

Reconsideration of the majorant collisional frequency schemes for the DSMC method

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Keywords: DSMC method, statistical error, variance

PACS: 02.70.Uu, 02.60.-x, 02.70.-c

INTRODUCTION

It may be currently considered that a new independent CFD direction (computational rarefied gas dynamics) has been formed. The leading role here belongs to the Direct Simulation Monte Carlo (DSMC) method [1]. The DSMC method is traditionally considered as a method of computer simulation of the rarefied gas flow as a set of a great number of model molecules with binary collisions. Usually the number of simulated molecules is large enough ($\sim 10^5 - 10^7$), but this is extremely small in comparison with the number of molecules that would be present in the real gas flow. Each simulated molecule is then regarded as representing an appropriate number (F_{num}) of actual molecules. The conventional treatment of the DSMC method is based on the principle of splitting of continuous motion and collisions of molecules within a small time step Δt into two consecutive stages: free-molecular transfer and uniform collisional relaxation at the time interval Δt .

Another approach to constructing numerical schemes for the DSMC method, based on the principle of the majorant collision frequency (MCF), was proposed in [2, 3, 4, 5]. These schemes were derived on the basis of the probability interpretation of the integral form of the master kinetic equation (Kac equation in the spatially uniform case and Leontovich equation in the spatially nonuniform case) for N -particle distribution function. The statistical estimate of gas dynamic parameters used in both uniform and nonuniform cases were proved there to be unbiased. In their nature, the MCF schemes obtained are "time-accurate," i.e., the principle of splitting was not used in their construction. These schemes without splitting, the so-called "splitless" MCF schemes, were applied for the first time in [5] for solving the problem of the shock-wave structure. Though the computational efficiency of these schemes depends linearly on the number of simulated particles, they are more CPU-expensive than the schemes that involve the splitting principle (NCT, NTC). Therefore, approximate MCF schemes based on the splitting principle were constructed in [3]. The main advantage of these schemes is the correct reproduction of the collision frequency with a small number (close to unity) of model particles in a collisional cell. More than 15-years experience of application of these MCF schemes with splitting for various problems of rarefied gas dynamics confirmed their high efficiency in solving multidimensional problems of high-altitude aerodynamics.

An important problem that arises in DSMC modeling is the evaluation of the numerical accuracy of the results obtained, and how far they are from the solution of the Boltzmann equation. This question is especially important for the near-continuum flows. One of the most important issues here is the analysis of solution convergence in terms of the timestep. Normally, this analysis reduces to performing a series of computations with decreasing Δt . For a near-continuum regime, the computations are often conducted using all available computer resources, and no additional accuracy-establishing computations are possible in this case. The use of splitless MCF schemes allows avoiding these difficulties and obtaining results containing no errors due to time discretization. The present paper describes the main stages of constructing splitless MCF schemes and gives examples of their combined application with MCF schemes with time splitting.

MAJORANT COLLISION FREQUENCY SCHEMES

DSMC computations always employ a finite system of model particles; hence, the n -particle master kinetic equation can be naturally used to construct modeling schemes. Our consideration is based on the master kinetic equation, for which the transition to the Boltzmann equation was examined in detail in [6]. Such an approach allows one to estimate the adequacy of modeling results to the solution of the Boltzmann equation.

The regularized master kinetic equation [3] is presented in the form

$$\frac{\partial}{\partial t} f_N + \sum_{i=1}^N \mathbf{v}_i \frac{\partial}{\partial \mathbf{r}_i} f_N = \sum_{i < j} \int \{f'_N - f_N\} \tilde{w}(\mathbf{v}'_i, \mathbf{v}'_j \rightarrow \mathbf{v}_i, \mathbf{v}_j | \mathbf{r}_i, \mathbf{r}_j, \rho) d\mathbf{v}'_i d\mathbf{v}'_j \quad (1)$$

