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ABSTRACT

In this paper, the basic ideas underlying the Direct Simulation Monte Carlo (DSMC) method are examined and a novel nonhomogeneous N-particle kinetic equation describing the randomized mathematical model of DSMC is derived. It is shown that different collision-partner selection schemes, including No-Time-Counter (NTC) and Bernoulli-trials schemes, are approximations of the general transition operator of the randomized model. The popular collision-partner selection schemes, represented by the standard NTC and Bernoulli-trials approximations of the general transition operator, represented by Simplified Bernoulli-trials and Generalized Bernoulli-trials schemes, are tested on the one-dimensional rarefied gas heat transfer problem against conditions of two approximation limits: first, leading to the Boltzmann equation and, second, leading to the novel N-particle kinetic one.

I. INTRODUCTION

The Direct Simulation Monte Carlo (DSMC) method was introduced by Bird[1] in the beginning of 1960s as a particle-based Monte Carlo technique for numerical simulation of molecular gas dynamics. Within the next several decades, the method gained a great popularity as a stable and confident numerical approach opened to applications in wide area ranged from the classical rarefied gas dynamics to the recently developing gaseous microfluidics. In spite of its great success and remarkable agreement with experiments, its deep essence was not well understood and a lot of theoretical work was done and still is ongoing to find a theoretical background of the DSMC method in the form of mathematical models and equations. Bird was always interested in finding relations between the DSMC and the Boltzmann equation.[2,3] In the course of time, it has been revealed that the DSMC was closely relevant to the kinetic Boltzmann equation under given conditions and could be considered as a numerical method for its resolution. As a result of the theoretical investigations, a number of different Monte Carlo schemes and modifications of the collision procedure (the more complicated part) of the DSMC method were developed and most popular among them became Bird's No time Counter (NTC)[4] and Nearest Neighbor (NN),[5] Ivanov and Rogasinsky's Majorant Collision Frequency (MCF),[6] and Koura's Null Collision (NC)[7] schemes because of their efficiency and linear algorithmic complexity (i.e., performance scaling) with respect to the number of particles per grid cell. A more comprehensive consideration of these collision schemes can be found in the work of Roohi and Stefanov.[8] All of them determine an estimation of a maximum number of randomly selected pairs of particles for each cell of the computational grid, which are checked for collision within a time step by using the Monte Carlo acceptance-rejection method. This procedure is closely related to the famous Boltzmann "*Stoßzahlansatz*" statement playing a crucial role in the Boltzmann equation derivation. Furthermore, in 1992, Wagner[9] published a rigorous mathematical proof of asymptotical convergence of the DSMC solution under certain conditions to the Boltzmann equation (BE) one for a number of particles (simulators) tending to infinity. Nanbu[10] suggested an alternative of the above collision schemes derived directly from the BE, in which the changes in particle velocities are independent events during each time step with algorithmic complexity $O(N^2)$. Later, Babovsky[11] proposed a modification with linear scaling $O(N)$. The convergence proof to the full Boltzmann equation of the latter was given by Babovsky and Illner.[12] Both Wagner' and Babovsky's convergence proofs are built on an analogous assumption that the vicinity of each point of any considered domain is occupied by a

large number of particles tending to infinity. These are solid arguments one to insist that the DSMC is a numerical method for solving the Boltzmann equation.

However, in real DSMC applications, one faces some basic issues, which cannot be easily ignored. The first issue concerns the number of particles (simulators) used in a simulation. The fact is that the DSMC calculations are performed with a limited total number of particles restricted to the available computational resources and a requirement for a reasonable computational time. From the successful application practice of numerous numerical simulations, it was found that the contemporary sophisticated DSMC method with collision schemes such as NTC, MCF, and NN requires more than 10 (often 20–30) particles per cell (PPC) to get reliable estimations of macroscopic variables corresponding to the solution of the Boltzmann solution. Nowadays, this requirement is not a problem for simple one-dimensional (1D) or two-dimensional (2D) simulations, but it is a problem for two-dimensional (2D) and three-dimensional (3D) simulations of nonequilibrium gas flow problems requiring very fine grids and subgrids where the actual average number of particles can go down to 1–2 particles per cell/subcell or even less. Good examples are the DSMC studies of flow instability[13–15] and transition to turbulence[16,17] in a rarefied gas at a low Knudsen number. A similar situation arises also in strong nonequilibrium complex gas flows with shock waves or large temperature gradients. Under these circumstances, the use of parallel and Graphics Processing Unit (GPU) DSMC algorithms and powerful computers within massive memory storage allowing a large enough number of particles in cells can help overcome the resource constraints in many cases but cannot resolve in general the problem with the particle number demands and cannot avoid some essential issues arising using the method with a small number of particles in grid cells. If that obtained by the DSMC result with a large number of particles per cell is considered as a solution of the Boltzmann equation, the deviations from it in simulations with a small number of particles should be considered as systematic errors of the method with respect to the BE solution. In the present paper, the conceivable sources of errors are analyzed and ways for eliminating them are discussed.

