

Analysis of Numerical Errors in the DSMC Method

D. A. Fedosov*, S. V. Rogasinsky†, M. I. Zeifman*, M. S. Ivanov**,
A. A. Alexeenko* and D. A. Levin*

**Department of Aerospace Engineering, Pennsylvania State University, State College, PA 16802, USA*

†*Laboratory of Stochastic Problems of Mathematical Physics, Institute of Computational Mathematics and
Mathematical Geophysics, 630090 Novosibirsk, Russia*

***Computational Aerodynamics Laboratory, Institute of Theoretical and Applied Mechanics, 630090
Novosibirsk, Russia*

Abstract. The direct simulation Monte Carlo (DSMC) method is one of the most popular numerical methods used to model rarefied gas environment flows. In order to predict the accuracy of a solution obtained by the DSMC method we have to be able to estimate its accuracy. In the work presented here we have developed a technique to estimate the numerical accuracy of the DSMC method. This paper presents a derivation of expressions of the variance of the DSMC estimators of number density and translational temperature, and the corresponding comparison with the empirical variance. A discussion of the deterministic numerical errors corresponding to typical DSMC parameters such as the time step, cell volume, and total number of simulated particles is given. Moreover, a comparison of two different DSMC schemes, No Time Counter (NTC) and Majorant Frequency (MF), is made.

INTRODUCTION

The direct simulation Monte Carlo (DSMC) method [1] has been developed gradually over the past three decades and has gained a large popularity and proven its reliability over that time. The DSMC method is a tool used to solve the Boltzmann equation numerically and is based on the direct statistical simulation of molecular processes described by kinetic theory. This method is traditionally considered a computer simulation of the behavior of a great number of particles, and because of its simplicity it can be used for a large range of applications. The flexibility of the method allows a user to implement different models for various processes such as binary elastic collisions of particles, multi-component mixtures, chemical reactions, and energy partition and relaxation. Moreover, the DSMC method conveniently allows us to deal with problems involving different boundary conditions and complex geometries.

As a numerical and stochastic method, DSMC has statistical and numerical errors, which have to be quantified to verify the accuracy of the obtained solution. Two types of error arise in this method: i) a statistical error which corresponds to the stochastic nature of the method, and ii) a deterministic error which depends on the selection of numerical parameters such as the time step Δt , cell volume ΔV , and the total number of simulated particles N . One has to be able to separate those errors in order to understand their influences on the flow results. A numerical testing was performed using No Time Counter (NTC) [1] and Majorant Frequency (MF) [2] schemes.

First, let us consider errors due to the stochastic nature of the DSMC method. The solution of the DSMC method for the macroparameters of a flow is obtained by averaging of particle properties over a number of time steps N_t . The source of the statistical errors is the process of taking a sample average in a finite volume. The errors have an asymptotic behavior and vanish when the sample size goes to infinity. Thus, these errors are inversely proportional to the sample size, and therefore they can be decreased by increasing of the sample size, i. e. number of particles in a computational domain or number of time steps used in the sample. Usually we can assume that the variance of a computed property X is independent of the sample size, and therefore this parameter has a statistical error

$$|X_{computed} - X_{true}| \leq 3 \cdot \sqrt{\frac{\sigma_X^2}{N_s}}, \quad (1)$$

where $\sigma_X^2 = E\{X^2\} - E^2\{X\}$ is the variance (dispersion) of X , $E\{X\}$ denotes the mean (expectation) of X , and N_s is

the sample size. Equation (1) is the so-called three-sigma rule [3]. All definitions and notations from statistics can be found in [3, 4, 5]. Thus, by estimation of the variance, σ_X^2 , one can make an error prediction for a given sample size.

Secondly, we consider errors that occur because the numerical parameters cannot be taken as infinitesimally small. These errors are not statistical in nature, and therefore cannot be reduced by use of a large sample size. The correct choice of these parameters guarantees that the numerical solution is in fact a solution of the Boltzmann equation. The method parameters Δt and ΔV should be chosen small enough compared to the characteristic time and length of the flow which are physical characteristics of the specific flow. In fact, this type of error may have a greater impact on the results than the statistical error, especially when a large sample size is used, and stochastic errors can be neglected.