Here $f_N = f_N(t, \mathbf{R}, \mathbf{C})$, $f'_N = f(t, \mathbf{R}, \mathbf{C}'_{ij})$ are the N -particle distribution functions; $\int f_N(t, \mathbf{R}, \mathbf{C}) d\mathbf{C} d\mathbf{R} = 1$; $(\mathbf{R}, \mathbf{C}) = (\mathbf{r}_1, \mathbf{v}_1, \dots, \mathbf{r}_N, \mathbf{v}_N)$, $(\mathbf{R}, \mathbf{C}'_{ij}) = (\mathbf{r}_1, \mathbf{v}_1, \dots, \mathbf{r}_i, \mathbf{v}'_i, \dots, \mathbf{r}_j, \mathbf{v}'_j, \dots, \mathbf{r}_N, \mathbf{v}_N)$ are the $6N$ -dimensional vectors of coordinates and particle velocities; $(\mathbf{v}'_i, \mathbf{v}'_j)$ and $(\mathbf{v}_i, \mathbf{v}_j)$ are the velocities of a pair of particles before and after their collision; $\tilde{w}(\mathbf{v}'_i, \mathbf{v}'_j \rightarrow \mathbf{v}_i, \mathbf{v}_j | \mathbf{r}_i, \mathbf{r}_j, \rho)$ is the probability density of the transition of the colliding pair (i, j) from the state $(\mathbf{v}'_i, \mathbf{v}'_j)$ to the state $(\mathbf{v}_i, \mathbf{v}_j)$ with fixed values of the coordinates $(\mathbf{r}_i, \mathbf{r}_j)$; ρ is a regularization parameter. We also have

$$\tilde{w}(\mathbf{v}'_i, \mathbf{v}'_j \rightarrow \mathbf{v}_i, \mathbf{v}_j | \mathbf{r}_i, \mathbf{r}_j, \rho) \rightarrow w(\mathbf{v}'_i, \mathbf{v}'_j \rightarrow \mathbf{v}_i, \mathbf{v}_j) \delta(\mathbf{r}_i - \mathbf{r}_j) \text{ when } \rho \rightarrow 0,$$

$$w(\mathbf{v}_i, \mathbf{v}_j \rightarrow \mathbf{v}'_i, \mathbf{v}'_j) d\mathbf{v}'_i d\mathbf{v}'_j = g_{ij} b_{ij} db_{ij} d\epsilon_{ij} = g_{ij} \sigma(g_{ij}, \chi_{ij}) \sin \chi_{ij} d\chi_{ij} d\epsilon_{ij},$$

$$\int w(\mathbf{v}_i, \mathbf{v}_j \rightarrow \mathbf{v}'_i, \mathbf{v}'_j) d\mathbf{v}'_i d\mathbf{v}'_j = g_{ij} \sigma_i(g_{ij}),$$

where b_{ij} and ϵ_{ij} are the collision parameters and χ_{ij} is the angle of deviation of the relative velocity after the collision. Then the total collision frequency is

$$\nu(\mathbf{R}, \mathbf{C}) = \sum_{i < j} h(\mathbf{r}_i, \mathbf{r}_j) \int w(\mathbf{v}_i, \mathbf{v}_j \rightarrow \mathbf{v}'_i, \mathbf{v}'_j) d\mathbf{v}'_i d\mathbf{v}'_j = \sum_{i < j} h(\mathbf{r}_i, \mathbf{r}_j) g_{ij} \sigma_i(g_{ij}).$$

It should be noted that the direct evaluation of $\nu(\mathbf{R}, \mathbf{C})$ would require a computational effort proportional to N^2 . This is very costly in terms of computational resources. To overcome this difficulty, a method for constructing numerical schemes of the DSMC method based on the majorant collision frequency was proposed in [3], which allowed the computational effort to grow linearly with N .

In constructing the Monte Carlo schemes on the basis of the majorant frequency principle [5], we transform Eq. (1) to the form

$$\begin{aligned} \frac{\partial}{\partial t} f_N + \sum_{i=1}^N \mathbf{v}_i \frac{\partial}{\partial \mathbf{r}_i} f_N + \nu_m f_N = \sum_{i < j} \int f'_N \{ \tilde{w}(\mathbf{v}'_i, \mathbf{v}'_j \rightarrow \mathbf{v}_i, \mathbf{v}_j | \mathbf{r}_i, \mathbf{r}_j, \rho) + \\ + ([v_{ij}]_m - v_{ij}(g_{ij} | \mathbf{r}_i, \mathbf{r}_j, \rho)) \delta(\mathbf{v}_i - \mathbf{v}'_i) \delta(\mathbf{v}_j - \mathbf{v}'_j) \} d\mathbf{v}'_i d\mathbf{v}'_j, \end{aligned} \quad (2)$$

