules interact with each other by force, σ is function of g_{ij}).

2) Time between two collisions τ is defined by the distribution function

$$F(\tau) = P[\delta t \leqslant \tau] = 1 - \exp(-\lambda\tau)$$

3) After the collision of molecules, initially with speed of $\vec{c}_i, \vec{c}_j$, their speed will change to $\vec{c}\,'_i$, $\vec{c}\,'_j$, while the total energy and momentum of the system of two molecules i, j remains conserved.

In general, DSMC methods are a set of procedures to simulate stochastic processes derived from the kinetic equations (Boltzmann or Kac equations). When using these methods, within the memory of the computer are stored all speed coordinates of the modelled molecules and those physical coordinates, in the direction of which occurs the change of characteristics (e.g. for a one-dimensional flow in the x direction it is only the x-coordinate). The macroscopic quantity, such as a density, a pressure, or a temperature are calculated from the positions and velocities of the molecules.

The methods, in general, solve non-stationary flows, the stationary problem is solved as a steady-state status of a conveniently chosen starting status.

The volume of the physical space being modeled is divided into cells. Such a cell may be a small volume with a given limit or a certain number of points. In such a case a molecule is present in a given cell if it is nearest to the point it represents. A net of points provides the opportunity to avoid the analytical description of the system's limits, and so it is more convenient for cases with geometrically sophisticated limits.

The change of time occurs with the step Δt, which is sufficiently small compared to the average time of collisions between molecules.

The algorithm of the method may be expressed as follows (Fig. 1):

1. All molecules are being transposed to a given distance determined by their speed $\vec{v}$ and the time step Δt.

$$\vec{r}(t+\Delta t)=\vec{r}(t)+\Delta t\vec{v}$$

An analysis would be performed as to whether the molecules cut the surface of a solid body or the outer limits of the flow. New molecules are being randomly generated on limits, through which the flow of molecules into the area of the cell exists.

2. Collisions between molecules, which correspond to the time Δt are performed. The velocity of molecules ahead of the collision $\vec{c}$ will be exchanged by the velocity after the collision $\vec{c}'$. The exchange of the energy of the intramolecular motions will occur respectively (chemical reaction). According to the choice of a molecule pair there exist different variants of this method.

If it is necessary to decrease the statistical deviation of the solution under non-stationary flows, the calculation should be repeated several times for each time step Δt

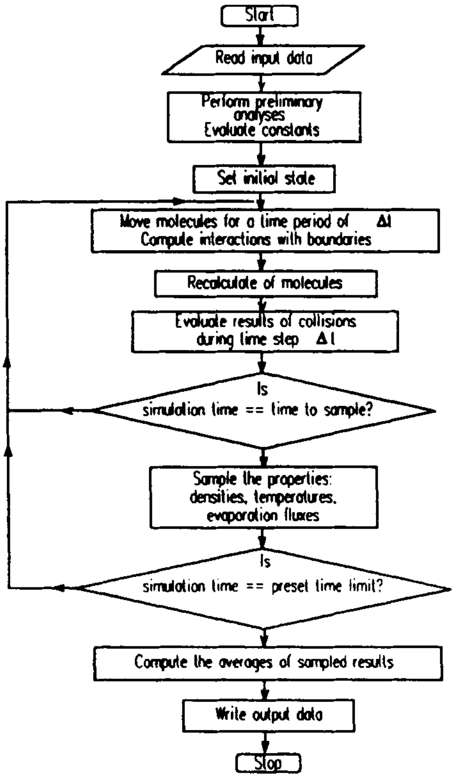

Figure 1 Scheme of DSMC method.

and the required results should be averaged, alternatively for stationary flows, after having reached a stationary status the solution for several steps Δt should also be averaged.

2.2 *The Treatment of Molecular Collision*

The central role in DSMC involves the "treatment of molecular collision", as a consequence of which all DSMC may be divided into two groups.

1) Where DSMC is applied to real gas flow simulation, i.e. mostly for technological applications, there is a tendency to reduce the mathematical sophistication of the algorithm, whilst simultaneously preserving a sufficient veracity of results. This group includes Bird's original time counter method (*TC*), which has played the primary role in technological applications of DSMC methods until recent times.

2) Where DSMC is a mathematical solution of the kinetic equations. Procedures for these methods are rigorously derived from the kinetic equations, this may be:

a) from the Kac equation which include the group of methods: Yanitskiy and Belotserkovskiy, its different variants-Koura, Desphande. Further it may include a group of null collision technique methods (Koura, Ivanov, Yanitskiy, Radev, Bird's no time counter) following from various starting considerations;

b) from the Boltzmann equation which include the original scheme by Nanbu and its variants by Babovsky or the method by Abe related to the null-collision technique.

