Analysis of Efficiency of Some Approaches of Solving Problems by the DSMC Method

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1 Introduction

In the first part of the work radial weighting factors (WFs) [1 – 3] used for simulation by the DSMC method [1] of axially symmetric flows are considered. WFs are introduced for compensation of large differences of cell volumes in the radial direction and determined in such a way that a molecule located far from the axis represents more real molecules than one near the axis. This can even up the number of molecules per cell and considerably decrease the total number of simulated molecules. But using WFs, there is observed a reduction of the simulated collisions in cells near the axis and considerable variations of the total number of simulated molecules during the computation. The objective of the first part was to investigate possibilities of various WFs and to make a comparative analysis of their efficiency.

The second part is dedicated to investigation of efficiency of some estimations used for calculation of macroscopic properties of gas flow. The following estimations are considered:

- The commonly employed estimation of parameters in a cell is performed by a "photograph" of the state of the molecules on each time step with an equal contribution of each molecule [1]. Further this estimation will be referred to as the photograph estimation.

- When using the intersection estimation [4], the summation of data required for calculation of gas properties occurs during the motion of the molecules, and the necessary values are determined at preset planes. As soon as a molecule crosses such a plane, the summation of the information with a weight \(1/u\) happens (here \(u\) is the velocity of the molecule in the direction perpendicular to the plane).

- For the time estimation the information is summed into cells that molecules passed through, and the contribution of a molecule is proportional to the time that the molecule stays in the cell. A similar
strategy is apparently employed at many applications of the Monte Carlo method, e.g. [5, 6].

For comparison of efficiency of these approaches computational cost is calculated. By the computational cost is meant a value $S = t \cdot V\xi/n$, which is generally taken in the Monte Carlo method for estimation of the algorithm quality [5]. Here $t$ is the total computer time spent on the simulation, $n$ is the number of events for counting the variance $V\xi$. The computational cost characterizes the computer time that is necessary for attainment of preassigned exactness.

2 Analysis of weighting factors

2.1 Correctness of the use of WFs

To estimate the correctness of the use of WFs, there were calculated the normalized collision number $\Theta$ and the ratio of the number of duplicate molecules to the total number of the molecules $\Omega = \sum (l - 1)/\sum l$ ($l$ is the number of identical particles in the cell) for cells located at different distances from the axis. Numerical experiments were performed for subsonic ($M = 0.01$) and supersonic ($M = 2$) flows.

WFs may be introduced by setting a maximum value of the WF $W_{max}$. Then a WF for a cell with a number $i$ is calculated as

$$W_i = \frac{1}{i_{max} - 1} [(W_{max} - 1)i + i_{max} - W_{max}] .$$

Here $i = 1$ corresponds to the axial cell; $i_{max}$, to the cell near the cylinder wall. The limiting cases of these WFs for the used net are $W_{max} = 31$, which corresponds to WFs proportional to cell volumes (WF $\sim$ cell), and $W_{max} = 1$, which corresponds to the computation without WFs.

When simulating without WFs, the total number of molecules is equal to 40,000, and the density deviation does not exceed of 1%. For WFs proportional to cell volumes the total number of molecules averages 2,500, and considerable variations of the density in the range 50 - 150% are observed in the process of the computation. Besides, a decrease of the collision number $\Theta$ near the axis by 60% is observed (fig.1a, WF $\sim$ cell). That may be believed to be the consequence of a large number of duplicate molecules (fig.1b). More satisfactory results have been obtained for less WF $W_{max} = 10$, but the small collision number near the axis does not allow to use even this WF (fig.1a, small WF).

To decrease the number of duplicate molecules near the axis, the case was considered when WFs were introduced from a reference radius $R_{ref}$. As an example, there was chosen $R_{ref} = 2$, so that WFs appear only beginning
Figure 1: The normalized collision number (a) and the ratio of the number of duplicate molecules to the total number of molecules (b) for various WFs.

with the ninth cell from the axis. The maximum value $W_{max}$ was taken equal to 5. The obtained collision number is close enough to the correct value, but despite the large number of simulated molecules ($\approx 19,800$), density fluctuations remain at the range from 80 to 120%.

The undesirable impact of the molecule duplication may be lessened in a steady flow by the imposition of a time delay on the appearance of the duplicate molecule [1]. In the present work there is used the delay by the dimensionless time unit $t' = 1/(2n_0\sigma)\sqrt{m/(kT_0)}$, which exceeds slightly the mean time between collisions of the molecules. It is worth noting that the introduction of such a buffer does not increase the time of the calculation and the necessary size of the computer storage. Using such a delay, even for WFs proportional to cell volumes there is a marked reduction of the number of duplicate molecules (fig.1b), and as the consequence there is almost the correct collision number (fig.1a).

The optimum way to use WFs should be considered as the introduction of WFs from a radius $R_{ref}$ with the time delay application. So for $R_{ref} = 2$ and $W_{max} = 5$ with the time delay, the right collision rate (fig.1a) and the minimum number of duplicate molecules (fig.1b) are obtained. But even in this case the density deviation during the computation reaches 20%, and this does not permit to calculate the density accurately using these WFs.

The similar results were obtained for WFs based not on the cell location but on the distance of a molecule from the axis [1].

By computation a supersonic flow with WFs proportional to cell volumes, a significant decrease of density variations during the computation was obtained (the maximum deviation was not exceed 10%). The behaviour of other calculated values is analogous to one for the subsonic flow.