where $v_{ij}(g_{ij} | \mathbf{r}_i, \mathbf{r}_j, \rho) = \int \tilde{w}(\mathbf{v}_i, \mathbf{v}_j \rightarrow \mathbf{v}'_i, \mathbf{v}'_j | \mathbf{r}_i, \mathbf{r}_j, \rho) d\mathbf{v}'_i d\mathbf{v}'_j$; $[v_{ij}]_m = \max_{g_{ij}, \mathbf{r}_i, \mathbf{r}_j} \{v_{ij}(g_{ij} | \mathbf{r}_i, \mathbf{r}_j, \rho)\}$, $\nu_m = \frac{N(N-1)}{2} [v_{ij}]_m$ is majorant collision frequency.

Equation (2) with the initial and boundary conditions can be presented as an integral equation. Then, as it follows from the general theory of Monte Carlo methods, the probabilistic treatment of the kernel and the free term of this equation yields the process of DSMC modeling. To avoid too many details of secondary importance, let us trace all considerations as applied to a particular case of a spatially inhomogeneous Cauchy problem for Eq. (1). All principal issues of modeling of particle collisions and transfer are retained. In the general case of the initial-boundary problem, modeling of collisions with the body surface and fluxes of particles entering the computational domain does not suffer any significant changes. Modeling of these processes was studied in detail in [3] and is naturally included into the scheme of the DSMC method for Eq. (2).

The integral equation for the collision density $\varphi(t, \mathbf{R}, \mathbf{C}) = \nu_m f_N(t, \mathbf{R}, \mathbf{C})$ has the form

$$\varphi(t, \mathbf{R}, \mathbf{C}) = \int_0^t dt' \int d\mathbf{R}' d\mathbf{C}' K_{123}(t', \mathbf{R}', \mathbf{C}' \rightarrow t, \mathbf{R}, \mathbf{C}) \varphi(t', \mathbf{R}', \mathbf{C}') + \varphi_0(t, \mathbf{R}, \mathbf{C}), \quad (3)$$

where $K_{123}(t', \mathbf{R}', \mathbf{C}' \rightarrow t, \mathbf{R}, \mathbf{C}) = K_1(\mathbf{C}' \rightarrow \mathbf{C} | \mathbf{R}') K_2(t' \rightarrow t | \mathbf{R}', \mathbf{C}) K_3(\mathbf{R} \rightarrow \mathbf{R} | \mathbf{C}, t)$, and

$$K_1(\mathbf{C}' \rightarrow \mathbf{C} | \mathbf{R}') = \sum_{i < j}^N \frac{2}{N(N-1)} \left\{ \frac{v_{ij}(\mathbf{v}'_i, \mathbf{v}'_j | \mathbf{r}'_i, \mathbf{r}'_j, \rho)}{[v_{ij}]_m} \frac{\tilde{w}(\mathbf{v}'_i, \mathbf{v}'_j \rightarrow \mathbf{v}_i, \mathbf{v}_j | \mathbf{r}'_i, \mathbf{r}'_j, \rho)}{v_{ij}(\mathbf{v}'_i, \mathbf{v}'_j | \mathbf{r}'_i, \mathbf{r}'_j, \rho)} + \right.$$

$$+ \left(1 - \frac{v_{ij}(\mathbf{v}'_i, \mathbf{v}'_j | \mathbf{r}'_i, \mathbf{r}'_j, \rho)}{[v_{ij}]_m} \right) \delta(\mathbf{v}_i - \mathbf{v}'_i) \delta(\mathbf{v}_j - \mathbf{v}'_j) \left\{ \prod_{k=1, k \neq i, j}^N \delta(\mathbf{v}_k - \mathbf{v}'_k) \right\}, \quad (4)$$

$$K_2(t' \rightarrow t | \mathbf{R}', \mathbf{C}) = v_m \exp\{-v_m(t - t')\}, \quad (5)$$

$$K_3(\mathbf{R}' \rightarrow \mathbf{R} | \mathbf{C}, t) = \delta(\mathbf{R} - \mathbf{R}' - \mathbf{C}(t - t')), \quad (6)$$

$$\varphi_0(t, \mathbf{R}, \mathbf{C}) = \int f_N(0, \mathbf{R}', \mathbf{C}) v_m \exp\{-v_m t\} K_3(\mathbf{R}' \rightarrow \mathbf{R} | t, \mathbf{C}).$$