2.2.1. *The method is a physical model of molecular collisions*

Bird's Time counter method (*TC*) [2, 15]

In the classic kinetic theory of ideal gases as the number of collisions, Z_{AA}, in the volume V with N molecules per unit time the following equation is valid

$$Z_{AA} = N(N-1)\langle g\sigma(g)\rangle/(2V)$$

where $\langle g\sigma(g)\rangle$ is the mean value of the expression $g\cdot\sigma(g)$. For the average time δt between two collisions

$$\delta t = 1/Z_{AA} = 2V/[N(N-1)\langle g\sigma(g)\rangle]$$

If the time counter method is substituted in to this relation instead of $\langle g\sigma(g)\rangle$ the value of $g_{ij}\sigma(g_{ij})$, where i, j determine a molecular pair chosen through a suitable criterion,

$$\delta t' = 2V/[N(N-1)g_{ij}\sigma(g_{ij})]$$

Summation over all possible combinations of molecular pairs gives

$$\Sigma\delta t' = \frac{2V}{N(N-1)}\Sigma[g_{ij}\sigma(g_{ij})]^{-1} = V\langle g\sigma(g)\rangle$$

$$\Sigma\delta t = [N(N-1)/2]\,2V/[N(N-1)\langle g\sigma(g)\rangle] = V\langle g\sigma(g)\rangle$$

and hence

$$\Sigma\delta t' = \Sigma\delta t$$

The number of collisions N_c may be determined from the condition

$$\sum_{i}^{Nc} \delta t_i' \leqslant \Delta t < \sum_{i}^{Nc+1} \delta t_i$$

It was found that for the correct determination of a number of collisions it is necessary that the number of molecules in the cell should be higher than 20.

The criterion for the choice of a molecular pair i, j is the ratio $g_{ij}\sigma(g_{ij})/g_{\max}\sigma(g_{\max})$. The expression $g_{\max}\sigma(g_{\max})$ is the maximum value of expression $g_{ij}\sigma(g_{ij})$, which has appeared during the calculation in a given cell. The scheme of the method for a one time step Δt in one cell is as follows:

(1) If the value of a variable time-counter is $> \Delta t$ go to the point (8) (none collision for this time step), else choose two molecules $i, j \in \langle 1, N \rangle$, $i \neq j$
(2) If $g_{\max}\sigma(g_{\max}) < g_{ij}\sigma(g_{ij})$ substitute the value $g_{ij}\sigma(g_{ij})$ to $g_{\max}\sigma(g_{\max})$
(3) Generate a random number $\mathscr{R} \in (0,1\rangle$
(4) If $g_{ij}\sigma(g_{ij})/g_{\max}\sigma(g_{\max}) < \mathscr{R}$, go to point (1), otherwise continue with the point (5)
(5) Perform the collision between the molecules i, j and substitute the speeds $\vec{c}_i, \vec{c}_j$ with $\vec{c}_i', \vec{c}_j'$.
(6) Add the value $2V/[N(N-1)g_{ij}\sigma(g_{ij})]$ to the variable time-counter
(7) Repeat the steps (1)–(6) until the time-counter is $< \Delta t$
(8) Subtract the value Δt from the value of the time-counter.

2.2.2 *Methods following from the Kac equation*

Yanitskiy and Belotserkovskiy's method [16, 27]

In accordance with the postulates upon which the Kac equation is based then for the time series $\tau_1, \tau_2, \tau_3, \ldots, \tau_k$, where τ_k is the time between the $(k-1)$th and k-th collision at a given time step Δt and in a given cell the following equation is valid:

$$P[\tau_k \leqslant \tau] = 1 - \exp(-\lambda\tau)$$

By means of a random number $\mathscr{R} \in (0, 1\rangle$ we may determine τ_k out of this formulation as follows

$$\tau_k = -\ln(\mathscr{R}) \Bigg/ \left[\sum_{i<j}^{N} g_{ij} \cdot \sigma(g_{ij})/V \right]$$

To generate a molecular pair for the collision a postulate stating that the probability of collision is proportional to

$$g_{ij}\sigma_{ij}(g_{ij})/\Sigma g_{kl}\sigma_{kl}(g_{kl})$$

is used.

The algorithm of the method may be written down in the following form:

(1) Calculate $\lambda(0)$ and τ_i from the above equation
(2) Choose a molecular pair i, j for the collision. Generate two numbers $i, j \in \langle 1, N \rangle$, $i \neq j$. Accept this choice if $\mathscr{R}_i \leqslant g_{ij}\sigma_{ij}(g_{ij})/\Sigma_{k<l}\, g_{kl}\sigma_{kl}(g_{kl})$, otherwise refuse it and generate a new i, j.
(3) Calculate post-collision speeds $\vec{c}_i', \vec{c}_j'$ out of $\vec{c}_i, \vec{c}_j$

(4) Modify the value $\lambda(\tau)$ in accordance with the change of $\vec{c}'_i\ \vec{c}'_j$ on to $\vec{c}_i, \vec{c}_j$
(5) Add the value $-\ln(\mathcal{R}_2)/\lambda$ to the sum $\tau_1 + \tau_2 + \cdots$
(6) Repeat the steps (2)–(5) until the sum $\tau_1 + \tau_2 + \cdots$ exceeds the value Δt.

In some programs a simplification often accepted used to be that the value $\lambda(t)$ changes during the time step Δt only negligibly, and that the step (4) could be omitted. The disadvantage of the method is that the calculation of λ by the summation throughout $N(N-1)/2$ members gives rise to a quadratic dependence of the computing time on the number of molecules in the cell.

Koura's method [27]

This method is a variant of the Yanitskiy-Belotserkovskiy scheme. It uses the simplification $\lambda(\tau) = \lambda(0)$, while $\lambda(0)$ is determined by the expression with a multi-component integral, calculated by the Monte Carlo method.

