Comparison of modern implementations of the direct simulation Monte Carlo method

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Abstract. In this work, collisional schemes of the direct simulation Monte Carlo (DSMC) method are compared. The sensitivity of the schemes to the number of simulated particles is investigated. The original No-Time-Counter (NTC) scheme, proposed by G.A. Bird, its modification NTC-2007 and majorant collision frequency (MCF) scheme, proposed by M. S. Ivanov and S.V. Rogasinsky are considered. For the high-speed Couette flow with parameters corresponding to a near-continuum regime (speed ratio $S$ is equal to 10, Knudsen number $Kn$ is equal to 0.01) the convergence of shear stress component is analysed. Calculations with different total number of the simulated particles (in the range from $500$ to $10^6$) were performed. It was shown, that the deviation of NTC-2007 scheme from the reference solution is about four times larger as compared to the MCF scheme. The original NTC scheme exhibits much higher sensitivity to the number of simulated particles.

1. Introduction
The direct simulation Monte Carlo (DSMC) method is a stochastic technique to solve the Boltzmann equation numerically [1]. The main area of DSMC method application is rarefied gas flows (when the continuum approach is not applicable): the high-altitude aerodynamics of spacecraft, vacuum systems, micromechanical devices. The DSMC method is based on the gas flow representation as a finite set of the simulated particles. Each simulated particle corresponds to a large amount of real molecules. The computational domain is split into the collisional cells. At the initial time, this domain is populated with the particles with the some initial distribution over the coordinates and velocities. During one time step the following stages are performed consequently: the free-molecular transfer of the simulated particles and the binary collision of the particles located in the same cell.

There are following error types in the numerical solution calculated by the DSMC method:
1) A statistical error, which depends on the size of the sample.
2) Deterministic errors, which depends on:
   − the time discretization,
   − the spatial discretization,
   − the number of simulated particles $N$.

The computational resources required by the DSMC computations linearly depend on the number of particles. All modern implementations of the DSMC method are mostly different from each other in the details of collision modeling. Practical applications of the DSMC method require intensive computations on powerful computers. Therefore, the ability to carry out calculations with a small number of particles without loss of accuracy is the most attractive property of the collision scheme.
this work, only the error connected to a number of simulated particles $N$ (particle discretization error) is investigated. The time step and cell size were small enough and the sample size was large enough for other errors being insignificant compared to the particle discretization error.

Until recently, one of the most popular DSMC collision schemes was the No-Time Counter (NTC) scheme, proposed by G.A. Bird in 1989 [2]. The NTC scheme allows getting the numerical solution of the Boltzmann equation, if the number of simulated particles in a collision cell is large enough.

Another collision scheme is the Majorant Collision Frequency (MCF) scheme, proposed by M. S. Ivanov and S. V. Rogasinsky [3]. The MCF scheme is used in the SMILE code family [4], [5], [6]. In [7] it was shown that the MCF scheme requires significantly fewer total particle number and does not depend on the particle number in the cell than conventional DSMC schemes. It means that more complicated problems can be solved with the same computational resources. The fraction of repeated collisions were introduced in [8] as indicator of the numerical solution convergences to the solution of the Boltzmann equation. The MFC scheme has been employed in the SMILE family codes for modelling various real gas effects, including energy transfer between different molecular modes, chemical reaction in the gas phase and on the vehicle surface and ionization [9] – [12].

In 2007, G.A. Bird proposed a modification of the NTC scheme [13], which, according to the author, makes the numerical modeling much more efficient. A comparison of NTC and MCF schemes was presented in [7]. However, the rigorous investigation of these schemes for classic problems of rarefied gas dynamics is still required.

The goal of this work was comparison of different schemes sensitivity to the total number of the simulated particles. Three schemes were considered:
- NTC, G.A. Bird,
- NTC-2007, G.A. Bird,
- MCF, M.S. Ivanov, S.V. Rogasinsky.

The dependence of the solution of the plane Couette flow problem on the simulated particle number is investigated. This classical problem of the rarefied gas dynamics is often used for the comparison between different DSMC schemes (see, e.g. [14]). The Couette flow problem is solved for the parameters corresponding to the near continuum high-speed gas flow.

2. Numerical results

Numerical simulation of the planar Couette flow of the monatomic dilute gas (argon) between two parallel plates was performed using different collisional schemes. This problem was considered in the following statement. Two plates are kept at constant temperature $T = 273$ K. The distance between plates is 1 m. One plate is stationary and the other one moves in its own plane with velocity of 3370 m/s. The $x$-axis is directed perpendicular to the walls, and the $y$-axis is in the direction of the motion. The gas motion occurs due to the viscous friction forces in the $y$-direction. The speed ratio (plate velocity divided by the most probable speed) is equal to 10, Knudsen number (ratio of the mean free path to the flow width) is equal to 0.01.