The probabilistic interpretation of the integral form of the master kinetic equation (3) with kernels (4)-(6) allows us to formulate a new scheme of DSMC modeling of a spatially inhomogeneous rarefied gas flow: a splitless MCF scheme [3, 4, 5]. We present this scheme for the general case, where the computational domain is bounded by the external surface Γ and by the body surface γ . We assume that the surface Γ is subjected to the steady conditions

$$f_1(\mathbf{r}_\Gamma, \mathbf{v}) = f_1^0(\mathbf{r}_\Gamma, \mathbf{v}), \quad (\mathbf{v}, \mathbf{n}_\Gamma) < 0, \quad \mathbf{r}_\Gamma \in \Gamma;$$

$$q^+(\mathbf{r}_\Gamma, \mathbf{v}) = |(\mathbf{v}, \mathbf{n}_\Gamma)| f_1^0(\mathbf{r}_\Gamma, \mathbf{v});$$

$$q^+(\mathbf{r}_\Gamma) = \int q^+(\mathbf{r}_\Gamma, \mathbf{v}) d\mathbf{v}, \quad v_\Gamma = \int \int q^+(\mathbf{r}_s, \mathbf{v}) d\mathbf{v} ds_\Gamma,$$

and the body surface γ is subjected to the condition

$$|(\mathbf{v}, \mathbf{n}_\gamma)| f_1(t, \mathbf{r}_\gamma, \mathbf{v}) = \int_{(\mathbf{v}', \mathbf{n}_\gamma) < 0} |(\mathbf{v}', \mathbf{n}_\gamma)| f_1(t, \mathbf{r}_\gamma, \mathbf{v}') \tilde{T}_\gamma(\mathbf{v}' \rightarrow \mathbf{v}) d\mathbf{v}'; \quad \int \tilde{T}_\gamma(\mathbf{v} \rightarrow \mathbf{v}') d\mathbf{v}' = 1; \quad \mathbf{r}_\gamma \in \gamma.$$

Here \mathbf{n}_Γ and \mathbf{n}_γ are the outward normals to the surfaces Γ and γ , respectively, at the points \mathbf{r}_Γ and \mathbf{r}_γ . The particle entry into the computational domain and interaction of particles with the body are modeled in a manner similar to that used in [1].

Thus, the general scheme of the DSMC method for a spatially inhomogeneous rarefied gas flow, based on the majorant frequency principle, can be presented as follows.

0. In accordance with the initial distribution $f_N(0, \mathbf{R}, \mathbf{C})$, the coordinates \mathbf{r}_i and velocities \mathbf{v}_i of particles for a given trajectory of the random process are sampled.

1. The time of the next transition in the system, caused either by intermolecular collisions or by generation of a new particle on the surface Γ , is sampled with a probability density $v_m^\Gamma \exp\{-v_m^\Gamma \tau\}$. Here $v_m^\Gamma = v_\Gamma + v_m$ and $v_m = \frac{N_n(N_n-1)}{2} [v_{ij}]_m$. All particles are transferred in accordance with the time $\tau_{\min} = \min\{\tau_\gamma, \tau\}$, where τ_γ is the time of the first intersection of the body surface after the time t_n . If $t_{n+1} = t_n + \tau_{\min} > T$ ($[0, T]$ is the time interval where the evolution of the N -particle model of the gas is considered), this trajectory is terminated, and one should go back to Step 0.

If the particles leave the computational domain owing to their displacement, then we have $N_{n+1} = N_n - \Delta N^-$, where ΔN^- is the number of particles left; otherwise $N_{n+1} = N_n$ and $\mathbf{R}_{n+1}(N_{n+1}) = \mathbf{R}_n(N_{n+1}) + \tau_{\min} \mathbf{C}_{n+1}(N_{n+1})$.

If $\tau_{\min} = \tau_\gamma$, one should go to Step 2; otherwise to Step 3

$\{t_{n+1}, N_{n+1}, \mathbf{R}_{n+1}(N_{n+1}), \mathbf{C}_{n+1}(N_{n+1})\}$, $n = 0, 1, 2, \dots$ 2. In the case of a collision with the body, the velocity of the reflected particle is sampled in accordance with the boundary transform \tilde{T}_γ , and one should go to Step 1.