Deshpande's method [18, 24, 27]

This method also uses the simplification $\lambda(\tau) = \lambda(0)$. The number of collisions N_c for the time interval $(0, \Delta t)$ is determined out of the Poisson probabilistic distribution

$$P(N_c = k) = e^{-\lambda\Delta t}(\lambda\Delta t)^k/k! \tag{3}$$

Kac (Direct) method—the scheme of collision simulation by a sequence of Bernoulli trials [22, 24]

In this method all possible combinations of molecules i, j are taken into consideration, which represents $N(N-1)/2$ pairs of molecules. The collision probability for each pair P_{ij} is proportional to the ratio of volume swept by their cross section, moving at the relative speed of the pair, to total volume of the cell

$$P_{ij} = g_{ij}\sigma(g_{ij})\Delta t/V = \omega_{ij}\Delta t$$

If this probability is higher than $\mathcal{R}$, the collision will take place and $\vec{c}_i, \vec{c}_j$ will be replaced by post-collision speeds $\vec{c}'_i, \vec{c}'_j$.

The algorithm is as follows:

(1) Perform the following for i from 1 to $N-1$
(2) Perform the following for j from $i+1$ to N
(3) Calculate $P_{ij} = g_{ij}\sigma(g_{ij})\Delta t/V$
(4) Generate a random number $\mathcal{R}$
(5) If $(\mathcal{R} \leqslant P_{ij})$ perform collision between the molecules i, j and exchange the velocities $\vec{c}_i, \vec{c}_j$ by new ones $\vec{c}'_i, \vec{c}'_j$
(6) Increase j by one
(7) Increase i by one

The method is also a time-dependent on the quadratic of the molecules number in the cell.

2.2.3 *Null collision techniques*

In null collision techniques, the null collision is introduced by replacing $\Sigma g_{ij}\sigma(g_{ij})$ by $g_{\max}\sigma(g_{\max})$ which is a constant larger then $\Sigma g_{ij}\sigma(g_{ij})$.

The value $g_{\max}\sigma(g_{\max})$ is determined in parallel during the calculation, in the same way as in the Bird's time counter method.

Koura's null-collision technique [20, 24]

This technique is a variant of the Yanitskiy-Belotserkovskiy method. A maximum estimation of $\lambda_{\max}$ for a given cell is determined as follows:

$$\lambda_{\max} = N(N-1)\, g_{\max}\sigma(g_{\max})/(2V)$$

This value is considered to be constant during the calculation and is taken as the entry value λ in to the Yanitskiy and Belotserkovskiy algorithm. In this way the number of pseudo-collisions is determined, while a pseudo-collision may not lead to a real collision. A pseudo-collision corresponds to a real collision with the probability $g_{ij}\sigma(g_{ij})/g_{\max}\,\sigma(g_{\max})$. Molecules for the collision are generated randomly, from the whole interval $\langle 1, N\rangle$. For a given pair i, j a collision occurs and $\vec{c}_i, \vec{c}_j$ are changed by $\vec{c}\,'_i, \vec{c}\,'_j$ if $g_{ij}\sigma(g_{ij})/g_{\max}\,\sigma(g_{\max}) \geqslant \mathcal{R}$. Unlike the original algorithm, λ is not calculated by the summation through $N(N-1)/2$ members, but it follows directly from one member, which significantly accelerates the calculation.

The algorithm of the method:

(1) Calculate $\lambda_{\max}$
(2) Choose a pair of molecules i, j for the collision, $i, j \in \langle 1, N\rangle$, $i \neq j$
(3) If $g_{ij}\sigma(g_{ij}) > g_{\max}\sigma(g_{\max})$ substitute the value $g_{\max}\sigma(g_{\max})$ with the value $g_{ij}\sigma(g_{ij})$ and recalculate the value $\lambda_{\max}$
(4) Generate random numbers $\mathcal{R}_1, \mathcal{R}_2$
(5) If $\mathcal{R}_1 \leqslant g_{ij}\sigma(g_{ij})/g_{\max}\sigma(g_{\max})$, calculate post-collision velocities $\vec{c}\,'_1, \vec{c}\,'_2$ out of $\vec{c}_i, \vec{c}_j$
(6) Add the value $-\ln(\mathcal{R}_2)/\lambda_{\max}$to the sum $\tau_1 + \tau_2 + \cdots$
(7) Repeat the steps (2)–(6), until the sum $\tau_1 + \tau_2 + \cdots$ exceeds the value Δt.

Ballot box scheme of simulation [17, 21, 24]

The time step Δt is divided into k time steps δt so that for any combination i, j $P_{ij}(\delta t) \leqslant 1$ is valid (normally $P_{ij}(\Delta t) \ll 1, \rightarrow k < 1$, out of which for δt and k follows

$$P_{ij,\max} = g_{\max}\,\sigma(g_{\max})\delta t/V = 1$$

$$\Downarrow$$

$$\delta t = V/[g_{\max}\,\sigma(g_{\max})]$$

$$k = \Delta t/\delta t = g_{\max}\,\sigma(g_{\max})\Delta t/V$$

where $g_{\max}$ is a maximum relative velocity, having occurred during the calculation in a given cell. The calculation is the analogy of the Kac method, k-multiple number of states are being generated so the number of generated pairs is

$$M = k\,N(N-1)/2 = [N(N-1)g_{\max}\sigma(g_{\max})\Delta t]/2V$$

and the collision probability P_{ij} is k-times decreased.

$$P'_{ij} = P_{ij}/k = g_{ij}\sigma(g_{ij})/[g_{\max}\sigma(g_{\max})]$$

For $k < 1$ is $M < N(N-1)$ and the calculation time compared with the Kac method decreases.