NUMERICAL ERROR ANALYSIS

Statistical errors

The numerical errors corresponding to the stochastic nature of the DSMC method can be characterized by the variance of numerical results. Here, we will carry out the analysis of variance for the translational temperature and number density for the case of a flow with zero mean velocity and simple monocomponent gas. To make the analysis simpler we will consider that the total number of simulated particles N in the computational domain is constant. The further analysis will be done for the flow macroparameters estimated in a some fixed cell ΔV .

Let us introduce notations

$$\zeta_k = \sum_{i=1}^{N_k} \overline{v_i^2}, \quad \xi_k = N_k, \quad k = 1, \dots, N_t,$$

where index k represents a time step, N_k is the number of particles presented in a cell ΔV at k -th time step, and $\overline{v_i}$ are velocities of particles in the cell. The statistical estimators for the calculation of translational temperature and number density in a fixed cell ΔV used in the DSMC method are

$$\hat{T} = C_T \cdot \frac{\sum_{i=1}^{N_t} \zeta_i}{\sum_{i=1}^{N_t} \xi_i}, \quad (2)$$

$$\hat{n} = C_n \cdot \frac{1}{N_t} \sum_{i=1}^{N_t} \xi_i, \quad (3)$$

where $C_T = \frac{m}{3k}$, m - molecular mass, k - Boltzmann constant, and $C_n = \frac{Fnum}{|\Delta V|}$, $Fnum$ - a number of real molecules represented by one simulated particle, $|\Delta V|$ - volume of the cell. It is well known from general Monte Carlo theory [5] that the statistical estimator of the form given in Eq. (2) is asymptotically unbiased [4, 5], i. e.

$$\hat{T} = C_T \cdot \frac{\sum_{i=1}^{N_t} \zeta_i}{\sum_{i=1}^{N_t} \xi_i} \rightarrow C_T \cdot \frac{E\{\zeta\}}{E\{\xi\}} = \overline{T} \quad as \quad N_t \rightarrow \infty,$$

and its variance has the following asymptotical form

$$\sigma_{\hat{T}}^2 = C_T^2 \cdot \frac{\sigma_{11} - 2\sigma_{12} \cdot (\overline{T}/C_T) + \sigma_{22} \cdot (\overline{T}/C_T)^2}{(\overline{N_k})^2}, \quad (4)$$

where $\sigma_{11} = E\{\zeta^2\} - E^2\{\zeta\}$, $\sigma_{12} = E\{\zeta\xi\} - E\{\zeta\} \cdot E\{\xi\}$, $\sigma_{22} = E\{\xi^2\} - E^2\{\xi\}$, and $\overline{N_k} = E\{\xi\}$. In other words Eq. (4) takes into account a two-term Taylor expansion for the estimator in Eq. (2). The variance of the estimator given in Eq. (3) can be calculated by $\sigma_{\hat{n}}^2 = C_n^2 (E\{\xi^2\} - E^2\{\xi\}) = C_n^2 \sigma_{22}$.

If we know the variance of temperature and number density, the statistical errors can be estimated using the three-sigma rule

$$|\hat{T} - T_{true}| \leq 3 \cdot \sqrt{\frac{\sigma_{\hat{T}}^2}{N_t}}, \quad |\hat{n} - n_{true}| \leq 3 \cdot \sqrt{\frac{\sigma_{\hat{n}}^2}{N_t}}. \quad (5)$$

The expressions for the variances of translational temperature and number density can be extended to the case of multiple species mixture, and non-zero flow velocity. However, these expressions become very cumbersome.