3. A collision of a pair of particles occurs with a probability v_m/v_m^Γ (Step 3.1), and a new particle is generated with an additional probability (Step 3.2).

3.1. The collision occurs in accordance with the kernel $K_1(\mathbf{C}_{n+1} \rightarrow \mathbf{C}_{n+2} | \mathbf{R}_{n+1})$:

3.1.1) Pairs (i, j) are uniformly chosen among N_{n+1} particles;

3.1.2) with a probability $1 - \frac{v_{ij}(\mathbf{R}_{n+1}, \mathbf{C}_{n+1})}{[v_{ij}]_m}$ there occurs a dummy collision, i.e., the particle velocities remain unchanged, and one should go to Step 1 $\{t_{n+1}, N_{n+1}, \mathbf{R}_{n+1}(N_{n+1}), \mathbf{C}_{n+2}(N_{n+1})\}$, $n = 0, 1, 2, \dots$;

3.1.3) with a probability $v_{ij}(\mathbf{R}_{n+1}, \mathbf{C}_{n+1})/[v_{ij}]_m$, there occurs a real collision.

The direction of the relative velocity vector after the collision is sampled with a probability density $\sigma(g_{ij}, \mathbf{e})/\sigma_i(g_{ij})$, and the velocities of the particles i, j are replaced by $\mathbf{v}_i = \frac{1}{2}(\mathbf{v}'_i + \mathbf{v}'_j) + \frac{1}{2}g'_{ij}\mathbf{e}$; $\mathbf{v}_j = \frac{1}{2}(\mathbf{v}'_i + \mathbf{v}'_j) - \frac{1}{2}g'_{ij}\mathbf{e}$; $g'_{ij} = |\mathbf{v}'_i - \mathbf{v}'_j|$.

Then one should go to Step 1: $\{t_{n+1}, N_{n+1}, \mathbf{R}_{n+1}(N_{n+1}), \mathbf{C}_{n+2}(N_{n+1})\}$, $n = 0, 1, 2, \dots$;

3.2 The coordinates of the new particle are sampled with a probability density $q^+(\mathbf{r}_\Gamma)/v_\Gamma$ and velocity with a probability density $q^+(\mathbf{r}_\Gamma, \mathbf{v})/q^+(\mathbf{r}_\Gamma)$. Number of particles $N_{n+2} = N_{n+1} + 1$. Then one should go to Step 1: $\{t_{n+1}, N_{n+2}, \mathbf{R}_{n+1}(N_{n+2}), \mathbf{C}_{n+2}(N_{n+2})\}$, $n = 0, 1, 2, \dots$;

Cyclic repetition of Steps 1-3 yields one trajectory of a random process on a time interval $[0, T]$. To determine the gas flow parameters, one should use L trajectories and standard estimates of the DSMC method.

Let us consider particular methods of regularization of the collision integral in Eq. (1). The structure of kernels (4)-(6) of the integral equation (3) remains unchanged for all types of regularization of the collision integral. Its particular form affects only the kernel $K_1(\mathbf{C}' \rightarrow \mathbf{C} | \mathbf{R}')$ responsible for particle collisions in the system. The global modeling

scheme for a particular type of regularization requires an additional description only on Step 3.1 to allow for the relative spatial positions of the colliding particles. Applying the regularization conventionally used for the Boltzmann equation, we obtain

$$\tilde{w}(\mathbf{v}'_i, \mathbf{v}'_j \rightarrow \mathbf{v}_i, \mathbf{v}_j | \mathbf{r}'_i, \mathbf{r}'_j, \rho) = h(\mathbf{r}_i, \mathbf{r}_j) w(\mathbf{v}'_i, \mathbf{v}'_j \rightarrow \mathbf{v}_i, \mathbf{v}_j)$$

where $h(\mathbf{r}_i, \mathbf{r}_j) = \sigma_0^{-1}$ if $|\mathbf{r}_i - \mathbf{r}_j| < \rho$ and 0 if $|\mathbf{r}_i - \mathbf{r}_j| > \rho$; $\sigma_0 = \frac{4}{3}\pi\rho^3$. The parameter ρ determines the size of the "region of particle interaction." We will call such regularization the free cell regularization.