No time counter (NTC) method (Bird) [22,24] and urn-scheme method (Yanitskiy) [19,23,25]

This method is a modification of a direct (Kac) method, where in a number of sampled pairs are reduced by a certain factor F, on the other hand the collision probability is increased by the same factor. This factor is chosen such that the maximum collision probability of a certain pair be unity.

$$M = N(N-1)/(2F)$$

$$P'_{ij} = P_{ij}F = N(N-1)g_{ij}\sigma(g_{ij})\Delta t/(2VM)$$

$$P'_{\max} = N(N-1)\,g_{\max}\sigma g(g_{\max})\Delta t/(2VM) = 1$$

$$\Downarrow$$

$$M = [N(N-1)\,g_{\max}\sigma(g_{\max})\Delta t]/2V$$

$$P'_{ij} = g_{ij}\sigma(g_{ij})/g_{\max}\sigma(g_{\max})$$

This result is identical with the Ballot box scheme of simulation technique.

The algorithm for both methods may be demonstrated as follows

(1) Calculate M out of the value $g_{\max}\sigma(g_{\max})$
(2) Perform the following for l from 1 to M
(3) Choose randomly two molecules $i, j \in \langle 1, N \rangle$, $i \neq j$
(4) If $g_{ij}\sigma(g_{ij}) > g_{\max}\,\sigma(g_{\max})$ substitute the value $g_{\max}\sigma(g_{\max})$ with the value $g_{ij}\sigma(g_{ij})$
(5) Generate a random number $\mathscr{R}$.
(6) If $\mathscr{R} \leqslant g_{ij}\sigma(g_{ij})/g_{\max}\,\sigma(g_{\max})$ perform the collision and replace the velocities $\vec{c}_i, \vec{c}_j$ by new $\vec{c}'_i, \vec{c}'_j$ aims
(7) Increase 1 by one.

2.2.4 *Methods following from the Boltzmann equation*

Nanbu's method [27]

For each molecule $i \in \langle 1, N \rangle$ the collision probability should be determined

$$P_i = \sum_j P_{ij}$$

If the random number $\mathscr{R} > P_i$, the molecule will not collide. If $\mathscr{R} \leqslant P_i$, for the molecule i with the probability criteria $g_{ij}\sigma(g_{ij})/\Sigma_k\, g_{ik}\sigma(g_{ik})$ will be a partner for the collision chosen and the collision occurs. After the collision the velocity $\vec{c}_i$ is replaced by $\vec{c}'_i$, the velocity $\vec{c}_j$ does not change.

The method is time-dependent on the quadratic of the number of molecules in the cell. Additionally, some authors have observed that the energy and momentum conservation law is broken at the collision [14]. Post-collision velocities are calculated from energy and momentum conservation law

$$\frac{1}{2}m_i c_i^2 + \frac{1}{2}m_j c_j^2 = \frac{1}{2}m_i c_i'^2 + \frac{1}{2}m_j c_j'^2$$

$$m_i\vec{c}_i + m_j\vec{c}_j = m_i\vec{c}_i' + m_j\vec{c}_j'$$

In this method for after the collision only the velocity of i-th molecule is replaced by the post-collision velocity and

$$\frac{1}{2}m_i c_i^2 + \frac{1}{2}m_j c_j^2 \neq \frac{1}{2}m_i c_i'^2 + \frac{1}{2}m_j c_j^2$$

$$m_i\vec{c}_i + m_j\vec{c}_j \neq m_i\vec{c}_i' + m_j\vec{c}_j$$

```
(1) Perform the following for $i$ from 1 to $N$
(2) $P_i = 0$
(3) Perform the steps (4), (5) for $j$ from 1 to $N$
(4) $P_i = P_i + g_{ij}\sigma(g_{ij})\Delta t/V$
(5) Increase $j$ by one
(6) Generate a random number $\mathscr{R}_1$
(7) If $\mathscr{R}_1 \leqslant P_i$ perform the steps (8), (9)
(8) Choose a molecule $j$ for the collision with a molecule $i$. Generate a number $j = \mathscr{R}_2 N$, $i \neq j$. Accept this choice, if $\mathscr{R}_3 \leqslant g_{ij}\sigma_{ij}(g_{ij})/\Sigma_k g_{ik}\sigma_{ik}(g_{ik})$, otherwise refuse it and generate a new $j$.
(9) Perform the collision between the molecules $i, j$, replace by $\vec{c}_i'$ the value $\vec{c}_i$
(10) Increase $i$ by one (test next molecule)
```

Babovsky's method [27]

