Application of parametric correction for improving of DSMC method results

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Abstract. In the article the deterministic errors of the numerical results received by DSMC method are considered. These errors are connected with finiteness of basic parameters of DSMC schemes. The manner of increase of the order of accuracy on basic parameters is offered. Application of the offered manner is shown on an example of a problem of heat transfer between two parallel plates.

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INTRODUCTION

As it is well known, the traditional interpretation of the DSMC method [1] is based on considering the rarefied gas as a set of N particles with binary interaction and on the principle of splitting of continuous motion and collisions of rarefied gas molecules within a small time step Δt . In the further for certainty, we consider a case with identical time step $\Delta\mathbf{t}$, constant general number particles N, and identical volume of spacial cell $\Delta\mathbf{r}$.

There are a lot of versions of numerical schemes realizations for the DSMC method. At present time numerical schemes such as NTC [1], MFS [2] and NC [3] are widely adopted. It is significant the fact which follows from the traditional interpretation and is general for all the numerical schemes Δt, $\Delta\mathbf{r}$, N are parameters of the DSMC method. Conditions which should be imposed on Δt, $\Delta\mathbf{r}$, N are well-known [1].

A correct choice of these parameters for heuristic schemes (for example NTC, NC) allows to interpret these schemes as approximations to physical model of rarefied gas.

For numerical schemes based on ŞMaster equationsŤ (for example MFS) the correct choice allows to speak about proximity between a calculated solution and solution of the Boltzmann equation.

In applications of the DSMC method we often have the following situation with parameters Δt, Δr, N. Making choice and changing considered parameters in the correct intervals we see that several calculated magnitudes donŠt vary at the same time other calculated magnitudes remain sensitivity from the parameter manipulations.

Naturally, this fact is explained by finiteness of magnitudes Δt, $\Delta\mathbf{r}$, N and hence the question about increase of accuracy for results obtained by the DSMC method appears. In this report we consider in details this question and recommend constructive manner increasing accuracy of numerical results obtained by the DSMC method up to second order on Δt, $\Delta\mathbf{r}$, N, and in some cases more.

We make two notes.

Parameter Δt can be absent in some versions of MFS which donŠt use the principle of the splitting. In this case these are two parameters Δr, N. Any numerical error of value obtained by the DSMC method has obviously two parts. First is statistical error and second is deterministic error connected with finiteness of the quantities Δt, Δr, N.

We assume that statistical error is enough suppressed, i.e. sample size is big enough and deterministic error is leader.

PARAMETRIC CORRECTION FOR DSMC METHOD

In the further consideration we shall not concretize numerical scheme of the DSMC method, but we shall use properties which have all numerical schemes of the DSMC method.

There are parameters of the DSMC method Δt, Δr, N (or Δr, N in case MFS). Calculated values have sensitivity from change of these parameters which we shall call basic parameters.

Naturally that the given statement of the question is general and hence requires general approach for its solution. On our opinion adequate method for solving this problem is parametric correction method which is widely known in deterministic numerical methods.

We use this method.

In applications of the DSMC method concrete values parameters Δt, $\Delta \mathbf{r}$, N are chosen that changes of calculated values are weakly (in perfectly donŠt change) [1]. It means analytical dependence of calculated values from these parameters. Starting from that we write a calculated value up to first order on Δt, $\Delta \mathbf{r}$, $1/N$ ($1/N$ is taken for convenience) :

$$F(\Delta t, \Delta \mathbf{r}, 1/N) = F_0 + A_1 \cdot \Delta t + A_2 \cdot \Delta \mathbf{r} + A_3 \cdot 1/N + O(\text{second order on basic parameters}) \tag{1}$$

Were F_0 is limit value F, i.e. value at $\Delta t = 0$, $\Delta \mathbf{r} = 0$, $N = \infty$. Coefficients A_1, A_2, A_3 describe sensitivity of $F()$ from Δt, $\Delta \mathbf{r}, N$ correspondingly.

From the formula (1) follows that if we have four results of calculations for value $F()$ at different magnitudes Δt, $\Delta \mathbf{r}, N$ then we can find values F_0, A_1, A_2, A_3.

In practical situation we usually interest magnitude F_0. We can obtain this value using two values of F, but choosing parameters of the DSMC method is coordinated, that is we shall change basic parameters Δt, $\Delta \mathbf{r}$, $1/N$ as follows $\alpha \Delta t$, $\alpha \Delta \mathbf{r}$, α/N (naturally, α it is necessary to take such that N/α is an integer) . Really, put in formula (1) the coordinated values of parameters, i.e. if $\alpha \neq 1$ we have

$$F_1(\Delta t, \Delta \mathbf{r}, 1/N) = F_0 + A_1 \cdot \Delta t + A_2 \cdot \Delta \mathbf{r} + A_3 \cdot 1/N + O(\text{second order on basic parameters});$$

$$F_2(\alpha \cdot \Delta t, \alpha \cdot \Delta \mathbf{r}, \alpha \cdot 1/N) = F_0 + A_1 \alpha \cdot \Delta t + A_2 \cdot \alpha \cdot \Delta \mathbf{r} + A_3 \cdot \alpha \cdot 1/N + O(\text{second order on basic parameters}),$$

from which

$$F_0 = (F_2 - \alpha \cdot F_1)/(1-\alpha) + O(\text{second order on basic parameters}). \tag{2}$$

Magnitude F_0 has numerical accuracy up to second order on parameters $\Delta t, \Delta \mathbf{r}, 1/N$.