In the considered flow all macroparameters change along the $x$-axis. The velocity, density and temperature profiles are shown in the figure 1. In the center of the flow, a maximum of temperature and a minimum of density are observed (figures 1b and 1c).

In this work $\tau_{xy}$ component of shear stress tensor was used for the comparison of the collision schemes:

$$\tau_{xy} = \rho c_x c_y,$$

where $c_x$, $c_y$ are the components of the particle thermal velocity vector, $\rho$ is the density. Since $\rho = n m$, where $n$ is the number density, $m$ is the molecular mass, and the flow velocity in $x$ direction is zero, $\tau_{xy}$ was estimated as $\tau_{xy} = n m u v$, where $u$, $v$ are the absolute molecule velocities in $x$, $y$ directions.
The calculations were performed using the DSMC1 demonstration code written by G.A. Bird. The collisional subroutine COLLMR was modified to implement each investigated scheme. The sample size, the time and spatial discretization were taken in such a way that the corresponding errors became significantly less than the particle discretization error. The number of the cells in the computational domain was equal to 2000, and the time step was $2\times10^{-7}$ s. The calculations using each scheme were performed for $N$ equal to 500, 1000, 2000, 4000, 6000, 8000, $10^4$, $5\times10^4$, $10^5$, $10^6$. For $N = 10^6$, the reference result was reproduced by all three schemes, as shown in figure 2.

![Figure 2](image)

**Figure 2.** The reference result ($N = 10^6$) for NTC, NTC-2007 and MCF schemes.

![Figure 3](image)

**Figure 3.** The solutions obtained using NTC (a), NTC-2007 (b) and MFS (c) schemes.
The figure 3 shows the deviation of the solution from the reference profile as the particle number decreases for each scheme. The different lines correspond to the results of the calculations with the particle number 500, 1000, 2000, 8000, and $10^6$. For the NTC scheme (figure 3a) with a decrease of the number of particles to 500 the solution deviates from the reference one severalfold. For NTC-2007, the deviation is about 12% if $N = 500$ (figure 3b). For MCF scheme, the deviation is only about 3% for $N = 500$ (figure 3c).

Since the linear convergence behavior $O(1/N)$ is observed for the parameter estimation during the increase of the simulated particle number, the dependence of the estimation of $\tau_{xy}$ parameter from $N$, obtained from the calculations, may be approximated by the function:

$$\tau_{xy}^* = \tau_{xy}^0 + CN^{-1},$$

(1)

where $\tau_{xy}^*$ is the reference value and $C$ is some coefficient. Symbols on figure 4 denote the results of the calculations with different $N$ (average $\tau_{xy}$ along x-axis), and lines represent the approximation (1). The figure 4 shows the convergence of the $\tau_{xy}$ estimation for all schemes as $N$ is large enough to the reference value. However, when $N$ is small, the deviation for the NTC scheme is significantly larger than for two other schemes, and the MCF scheme has smaller deviation than NTC-2007.

The smaller is absolute value of coefficient $C$ in formula (1), the smaller is deviation of $\tau_{xy}$ parameter from the reference value for any fixed $N$. Therefore, the value of $C$ can characterize the scheme sensitivity to the particle number for the flow considered. In table 1, the values of $C$ normalized by the reference value $\tau_{xy}^*$ are shown.

![Figure 4. The estimation of the shear stress $\tau_{xy}$ value as a function of total number of the particles. Points – DSMC computations, lines – approximation.](image)

| Scheme    | $|C/\tau_{xy}^*|$ |
|-----------|-----------------|
| NTC       | 1460            |
| NTC-2007  | 70              |
| MFC       | 18              |
3. Conclusions
By the test case of the high-speed Couette flow in the near-continuum regime (Kn = 0.01, S = 10), the sensitivity of three collision schemes of the DSMC method to the total number of simulated particles was studied. The NTC, NTC-2007 and MCF schemes were considered. The calculations with different simulated particle number (from 500 to 10^6) were performed. The values of the shear stress $\tau_{xy}$ was calculated using each scheme. For the case of large particle number N = 10^6, the same results for all schemes were obtained. The deviation of the computational results from the reference value for decreased total number of the simulated particles was demonstrated for the considered schemes.

The numerical results demonstrate that the MCF scheme has the lowest error growth with a decrease of the number of simulated particles. The deviation from the reference solution obtained for the MCF scheme is approximately four times lower than for the NTC-2007 scheme and 80 times lower that for the NTC.

These results have the implications for the practical applications of the DSMC method, particularly, for the high-altitude aerothermodynamics problems. The smaller sensitivity to the particle number is important in the big supercomputer computations performed with all available computational resources.

The investigation of the convergence behavior for the different flow parameters (Kn, S), and for other classical problems of the rarefied gas dynamic (e.g. the Fourier problem), and interaction of the considered deterministic error with other DSMC errors will allow to extend and generalize present results.

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