Monte Carlo Method and Numerical Simulation
2.2 Correlation functions

When solving problems by the DSMC method, it is important to know what is the relationship between simulated molecules and how large is the contribution of the statistical correlation to the property estimation. For this purpose the spatial and time correlation functions [1] were calculated, and it was investigated how WFs influence on their behaviour. The normalized time correlation function of the number density is \( \hat{K}(t) = \langle \delta N_0 \delta N_t \rangle / \langle N \rangle \), where \( \delta N_0 \) is the departure of the instantaneous number of molecules \( N \) in a cell from the average number \( \langle N \rangle \) at the initial moment of time, \( \delta N_t \) is the departure at the time moment \( t \). In a similar manner the spatial correlation function is calculated \( \hat{K}(x) = \langle \delta N_0 \delta N_x \rangle / \langle N \rangle \).

The spatial correlation function for the density between the axial cell and radial cells and the time correlation function for the density in the axial cell are presented in fig.2a and 2b, respectively. When introducing WFs, there is an evident relationship between density variations in cells with space and time. When a reference radius \( R_{ref} \) is used, the similar results have been obtained. The calculations of the correlation functions for the velocity have shown that the WFs almost do not increase the velocity correlation.

2.3 Comparison of efficiency of different WFs

To compare the efficiency, there were calculated variances of density, velocity, and temperature and computational costs during the calculation of the considered quantities. When calculating without WFs, the density variance along the radius is constant, for WFs proportional to cell volumes its increase near the axis approximately by the order is observed, and the use of the time buffer causes its large decrease (fig.3a). The maximum computational cost at the calculation of the density is seen for the simulation
without WFs, at WFs proportional to cell volumes its decrease takes place, and when using the time delay, the value of the computational cost reaches the minimum (fig.3b). The minimum variance and computational cost are observed when the time delay is used.

When calculating the variance of the velocity with the use of various WFs, there is not any increase of the variance near the axis, and even its small reduction is observed. Accordingly a decrease of the computational cost for WFs occurs. Similar results have been obtained for the temperature.

3 Comparison of different estimations

The analysis of use of various estimations was performed for the stationary one-dimensional problem of heat transfer between parallel infinite planes. The gas is assumed to be enclosed between two planes located at points \( x = 0 \) and \( x = h \). The temperature of planes is equal to \( T_0 \) and \( T_1 \), respectively. The law of interaction of molecules with walls is assumed to be diffusive one with full accommodation of impulse and energy. The problem is determined by two parameters: the Knudsen number \( Kn = l_0 / h \) (\( l_0 \) is the mean free path) and the temperature ratio \( T_1 / T_0 \). At the present paper \( Kn = 1 \).

To avoid influence of gradients of macroscopic properties, at the first stage of the investigation the case of equal temperatures of the plates was considered \( (T_1 / T_0 = 1) \). There were varied the time step for the fixed cell number \( N = 10 \) and the cell number for the fixed time step \( \Delta t / t' = 0.1 \).

In figure 4 there are presented dependencies of computational cost for \( u^2 \) and
Figure 4: Dependence of computational cost on the time step for the fixed cell number $M = 10$ (a) and on the cell number for the fixed time step $\Delta t/t' = 0.1$ (b) for the second and the third moments of the distribution function.

$u^3$ calculation on the time step and on the cell number. It should be pointed out that the time estimation becomes more efficient in comparison with the photograph estimation with rise of calculated moments of the distribution function.

It is seen from comparative analysis that efficiency of the time estimation relative to the other estimations increases with the time step rise. But it is well known that correct realization of the DSMC method requires $\Delta t$ to be considerably less in compare with the mean collision time. Therefore, there was conducted an investigation of influence of the time step increase on the exactness of results for the time estimation. Sometimes it is profitable to use a large time step for simulation of nonstationary flows, and so, the same investigation was carried out for the photograph estimation also.

- At temperature computation the solution obtained by the simulation using the time estimation with the time step of $0.07t'$ was considered standard. For the time estimation solution obtained with $\Delta t/t' = 0.5$ practically coincides with the standard one, whereas for the photograph estimation even for the less time step $\Delta t/t' = 0.3$ some deviations of results are noticed (fig.5a).

- At heat flux computation the solution obtained by the simulation using the time estimation with the time step of $0.01t'$ was considered standard. Beginning with the $\Delta t/t' \leq 0.1$, results for this estimation practically coincide with the standard solution (fig.5b). For the photograph estimation, although a much smaller time step was used, even for $\Delta t/t' = 0.005$ the obtained profile distinctly differs from the
Figure 5: Temperature (a) and heat flux (b) profiles for various time steps for time and photograph estimations when solving the heat transfer problem for the temperature ratio $T_1/T_0 = 4. Kn = 1$, 20 cells by 40 molecules.

So the time estimation allows to use much larger time steps than the photograph estimation, with more accurate results being obtained.

4 Conclusion

- The performed investigation has shown that the computational cost can be decreased on retention of the correct collision rate by the proper selection of WFs. But simulating a subsonic flow in which the motion of the molecules towards the axis is expressed significantly, for any WFs large density variations are observed during the computation. So, for such subsonic flows it is not recommended to use WFs.

- The density fluctuations become minor when modelling supersonic flow. It can be deduced that WFs with the proper selected maximum value $W_{max}$, reference radius, and time delay may be sufficiently profitably used for the simulation of steady supersonic flows.

- The photograph estimation seems to be the most natural and can be readily realized, but its efficiency decreases at calculation of high moments in comparison with the time estimation.

- The advantage of the intersection estimation is the opportunity to obtain the solution precisely in a predetermined point that may be especially important for calculation of boundary conditions. Its shortcoming is large variance.
• The performed computations demonstrate high efficiency of the time estimation, particularly for calculation of the highest moments of the distribution function. It should be remarked that its efficiency increases with the rise of the number of cells passed through by a molecule at the time step. But this procedure is hardly applicable for the simulation of many-dimensional flows.

5 Acknowledgements

This work was supported by the Russian Foundation for Basic Research through Grant 97-01-00878

References