In the case of regularization corresponding to decomposition of the computational domain into non-intersecting cells d_k , ($k = 1, \dots, M$); $\sum_{k=1}^M d_k = V_0$, the so-called cell regularization, collisions occur between particles that belong to one cell. In this case,

$$\tilde{w}(\mathbf{v}'_i, \mathbf{v}'_j \rightarrow \mathbf{v}_i, \mathbf{v}_j | \mathbf{r}'_i, \mathbf{r}'_j, \rho) = \left\{ \sum_{k=1}^M h_k(\mathbf{r}_i) h_k(\mathbf{r}_j) d_k^{-1} \right\} w(\mathbf{v}'_i, \mathbf{v}'_j \rightarrow \mathbf{v}_i, \mathbf{v}_j).$$

Three numerical schemes of the DSMC method implementing the above-mentioned types of regularization were developed in [5]. The first two schemes (free cell and cell schemes) do not use sorting of particles over the cells, and the computation efficiency is increased by using a special organization of the computational process (the so-called delayed transfer of particles). The third scheme (cell scheme) involves sorting of particles over the cells, which leads to a significant decrease in the majorant frequency of collisions and, hence, to substantial improvement of computational efficiency. It was the third scheme that was used in computations described below.

COMPUTATIONAL EXAMPLES

Some examples computed with the use of the splitless MCF scheme are described below and compared with data obtained by the MCF scheme with time splitting (for brevity, the latter scheme will be further called the MCF scheme or the split MCF scheme).

The first example was a one-dimensional Couette flow between two infinite parallel plates with a distance D from each other. One of the plates moves with respect to the other plate with a constant velocity v (the velocity vector lies in the plane of the plate). Both plates have an identical temperature T_w , and the law of diffuse reflection of molecules with full accommodation of energy is defined on the surface. Molecules are assumed to interact as hard spheres. In such a formulation, the problem of the Couette flow depends on two dimensionless parameters: Knudsen number $Kn = \lambda/D$, where λ is the mean free path, and speed ratio $s = v/\sqrt{2RT_w}$. In the study described, the values of these parameters were $Kn=0.1$ and $s = 10$.

The DSMC results are plotted in Figs. 1 and 2. The computations involved 50 collisional cells and 10,000 model particles. The curves in the figures refer to $\Delta t=0.16$ (1), $\Delta t=0.04$ (2), $\Delta t=0.004$ (3), $\Delta t=0.0004$ (4), and splitless MCF scheme (5). All curves except for curve 5 show the results obtained by the MCF scheme with splitting, using different time steps nondimensionalized by the mean collisional time τ_λ . All values of Δt used were smaller than the residence time (mean time needed for the particle to cross the cell). Thus, the formal constraints on the time step in the DSMC method were satisfied even for the greatest value of Δt .

All the presented gas-dynamic parameters were non-dimensionalized as follows: temperature $T' = T/T_w$, stress-tensor components $p'_{xx} = p_{xx}/(\rho_0 c^2)$, $p'_{xy} = p_{xy}/(\rho_0 c^2)$, and heat-flux vector components $S'_x = S_x/(\rho c^3)$, $S'_y = S_y/(\rho c^3)$, where $c = \sqrt{2RT_w}$.

The left part of Fig. 1 shows the temperature profiles. The temperature is seen to comparatively weakly depend on the time step and to coincide, almost in all cases, with the splitless MCF result. The heat-flux profiles S'_x in the right part of Fig. 1 are more sensitive to the value of Δt . For a large time step (curve 1), the difference in the heat flux obtained by the MCF and splitless MCF schemes can reach 20%. This difference tends to zero with decreasing time step.

The most sensitive indicators of the error due to a finite time step are the stress-tensor components plotted in Fig. 2. For high values of Δt , the values of P_{xx} and P_{xy} (curves 1 and 2) are no longer constant in terms of x , which is qualitatively incorrect. It is only after a significant decrease in Δt that the distributions of the stress-tensor components become constant and approach the result obtained by the splitless MCF scheme.