The Nanbu's method was modified by Babovsky with the aim to decrease the time-requirement proportional to N^2 to one proportional N. The interval $\langle 0,1\rangle$ is divided on N equal segments. A random number $\mathscr{R}$ will determine by its size j-segment (it is within its interval-Figure 2). For molecules i, j P_{ij} is calculated and if $\mathscr{R} \geqslant (j/N) - P_{ij}$, a collision occurs between the given pair and the value $\vec{c}_i$ is substituted by $\vec{c}'_j$. It is necessary to note that for the successful use of this method the condition $P_{ij} < 1/N$ for any j must be fulfilled. This is fulfilled if Δt is sufficiently low compared to the mean time between two collisions.

```
(1) Perform the following for $i$ from 1 to $N$
(2) Choose randomly a molecule $j \in \langle 1, N\rangle$, $i \neq j$
(3) $P = \Delta t\, g_{ij}\sigma(g_{ij})/V$
(4) Generate a random number $\mathscr{R}$
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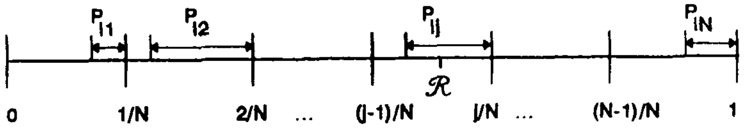

Figure 2 Scheme of Babovsky's variant of DSMC.

(5) If $P \geqslant j/N - \mathscr{R}$ perform the collision between the molecules i, j and replace by $\vec{c}_i'$ the value $\vec{c}_i$
(6) Increase i by one (test a next molecule)

Abe's method [26]
This method is a modification of the Nanbu's method of DSMC using the null-collision technique. Similarly, as with the ballot box scheme or NTC scheme, only a certain fraction of the total possible number of combinations of states is generated, however, the collision probability is increased by the same factor. By an analogous procedure as with the ballot box scheme for number of samples is:

$$M = N(N-1)\, g_{\max}\sigma(g_{\max})\Delta t/V$$

M couples $i, j \in \langle 1, \ldots, i \neq j, \ldots, N \rangle$ are generated. If $g_{ij}\sigma(g_{ij})/g_{\max}\sigma(g_{\max}) \leqslant \mathscr{R}$, the collision occurs and $\vec{c}_i$ is replaced by $\vec{c}_i'$. Unlike as with the NTC or ballot-box scheme the double number of states is generated and at the collision only the velocity of i-molecule is modified by the post-collision velocity.

(1) Calculate M out of the value $g_{\max}\sigma(g_{\max})$
(2) Perform the following for l from 1 to M
(3) Choose randomly two molecules $i, j \in \langle 1, N \rangle, i \neq j$
(4) If $g_{ij}\sigma(g_{ij}) > g_{\max}\sigma(g_{\max})$, substitute the value $g_{\max}\sigma(g_{\max})$ with the value $g_{ij}\sigma(g_{ij})$
(5) Generate a random number $\mathscr{R}$
(6) If $R \leqslant g_{ij}\sigma(g_{ij})/g_{\max}\sigma(g_{\max})$ perform the collision and replace the velocity $\vec{c}_i$ by $\vec{c}_i'$
(7) Increase l by one.

3 RESULTS AND DISCUSSION

We have tested by computer the following methods: Bird's time counter, no time counter, Babovsky, Nanbu, Koura null collision technique, Yanitskiy, Abe and direct (Kac) schemes.