A second key issue concerns the origin of the stochastic process linked to the DSMC algorithm for an arbitrary number of particles per cell. A deeper insight reveals details, which suggest that in the general case the DSMC algorithm is consistent with a stochastic model that only asymptotically converges to the BE solution. The main point here refers to the obvious circumstance that in the DSMC algorithm a requirement for "*molecular chaos*" (statistical independency of molecular velocities) is not stated within the binary collision process and the statistical independency of postcollision velocities of the collided particles can be achieved only if their precollision velocities are uncorrelated. Thus, the presumption for the existence of "*molecular chaos*" embodied in the Boltzmann equation is not generally met in the collision process released by the method. This is supported by some DSMC calculations[4,18–20] illustrating the applicability of the method for obtaining correct numerical estimations of fluctuations and correlations of macroscopic variables. On the other hand, it is known that the imposed in the Boltzmann equation statistical independency of molecular velocities a priori excludes the consideration of macroscopic fluctuations and correlations. Precisely speaking, as pointed out by Cercignani,[21] the linearized Boltzmann equation can be used for calculation of density fluctuations but only in case small perturbations (with Gaussian distribution) are imposed in the initial state and the evolution of the solution is averaged over the whole set of solutions starting from different initial states. Only then, the linearization ensures linear functionality in time and space between the correlation functions of macroscopic variables and the corresponding set of one-particle distribution functions. Summarizing the remarks above, one must conclude that the mathematical model that fully described the DSMC algorithm for an arbitrary finite number of particles per cell should be a stochastic model without a general requirement for local "*molecular chaos*" that asymptotically approaches the statistical independency of molecular velocities under certain conditions and converges to the BE solution for a large particle number $N \to \infty$. Thus, the stochastic model would avoid the above assumptions, leading to the use of a large number of particles per cell. It was found out that in the spatially homogeneous state the stochastic Kac master equation[22] satisfies the above requirements. The first construction of a computational algorithm corresponding to the Kac equation was developed by Denisik *et al.*[23] for Monte Carlo simulation of homogeneous nonequilibrium gas relaxation. The proposed algorithm following the exact Markov stochastic process of the Kac model was cumbersome and inefficient with algorithmic complexity $O(N^3)$. Belotserkovskii and Yanitskii[24] extended the application of the Kac model to the spatially inhomogeneous case and proposed the Bernoulli-trials (BT) scheme with a number of selected pairs checked for collision equal to $N_{sel} = N(N-1)/2$ with computational effort proportional to $O(N^2)$. The BT scheme was derived as a first order approximation of the Kac stochastic model for simulation of the collision step of the splitting algorithm. Furthermore, Yanitskii in a sequence of papers[25,26] has developed a general approach for construction of stochastic collision models on the basis of the Kac master equation and suggested the "Ballot-Box" (BB) collision scheme with $N_{sel} = 1$ and linear algorithmic complexity $O(N)$, which, however, required a very small time step. Following Yanitskiiz's approach, Stefanov[27–29] has proposed a simplified version of the Bernoulli trials, called Simplified Bernoulli-trials (SBT) with $N_{sel} = N - 1$ and algorithmic complexity $O(N)$comparable with the NTC one. A detailed description of the derivation of the set of Bernoulli trials schemes is given in the review paper of Roohi and Stefanov.[8] Furthermore, Roohi and Stefanov[30] have presented a Generalized Bernoulli-trials scheme using an arbitrary number of selected pairs $N - 1 > N_{sel} \geq 1$ and complexity $O(N)$. The above remarks concern the Kac model with a fixed number of particles in the system. Implementing a Bernoulli-trials scheme in the general DSMC algorithm, one should take into account that the method includes two steps—ballistic motion of all particles in the computational domain and collisions of particles in cells and, respectively, the number of particles is not fixed any more. In cells of the grid, it varies randomly during the simulation. To account for this circumstance, one should consider a randomized Kac model with a number of particles that varies in time according to some probability distribution. A number of numerical simulations[8,27,31–36] have revealed a new distinct feature of the randomized Kac model and its approximations—the BT and SBT collision schemes. If in a computational domain covered with a coarse grid the system with a large number of particles in cells fulfills asymptotically the properties of a Boltzmann gas ("*molecular chaos*" and Boltzmann collision frequency), the randomized Kac stochastic model keeps these