To simplify the variance expressions we use the molecular chaos approximation [6] and assume smallness of the method parameters, in particular $\Delta V \rightarrow 0$ and $N^{-1} \rightarrow 0$. For these assumptions all covariations from different variables vanish. The expression for the temperature calculated at a given time step k in a cell is

$$\hat{T} = \frac{m}{3k} \cdot \frac{v_{x_1}^2 + v_{y_1}^2 + v_{z_1}^2 + \dots + v_{x_{N_k}}^2 + v_{y_{N_k}}^2 + v_{z_{N_k}}^2}{N_k} \equiv C_T \cdot \frac{X}{Y}, \quad (6)$$

where N_k is the number of particles present in the cell during the k -th time step. If we express Eq. (6) in a Taylor series about the means of X , Y , and assume molecular chaos approximation, we obtain simple expression for the temperature variance

$$\sigma_{\hat{T}}^2 = C_T^2 \left(\frac{\sigma_X^2}{\mu_Y^2} + \sigma_Y^2 \frac{\mu_X^2}{\mu_Y^4} \right),$$

where $\mu_X = E\{X\}$ and $\mu_Y = E\{Y\}$. The number of particles N_k in the cell has a Poisson distribution, and therefore $E[Y] = \mu_Y = \bar{N}_k$ and $\sigma_Y^2 = \bar{N}_k$. All v_{x,y,z_k} , $k = 1, \dots, N_t$ have a local Maxwellian distribution which in this case is a normal distribution with zero mean, and variance σ^2 . It is known from probability theory [4] that v_{x,y,z_k}^2 will have a chi-squared distribution with one degree of freedom, the mean σ^2 and variance $2\sigma^2$. Thus, we obtain the following expressions:

$$Err(\hat{T}) = 3 \cdot \sqrt{\frac{\sigma_{\hat{T}}^2}{N_t}}, \quad \frac{\sigma_{\hat{T}}}{\hat{T}} = C_1 \sqrt{\frac{Fnum}{|\Delta V| \cdot \hat{n}}} = \frac{C_1}{\bar{N}_k}, \quad (7)$$

$$Err(\hat{n}) = 3 \cdot \sqrt{\frac{\sigma_{\hat{n}}^2}{N_t}}, \quad \frac{\sigma_{\hat{n}}}{\hat{n}} = C_2 \sqrt{\frac{Fnum}{|\Delta V| \cdot \hat{n}}} = \frac{C_2}{\bar{N}_k}, \quad (8)$$

where $C_1 = \sqrt{\frac{2}{3}}$, and $C_2 = 1$.

The variance of the translational temperature can be also calculated empirically in the DSMC calculation. The temperature estimated over M_s time steps is

$$T_{M_s} = \frac{m}{3 \cdot k} \frac{\sum_{k=1}^{M_s} \sum_{i=1}^{N_k} (v_{x_i}^2 + v_{y_i}^2 + v_{z_i}^2)}{\sum_{k=1}^{M_s} N_k},$$

and one obtains L of such temperatures. Then, the empirical variance of the temperature series is calculated as $\sigma_{T_{M_s}}^2 = E\{T_{M_s}^2\} - E^2\{T_{M_s}\}$, which represents the variance of temperature computed over M_s time steps. Thus, the error of temperature for one time step normalized by $\bar{T}_{M_s} = E\{T_{M_s}\}$ is $Err(T_{M_s}) = 3 \cdot \frac{\sqrt{\sigma_{T_{M_s}}^2 \cdot M_s}}{\sqrt{L \cdot \bar{T}_{M_s}}}$. However, the estimation of this error is very expensive numerically, and will be used only for the comparison.

Deterministic errors

Numerical errors due to the finite values of the DSMC method parameters play an important role when the sample size N_s is large enough such that statistical errors become small compared to deterministic errors. Assuming that the parameters Δt , ΔV , and N^{-1} are small, the estimated flow macroparameter A in each cell can be approximated as a linear function (neglecting cross terms and higher order terms) of these parameters as,

$$A(\Delta t, \Delta V, N^{-1}) = A_0 + A_1 \cdot \Delta t + A_2 \cdot |\Delta V| + A_3 \cdot N^{-1}, \quad (9)$$

where coefficients A_0, A_1, A_2, A_3 are functions of the cell location in the computational grid. In particular, A_0 stands for the exact solution, and the rest of the terms in Eq. (9) represent the deviation of A from the exact solution. By varying each of the method parameters, one can study the dependence of the flow solution on these parameters.