The modeled system was represented by an gas in equilibrium formed by molecules modelled as elastic spheres with collision diameter $d = 1 \times 10^{-9}$ m and molecular weight $m = 5.62 \times 10^{-25}$ kg. The pressure of the system was 1 Pa and its temperature 400 K. The velocities for the molecules were generated based on the Maxwell distribution function. The conditions chosen were such that it was possible to omit from the DSMC scheme part of the solution for molecular movement and the change in molecular velocity during the collision whilst at the same time ensured a constant value of λ during the calculation. For the selected algorithms the number of collisions N_c which took place in the cell of N molecules per time step of the calculation $\Delta t = 1 \times 10^{-6}$ s was determined. For each method the calculation was repeated, $M = 10000$, in total for the number of molecules in the cell N less than or equal 100 and $M = 1000$ for $N > 100$. The arithmetic mean value out of these values was calculated

$$\langle N_c \rangle = \sum_{i=1}^{M} N_{Ci}/M$$

dispersion

$$\sigma^2(N_c) = \sum_{i=1}^{M} (N_{Ci} - \langle N_c \rangle)^2/(M-1)$$

and constructed distribution function $f(N_c)$. The results are given in the Table 1.

The calculations were performed on the computer PC 386/25, 8 MB RAM under OS SCO UNIX V/386 release 3.2. Programs were created in the programming language *C*, whereby programs for individual methods differ only in the method of determining the number of collisions. The time of calculation was determined by the command OS UNIX "time", the results are illustrated in the Figure 3. It is obvious, that the most time-demanding methods are those which contain a cycle through $N(N-1)/2$ members-Nanbu, direct (Kac) and Yanitskiy, the quickest are Bird's time counter and no time counter. For a cell containing 100 molecules the difference in the velocity between the quickest and the slowest method is two range.

The Figure 4 shows the absolute, and the Figure 5 a relative difference between the number of collisions calculated out of the analytical relation for equilibrium

$$N_{c\,\text{theor}} = \sqrt{2}\pi d^2 \langle c \rangle n N \Delta t/2$$

$$\langle c \rangle = \sqrt{\frac{8kT}{\pi m}}$$

and the mean value $\langle N_c \rangle$ where n is the number density (number of molecules in m^3), k is the Boltzmann constant. For the absolute difference, the differences up to the value $N = 500$ are lower than 1. Above this value the absolute difference increases and the relative difference decreases (Figure 5). On the other hand, the relative deviation is

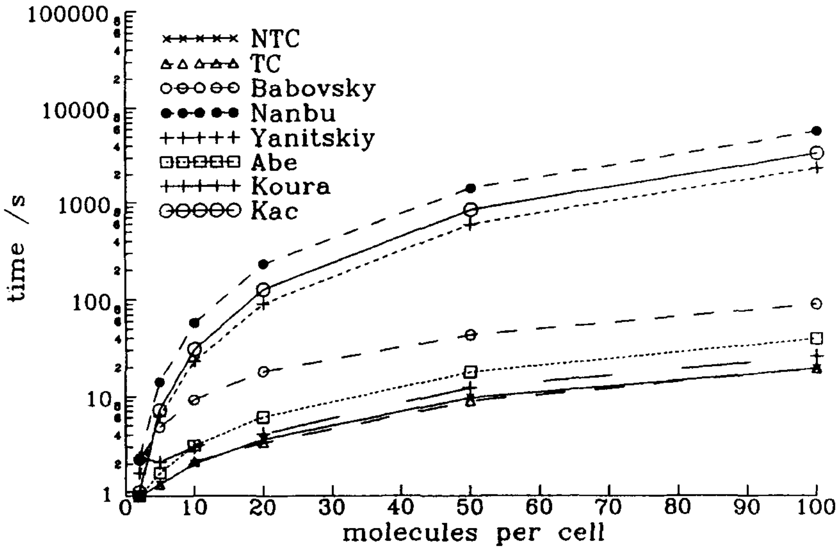

Figure 3 Dependence of the calculation time on number of molecules per cell for various variants of DSMC.

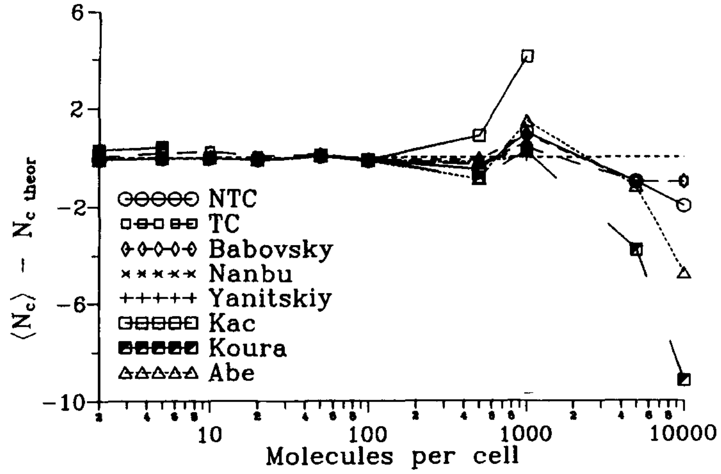

Figure 4 Dependence of absolute difference $\langle N_c \rangle - N_{theor}$ on number of molecules per cell for various variants of DSMC.

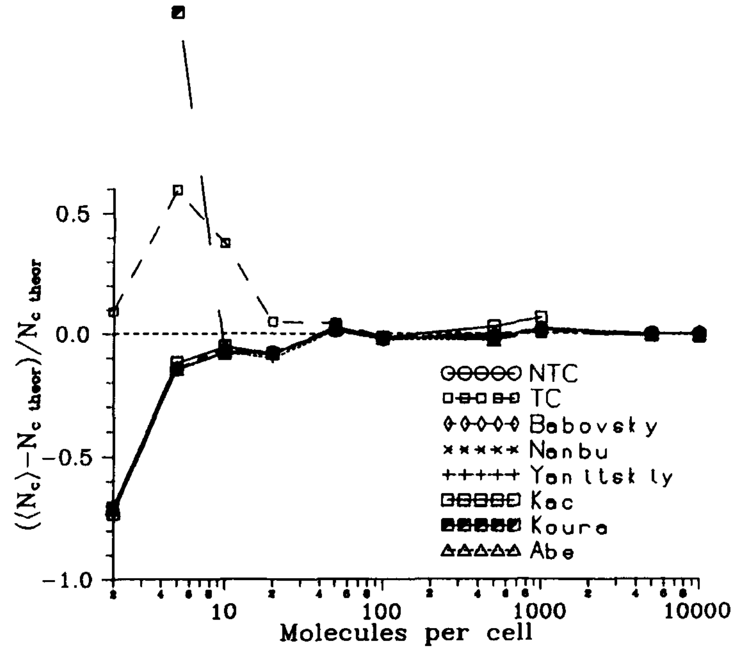

Figure 5 Dependence of relative difference $(\langle N_c \rangle - N_{theor})/N_{theor}$ on number of molecules per cell for various variants of DSMC.

significant for $N \leqslant 20$ which corresponds to the value $N_{C\,theor} \leqslant 1$. In these cases all methods fail (Table 1).

The Figure 6 shows the dependence $\sigma^2(N_C)$ on N for individual methods. Yanitskiy, Kac and Koura methods directly following from the Kac equation show that for given