A comparison of CPU costs for split/splitless schemes reveals the advantages of the split scheme: even with the minimum time step, the split scheme is several times faster than the splitless scheme. Nevertheless, if we take into account that a series of computations is needed to verify the convergence of the numerical solution in terms of Δt , the use of the splitless scheme is preferable in the one-dimensional case. In two-dimensional and three-dimensional

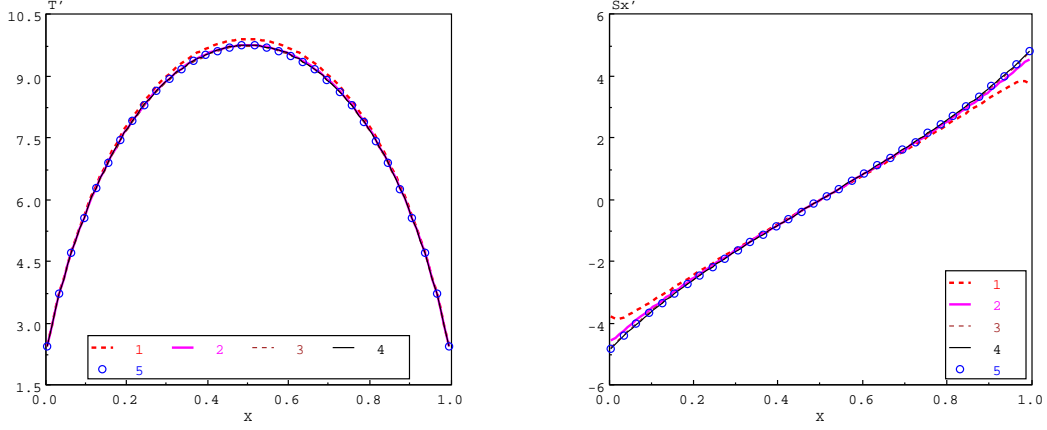


FIGURE 1. Temperature and heat flux.

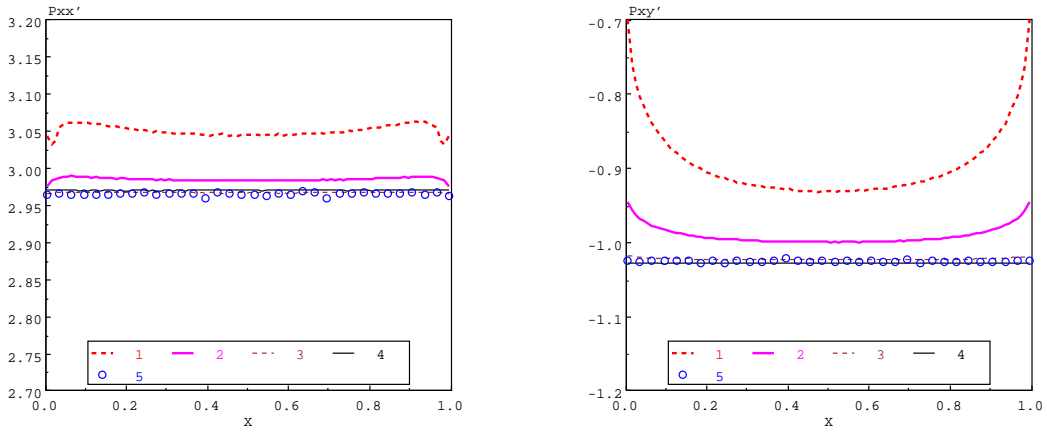


FIGURE 2. Stress-tensor components.

cases, straightforward application of the splitless scheme is too CPU-expensive. Thus, a combined use of the split and splitless schemes is implied. The flow is first computed by the conventional MCF scheme until a steady state was reached, and then the splitless MCF scheme is used. Such an approach allows obtaining a numerical solution independent of Δt with reasonable CPU-costs.

This approach was demonstrated by considering a two-dimensional argon flow around a cylinder with a diameter $d = 0.3048$ m. The flow had the following parameters: Mach number $M=10$, Knudsen number $Kn=0.25$ (based on the cylinder diameter), and free-stream temperature 200 K. The cylinder temperature was 500 K, and the law of diffuse reflection was set on the cylinder surface.