In case statistical errors are suppressed considerably it has meaning to make three calculations of value F at various magnitudes coordinating parameter α. Then, as it is easy to check up, it is possible to receive the third order of accuracy on basic parameters. The given circumstance is connected by that terms of identical order in Taylor series for F represent homogeneous polynomials from basic parameters. Formula of F_0 is follows

$$F_0 = \frac{\alpha\beta}{\beta-\alpha}\left[\frac{F_2 - \alpha^2 \cdot F_1)}{\alpha(1-\alpha)} - \frac{F_3 - \beta^2 \cdot F_1)}{\beta(1-\beta)}\right] + O(\text{third order on basic parameters}). \tag{3}$$

where F_2 corresponds to magnitude of coordinating parameter equals α and F_3 corresponds to magnitude of coordinating parameter equals β.

NUMERICAL RESULTS

Below results of calculations for a classical problem of heat transfer between two parallel plates are present. Model of molecules was hard spheres and Knudsen number was 0.1. Calculations of the profiles of temperature between two plates by the DSMC method are shown in Figures 1-3. The ratio of the plate temperatures was equal to 4. For recalculation the formula (2) with $\alpha = 0.5$ was used.

Distinction in behavior of the temperature structures after recalculation on Figure 1 and Figure 2 is explained by influence of number particles finiteness. In the first case accuracy of a recalculated curve has the order $(\frac{1}{20})^2$, while in the second case has $(\frac{1}{75})^2$. In Figure 4 the behavior in time of 10-th moment of speed for a problem of a homogeneous gas relaxation with the Bobylev initial conditions for maxwellian molecules is shown. The results show an opportunity of increase of accuracy of calculations at use of formulas for recalculation (2), (3).

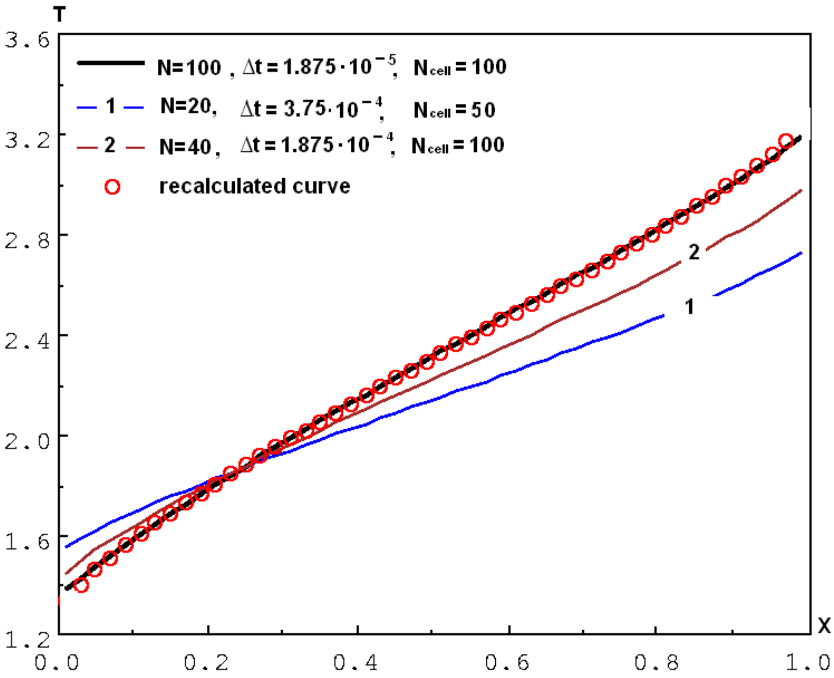

FIGURE 1.