RESULTS OF NUMERICAL CALCULATIONS

The main goals of the numerical calculations were *four*. The first goal was the verification of Eq. (4) for the temperature variance by comparison with the variance of T_{M_s} calculated empirically. The second was the test of Eqs. (7) and (8) which are based on molecular chaos approximation and local Maxwellian distribution by comparison with the variance in Eq. (4). The third goal was the numerical investigation of the linear dependence on the method parameters Δt , ΔV , and N^{-1} by applying linear approximation Eq. (9). Finally we compared the NTC and MF schemes for the case of a different total number of simulated particles.

The heat transfer problem between two parallel plates was selected as the testing problem. The distance between the plates is 1 m, the initial number density and temperature of a nitrogen gas is $n_0 = 1.0 \times 10^{20} \text{ m}^{-3}$ and $T_0 = 300 \text{ K}$. The temperature of the left and right plates are $T_l = 300 \text{ K}$ and $T_r = 500 \text{ K}$, respectively. The system has a zero flow velocity and corresponds to a Knudsen number of 0.013. The basic numerical calculation has been made for the specific values Δt_0 , ΔV_0 , and N_0 , which were chosen according to the typical DSMC requirements [1]. The magnitudes of the parameters used here were $\Delta t_0 = 10^{-5} \text{ sec}$, $\Delta V_0 = 0.005 \text{ m}^3$, and $N_0 = 1000$ particles.

Two different DSMC codes were used for these calculations, a newly developed one-dimensional java code, and the two-dimensional SMILE code [2]. The java code has only one layer of cells along the x axis, thus the cell size ΔV is equal to the cell length Δx , and particles are able to move either to the left or right neighboring cell. The total number of cells for the $\Delta x_0 = 0.005 \text{ m}^3$ was 200. The computational domain for the calculations using the SMILE code had the form of a closed box with 200 horizontal cells, and 50 vertical cell layers. The left and right walls assumed diffuse reflection, and a unit energy accommodation coefficient. The upper and lower walls assumed specular reflection and a zero energy accommodation coefficient. Thus, the conditions for the 2-D system give an approximation for 1-D calculations.

Figure 1 shows the square root of temperature variance for the test problem normalized by the cell local temperature using the 1-D java code. The first four curves represent the variance estimated empirically for different sample sizes M_s . As one can see the variance increases as the sample size increases. This shows that the variance appears to be dependent on the sample size, and Eq. (1) fails in this case. The thick solid line gives the variance estimated by Eq. (4), and the dash-dot line by Eq. (7). Both expressions give results much lower than the variation calculated empirically, and they are very close to each other. Figure 2 shows the analogous calculations using the 2-D SMILE code. The variance calculated empirically in this case does not increase as in Fig. 1, and therefore the Eq. (1) appears to be valid, and the variance can be considered as sample size independent. The only difference between the calculations is the computational domain. In the 2-D case there are 50 vertical layers of cells. When, it was checked if this two codes would give equivalent results by setting the domain for the 2-D case to have only one vertical layer of cells, the result was found to be in good agreement with the 1-D java calculations. Also, the empirical variance in Fig. 2 does not depend on the chosen vertical layer, and is very close to the prediction (thick solid line) of Eq. (4). Thus, the large difference in the 1-D code prediction is due to the domain structure. By using several vertical layers of cells in the 2-D case the domain structure dependence disappears, because particles are able to penetrate from one layer to another. Moreover, the approximate Eq. (4) agrees well with the empirical result.