Table 1 Dependence of the calculation time, $\langle N_c \rangle$ and σ^2_{Nc} on number of molecules per cell for various variants of DSMC

N	*Method*	*NTC*	*TC*	*Babov.*	*Nanbu*	*Yanit*	*Kac*	*Koura*	*Abe*	*Theor*
2	t/s	0.9	0.9	2.2	2.3	1.6	1.0	2.3	0.9	–
	$\langle N_c \rangle$	0.0337	0.1364	0.0354	0.0376	0.0370	0.0368	0.411	0.0337	0.125
	σ^2_{Nc}	0.0326	0.1178	0.0170	0.0182	0.0376	0.0355	0.2422	0.0157	0.125
5	t/s	1.2	1.2	4.8	14.2	6.2	7.2	2.1	1.6	–
	$\langle N_c \rangle$	0.267	0.499	0.268	0.267	0.266	0.275	0.728	0.267	0.313
	σ^2_{Nc}	0.196	0.250	0.118	0.119	0.256	0.267	0.1981	0.622	0.313
10	t/s	2.0	2.1	9.2	57.5	23.2	30.6	2.1	3.1	–
	$\langle N_c \rangle$	0.578	0.861	0.588	0.578	0.577	0.592	0.573	0.578	0.625
	σ^2_{Nc}	0.278	0.508	0.258	0.256	0.672	0.575	0.291	0.137	0.625
20	t/s	3.6	3.3	18.1	230	90.9	126	4.1	6.1	–
	$\langle N_c \rangle$	1.15	1.31	1.15	1.14	1.12	1.14	1.15	1.15	1.25
	σ^2_{Nc}	0.641	0.547	0.500	0.501	1.47	1.12	1.08	0.30	1.25
50	t/s	9.6	8.8	42.4	$1.39\ 10^3$	574.7	828	12.2	17.7	–
	$\langle N_c \rangle$	3.17	3.26	3.21	3.17	3.17	3.21	3.17	3.19	3.13
	σ^2_{Nc}	1.89	0.946	1.40	1.39	4.33	3.21	3.21	0.959	3.13
100	t/s	19.2	19.2	87.0	$5.59\ 10^3$	$2.26\ 10^3$	$3.26\ 10^3$	25.6	38.5	–
	$\langle N_c \rangle$	6.12	6.17	6.14	6.12	6.09	6.15	6.13	6.11	6.26
	σ^2_{Nc}	3.96	1.59	2.67	2.69	6.09	6.23	6.10	1.98	6.26
500	$\langle N_c \rangle$	30.8	31.0	31.2	31.0	31.1	32.2	30.5	30.4	31.3
	σ^2_{Nc}	22.3	7.99	13.3	13.5	31.5	25.3	29.1	11.5	31.3
1000	$\langle N_c \rangle$	63.6	63.0	63.5	63.2	62.6	66.7	62.8	64.1	62.7
	σ^2_{Nc}	39.5	18.8	26.2	29.2	81.6	58.1	65.2	27.0	62.7
5000	$\langle N_c \rangle$	312	312	312	–	–	–	309	311	313
	σ^2_{Nc}	250	83.4	141	–	–	–	446	240	313
10000	$\langle N_c \rangle$	624	625	625	–	–	–	617	621	626
	σ^2_{Nc}	503	163	263	–	–	–	1288	825	626

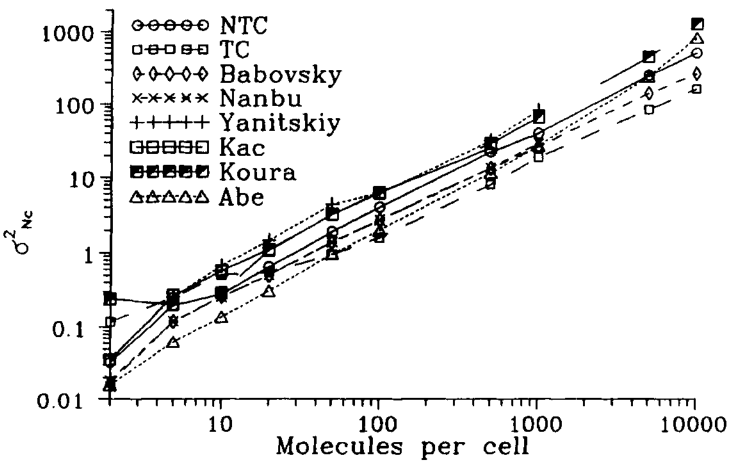

Figure 6 Dependence of σ^2_{Nc} on number of molecules per cell for various variants of DSMC.

conditions theoretical values of the dispersion near the mean value are obtained. The dispersion of the other methods is lower. Figure 7 and Figure 8 show the distribution functions $f(N_c)$ of individual methods compared with the theoretical Poisson distribution (Kac equation–eq. (3)). The shapes of numerically determined distribution functions are for Yanitskiy, Kac and Koura methods well consistent with the theoretical Poisson distribution, the other methods show a sharper distribution function (see Figure 6). Among these methods the lowest deviation from the Poisson distribution was shown by the no time counter algorithm, the biggest with the Bird's time counter algorithm.

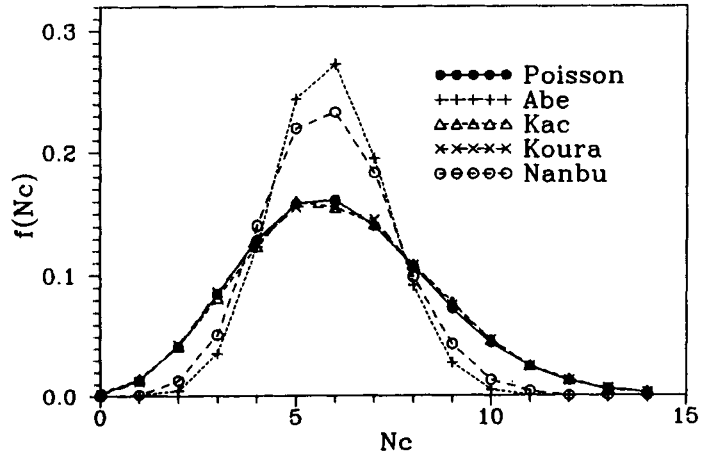

Figure 7 Comparison of Poisson distribution function with distribution functions $f(N_c)$ for Abe's, Kac's, Koura's and Nanbu's variant of DSMC.

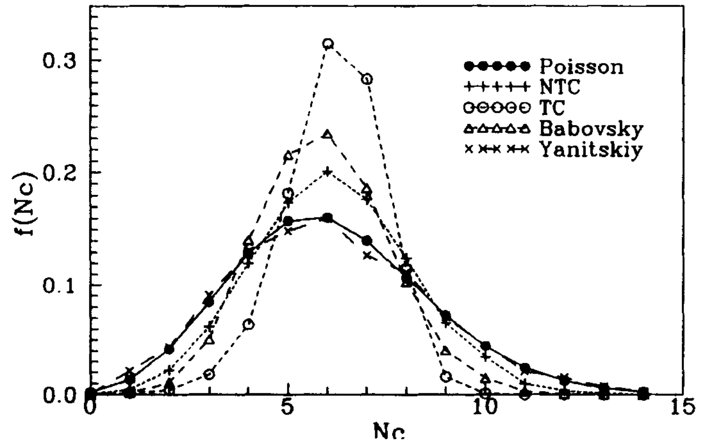

Figure 8 Comparison of Poisson distribution function with distribution functions $f(N_c)$ for no time counter time counter, Babovky's ans Yanitskiy's variant of DSMC.