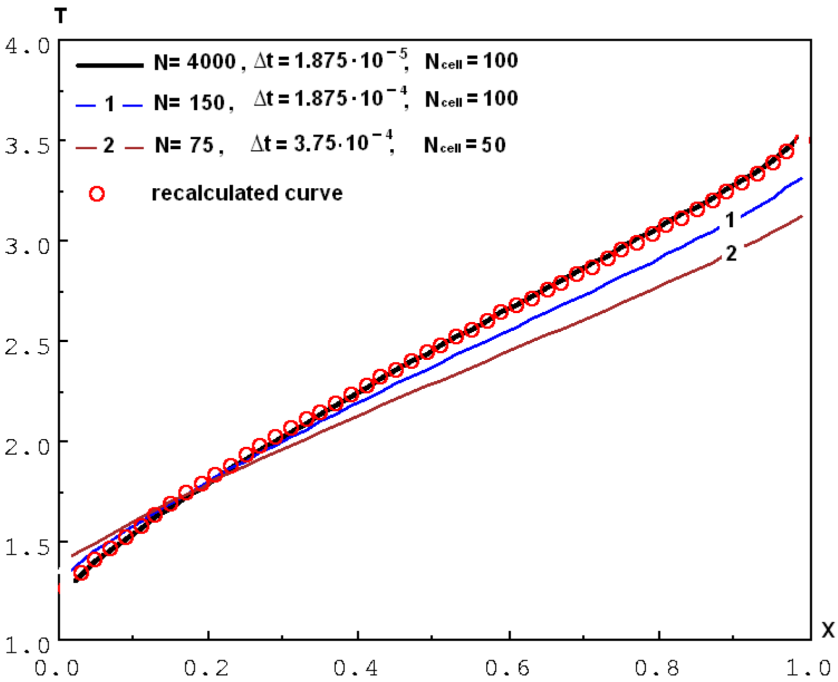

FIGURE 2.

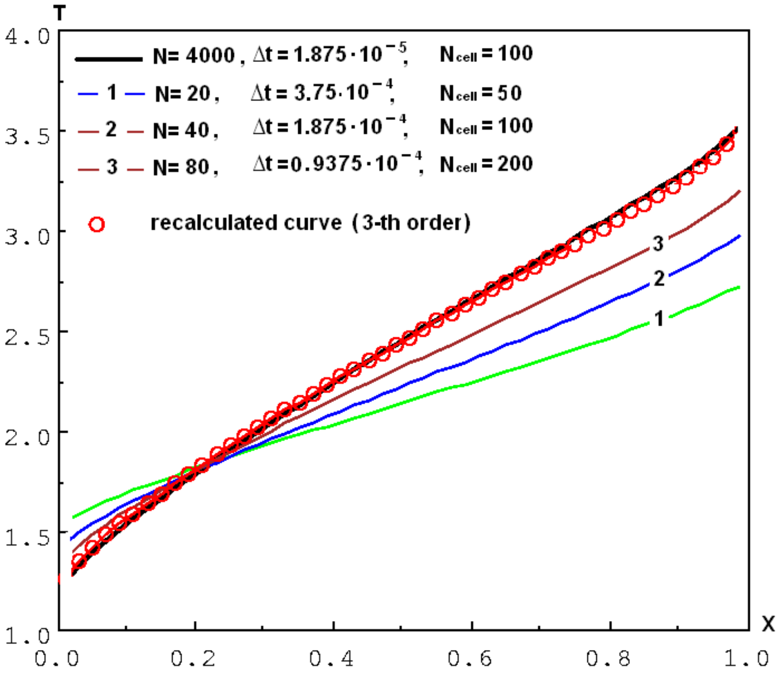

FIGURE 3.

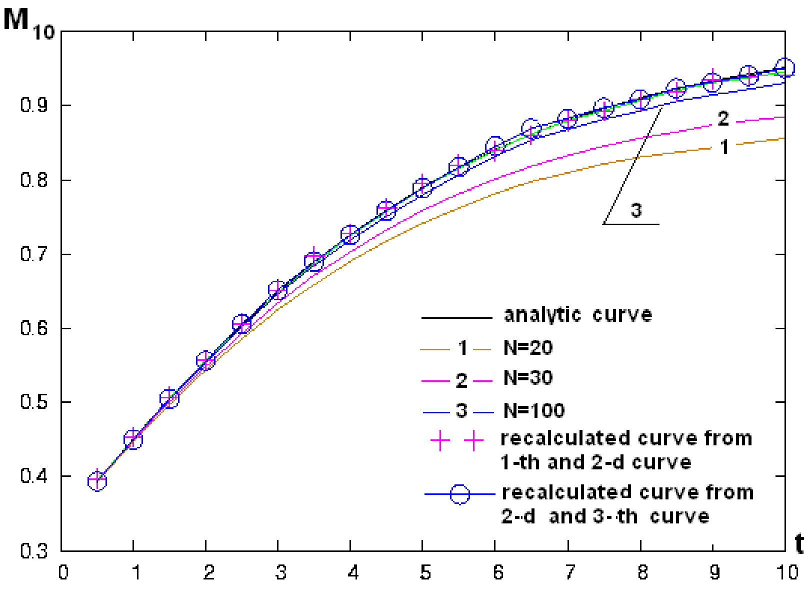

FIGURE 4.

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