Other observation is that the maximum variance is in the middle of the domain instead of expected region close to the hot wall. For example in the 2-D calculations the maximum of the variance is close to the hot wall. The reason of this is that the collisions of particles with the walls are performed using diffuse reflection, which is equivalent to the loss of all previous correlations in particle's moving history. This fact reduces the dependence of variance from domain structure. To check this idea the calculation of the problem with the same temperature on the walls, but different wall reflections, specular and diffuse, was made using the 1-D code. Figure 3 shows the result of the calculation. As it is was expected for specular wall reflection we have the maximum variation at the wall regions, in contrast to diffusion wall reflection case. However, Eqs. (4) and (7) does not take into account this domain structure dependence.

To verify Eq. (9) we tested the linear dependence of the calculated macroparameters on the method parameters. The sample size was chosen large enough to keep statistical errors of the results about one per cent in order to estimate deterministic errors. The main calculation is made using Δt_0 , Δx_0 , N_0 values, and assumed to be an exact solution. Figures 4 and 5 show the temperature and number density profiles for different time step Δt . In this case Eq. (9) is reduced to $T = T_0 + A_1 \cdot \Delta t$. With increase of time step discrepancy becomes larger comparing to the solution with Δt_0 . The "squares" curve represents the linear combination of $8\Delta t_0$ and $16\Delta t_0$ results in order to obtain new Δt_0 solution. This line is in a good agreement with the main result. Figures 6 and 7 show the temperature and number density profiles for different total number of simulated particles. The behavior of the solutions is qualitatively close as for the time step varying. Moreover, the linear combination lies very close to the main solution. These facts prove that a finite value of Δt , ΔV , and N is the source of the error which is different from statistical error. Applying Eq. (9) we are able

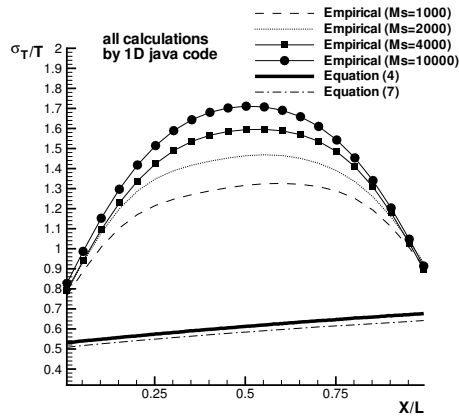


FIGURE 1. Comparison of temperature variations calculated empirically and by Eqs. (3) and (7) using 1D java code.

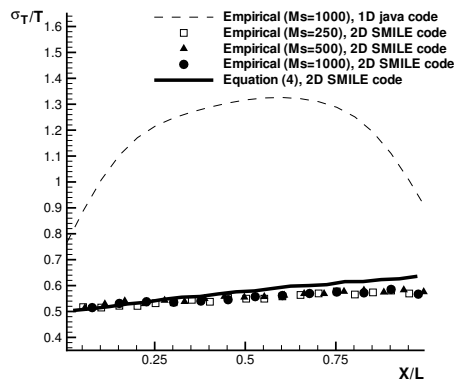


FIGURE 2. Comparison of temperature variations calculated empirically and by Eq. (3) using 2D SMILE code.

to get rid of the error corresponding to the first terms in Taylor series.

The analogous calculations were performed using NTC method. The comparison of these two methods gives a close behavior of results. However, when the average number of particles per cell is order of 1 or less, it was noticed a different behavior of temperature for MF and NTC methods. This result is presented in Fig. 8. MF method gives less discrepancy than NTC method due to a different structure of the methods.

ACKNOWLEDGMENTS

The research performed at the Pennsylvania State University was supported by the Air Force Office of Scientific Research Grant No. F49620-02-1-0104 administered by Dr. Mitat Birkan and the Army Research Office Grant No. DAAD19-02-1-0196 administered by Dr. David Mann.