properties as well in the cells of a finer or transient adaptive subcell (TAS) grid covering the domain with an arbitrary small number of particles in the cells when the total number of particles in the domain remains large enough.

In this study, the main basic concepts and numerical schemes built in the DSMC are considered in the light of the above commented issues. By using the basic concepts, a novel nonhomogeneous N-particle kinetic equation governing the evolution of the DSMC solution is obtained. Its local three-dimensional character in physical space and 3N-dimensions in velocity space requires introduction of a randomized model of particle sets in cells of the mesh covering the computational domain. It has been found that the randomized model asymptotically approximated the Boltzmann equation properties under specific conditions. The sources of systematic errors in both groups of schemes are considered with respect to the conditions of two approximation limits: first, leading to the Boltzmann equation and, second, leading to the novel N-particle kinetic one. Some theoretical arguments, numerical examples, and comparisons complete the analysis. The main part of the theoretical background of the BT and SBT has been given in the review paper.[8] In this paper, the author gives the derivation of the novel N-particle kinetic equation governing the evolution of DSMC solution along with additional arguments and proofs with regard to its asymptotic approach to the Boltzmann equation. For brevity and simplicity of the explanations, the author avoids involving mathematical rigor usually required in mathematical proofs assuming that the mathematical definitions and conditions, where needed, are fulfilled without accounting for them explicitly.

II. RELATIONSHIP BETWEEN DSMC STOCHASTIC MODEL AND KINETIC EQUATIONS

As stated originally by its creator, Bird,[2] the DSMC is a particle-based method that uses a finite set of N model particles (simulators) denoted by their positions $\mathbb{R} = \{\mathbf{r}_1, \ldots, \mathbf{r}_i, \ldots, \mathbf{r}_j, \ldots, \mathbf{r}_N\}$ and velocities $\mathbb{C} = \{\mathbf{c}_1, \ldots, \mathbf{c}_i, \ldots, \mathbf{c}_j, \ldots, \mathbf{c}_N\}$ that move and collide in physical space domain $D(\mathbf{r})$ to perform a direct simulation of the molecular gas dynamics. Binary intermolecular collisions as well as interactions with boundaries $\partial D(\mathbf{r})$ are modeled using a stochastic approach, and this distinguishes the DSMC technique from the molecular dynamics method. In general, a detailed description of such an arbitrary N-particle system is based on the Liouville equation for N-particle probability distribution density $F_N = F_N(t, \mathbb{R}, \mathbb{C})$ that in the case of no external force acting on the molecules takes the form[37]

$$\frac{\partial F_N}{\partial t} + \sum_{i=1}^{N} \mathbf{c}_i \frac{\partial F_N}{\partial \mathbf{r}_i} - \sum_{1 \le i < j \le N} \Phi_{i,j} F_N = 0, \tag{1}$$

where $\Phi_{i,j}$ is the binary molecular interaction operator that reads

$$\Phi_{i,j} = \frac{1}{m}\left(\frac{\partial \pi_{i,j}}{\partial \mathbf{r}_i}\frac{\partial}{\partial \mathbf{c}_i} + \frac{\partial \pi_{i,j}}{\partial \mathbf{r}_j}\frac{\partial}{\partial \mathbf{c}_j}\right). \tag{2}$$