For the Babovsky scheme the total kinetic energy of the system $E_{kin} = mc^2/2$ and its time development was followed (Figure 9). Contrary to the previous calculations it was necessary to include into the scheme a part calculating post-collision velocities. In the model cell $N = 100$ molecules were found, the total simulation time was 1×10^{-3} s. The system energy difference in time $E(t)$ and at the beginning of the simulation $E(0) = 2.7 \times 10^6$ J is shown in the Fig. 9. It is obvious that with this method a change of total system energy occurs, whereby for longer period of the simulation this difference becomes significant. Similar behavior was observed for both the Nanbu's and Abe's methods. With the no time counter method is maximum difference in energy 1×10^{-9} J is at the same input parameters as above. In this method the only numerical error is in the calculation of the post-collision velocities.

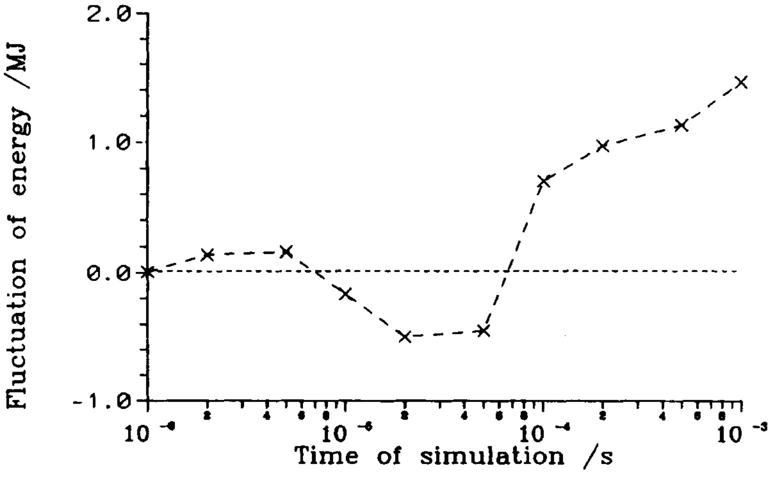

Figure 9 Dependence of fluctuation of energy on time of simulation for Babovsky's variant of DSMC.

4 CONCLUSIONS

From the comparison of the tested algorithms it follows that:

The Bird's time counter method is one of oldest, until recently the most used method in technical applications. The distribution function of the number of collisions in the cell is significantly sharper than the theoretical Poisson function. This method is one of the quickest ones, but it is not suitable for parallel computers (cycle do ... while (logical condition)).

The Yanitskiy and Belotserkovskiy method shows an excellent conformity of the distribution function $f(N_c)$ with the Poisson distribution, but it belongs to the group of slowest methods and again it is not suitable for use with parallel computers.

The Kac (direct) method shows an excellent $f(N_c)$ conformity with the Poisson distribution, it is slow but suitable for the use with parallel computers.

The Koura's null-collision technique belongs to the methods with an excellent $f(N_c)$ conformity with the Poisson distribution, it belongs to quick methods, but its algorithm again is not suitable for parallel computers.

Ballot-box, no time counter and Yanitskiy urn schemes show relatively good $f(N_c)$ conformity with the Poisson distribution, though it does not reach the quality of the Yanitskiy-Belotserkovskiy, Kac and Koura'a methods. Among the tested methods this method is together with the Bird's time counter the quickest method. It is also suitable for the use with parallel computers.

The Nanbu's procedure was the slowest one from the tested methods, it shows a $f(N_c)$ deviation from the Poisson distribution, additionally the change of the total system energy occurs during its use. It is not suitable for parallel computers.

The Babovsky's method was reasonably fast. It is suitable for use with parallel computers. The total energy is not conserved.

The Abe's method was the quickest from among the tested methods, it is suitable for use with parallel computer. The total energy is not conserved.

From the results presented here it follows that, for provided applications, the best method may be considered to be the no time counter (Ballot-box or Yanitskiy urn-scheme). The Bird's time counter, no time counter and Koura's null-collision technique are the best methods for use with one-processor computers.

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