REFERENCES

1. G. A. Bird. *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. Clarendon Press, Oxford, 1994.
2. M. S. Ivanov and S. V. Rogasinsky. Analysis of numerical techniques of the Direct Simulation Monte Carlo method in the rarefied gas dynamics. *Sov. J. Numer. Anal. Math. Modeling*, Vol. 3, No. 6, 1988, pp. 453-465.
3. Y. A. Shreider. *Method of Statistical Testing, Monte Carlo Method*. Elsevier Publishing Company, Amsterdam - London - New York, 1964.
4. E. Parzen. *Modern Probability Theory and Its Applications*. John Wiley & Sons, Inc., New York - London, 1960.
5. S. M. Ermakov and G. A. Mikhailov. *Statistical modeling*. Nauka, Moscow, 1982, (Russian).
6. M. Kac. *Probability and Related Topics in Physical Sciences*. Interscience Publishers, London - New York, 1959.

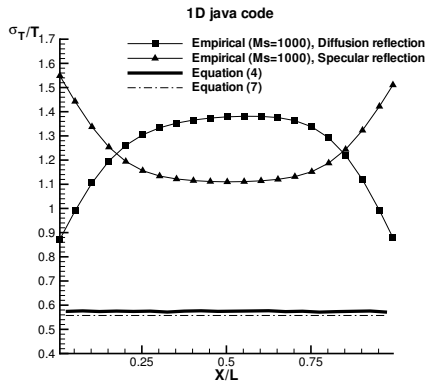


FIGURE 3. Check of wall reflection influence on the temperature variation.

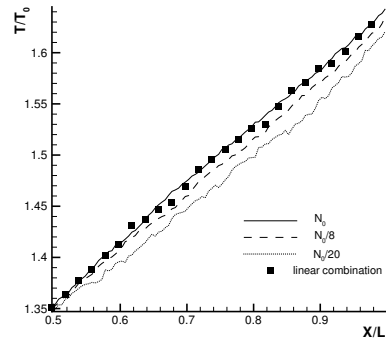


FIGURE 6. Temperature calculated using different total number of simulated particles.

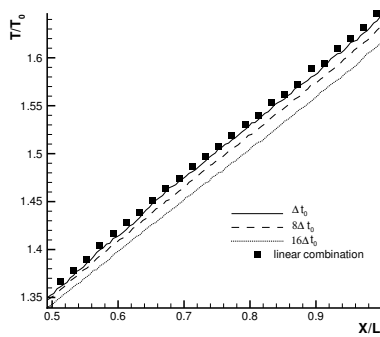


FIGURE 4. Temperature calculated using different time steps.

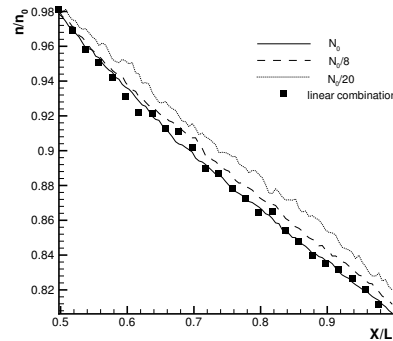


FIGURE 7. Number density calculated using different total number of simulated particles.

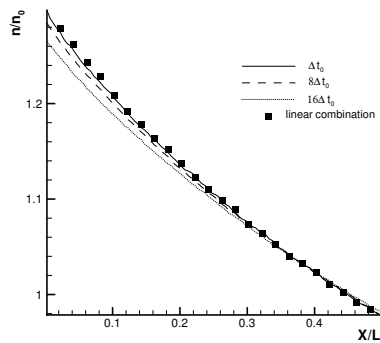


FIGURE 5. Number density calculated using different time steps.

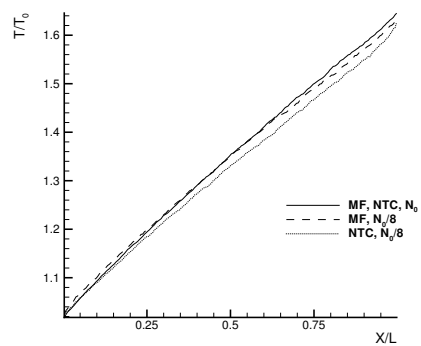


FIGURE 8. Comparison of MF and NTC schemes.