A series of computations was performed with the split scheme with a decreasing time step. The maximum time step was chosen to be 0.2 of the mean collisional time in the free stream. Below, the time steps are normalized to their maximum value. As it could be expected, the distribution of the pressure coefficient over the cylinder surface is almost independent of the time step, whereas the distributions of the friction coefficient (Fig. 3, left part) and heat-transfer coefficient (Fig. 3, right part) are extremely sensitive to the value of Δt . The maximum difference is 20% for the friction coefficient and 15% for the heat-transfer coefficient. This fact confirms that it is necessary to perform a series of computations with different time steps to verify their convergence. The results obtained by the above-described approach with a combined use of the split/splitless MCF schemes are also plotted in these figures (the solution with $\Delta t = 1/2$ was used as the initial data for splitless computations). The fields of temperature, which is one of the most sensitive parameters to the time step, are shown in Fig. 4 for the splitless computation and for the computation with the minimum time step. Though there are some differences observed far from the cylinder, the results in the vicinity of the stagnation point, i.e., in the zone of strong gradients, are identical. The computed results presented here illustrate

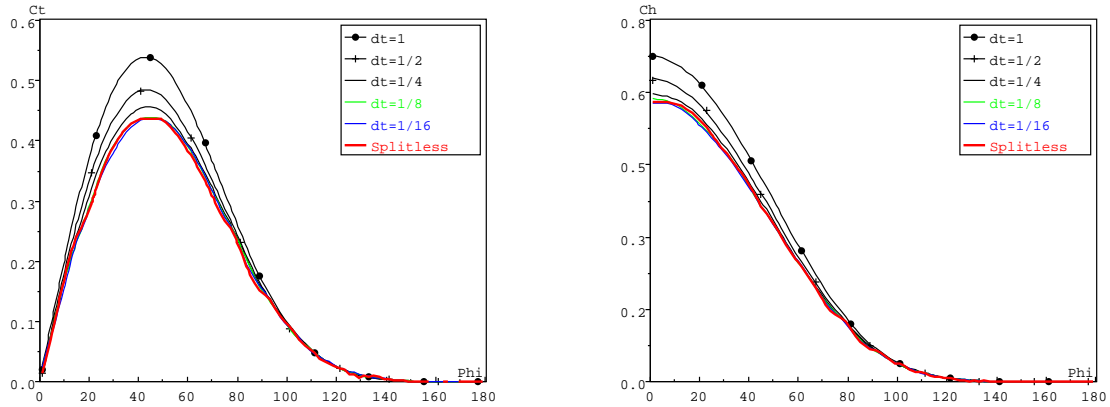


FIGURE 3. Skin-friction and heat-transfer coefficients.

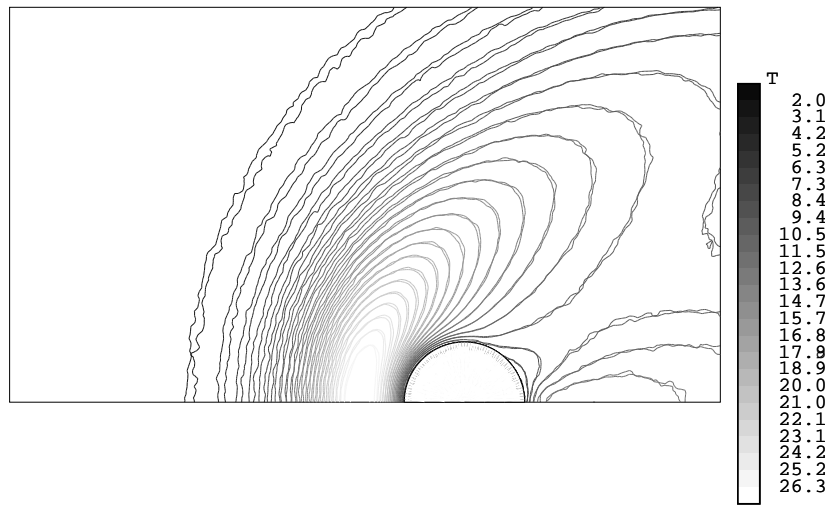


FIGURE 4. Translational temperature.

the feasibility of the combined use of the split/splitless MCF schemes, which allows one to avoid the procedure of verification of the convergence in terms of Δt in the analysis of the accuracy of DSMC simulations.

Acknowledgments. The present work was supported by the Russian Foundation for Basic Research (Project Nos. 06-08-00687 and 06-01-22000) and by the International Science and Technology Center (Project No. 3151). This support is gratefully acknowledged.

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