Particles are molecules assumed as force centers with masses m, with $\pi_{i,j}$ denoted the binary potential of molecular interaction between particle pair (i, j). The function F_N is normalized to give $\int F_N \prod_{i=1}^{N} d\mathbf{r}_i d\mathbf{c}_i = 1$. A general way to derive the Boltzmann equation from the Liouville equation (1) is to use the reduced distribution function

$$F_s(t, \mathbf{r}_1, \ldots, \mathbf{r}_s, \mathbf{c}_1, \ldots, \mathbf{c}_s) = \int F_N(t, \mathbb{R}, \mathbb{C}) \prod_{i=s+1}^{N} d\mathbf{r}_i d\mathbf{c}_i \tag{3}$$

to obtain a system of equations

$$\frac{\partial F_s}{\partial t} + \sum_{i=1}^{N} \mathbf{c}_i \frac{\partial F_s}{\partial \mathbf{r}_i} - (N-s)\sum_{i=1}^{s} \int \Phi_{i,s+1} F_{s+1} d\mathbf{r}_{s+1} d\mathbf{c}_{s+1} = 0, \quad s = 1, \ldots, N-1 \tag{4}$$

known as the Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY)-hierarchy of equations. For $s = 1$, under Boltzmann-Grad limit conditions ($N \to \infty$, $d_{12} \to 0$, Nd_{12}^2– bounded) and the Boltzmann assumption of "*molecular chaos*"

$$F_2(t, \mathbf{r}_1, \mathbf{r}_2, \mathbf{c}_1, \mathbf{c}_2) = F_1(t, \mathbf{r}, \mathbf{c}_1) F_1(t, \mathbf{r}, \mathbf{c}_2) \tag{5}$$

after some mathematical transformations,[21] Eq. (4) adopts the form of the Boltzmann equation,

$$\frac{\partial f(t, \mathbf{r}, \mathbf{c}_1)}{\partial t} + \mathbf{c} \cdot \frac{\partial f(t, \mathbf{r}, \mathbf{c}_1)}{\partial \mathbf{r}} = \int \left(f(t, \mathbf{r}, \mathbf{c}_1') f(t, \mathbf{r}, \mathbf{c}_2') - f(t, \mathbf{r}, \mathbf{c}_1) f(t, \mathbf{r}, \mathbf{c}_2) \right) |\mathbf{g} \cdot \mathbf{n}_{12}| d\mathbf{n}_{12} d\mathbf{c}_2, \tag{6}$$

where $|\mathbf{r}_1 - \mathbf{r}_2| = d_{12} \to 0$ leads to $\mathbf{r}_1 \to \mathbf{r}$, $\mathbf{r}_2 \to \mathbf{r}$ (for hard spheres the collision cross section is equal to d^2), $\mathbf{g} = \mathbf{c}_1 - \mathbf{c}_2$ is the relative velocity between two particles, and $\mathbf{n}_{12}$ is the outer normal of the sphere $|\mathbf{r}_1 - \mathbf{r}_2| = d_{12}$. The relation $|\mathbf{g}_{12} \cdot \mathbf{n}_{12}| d\mathbf{n}_{12} = \Phi_{12}(g, \theta) d\theta d\varepsilon$ is assumed for a short range binary interaction potential with central symmetry. Here, the Boltzmann velocity distribution function f is related to the single-particle probability distribution function as $f(t, \mathbf{r}, \mathbf{c}) = NF_1(t, \mathbf{r}, \mathbf{c})$. The postcollision velocities $\mathbf{c}_1', \mathbf{c}_2'$ are equal to[21,38]

$$\mathbf{c}_1' = \mathbf{c}_1 - \mathbf{n}_{12}(\mathbf{g}_{12} \cdot \mathbf{n}_{12}), \quad \mathbf{c}_2' = \mathbf{c}_2 + \mathbf{n}_{12}(\mathbf{g}_{12} \cdot \mathbf{n}_{12}). \tag{7}$$

The following form of the Boltzmann equation[38] contains the local collision frequency explicitly:

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \frac{\partial f}{\partial \mathbf{r}} = J_G - J_L = J_G - \nu_c f. \tag{8}$$

The first term on the right hand side $J_G = \int f(t, \mathbf{r}, \mathbf{c}_1') f(t, \mathbf{r}, \mathbf{c}_2') |\mathbf{g} \cdot \mathbf{n}_{12}| d\mathbf{n}_{12} d\mathbf{c}_2$ is called the gain term, the second is called the loss term, and $\nu_c = \int f(t, \mathbf{r}, \mathbf{c}_2) |\mathbf{g} \cdot \mathbf{n}_{12}| d\mathbf{n}_{12} d\mathbf{c}_2$ is the collision frequency. The explicit appearance of the collision frequency calculated as a linear functional of velocity distribution function f is a straightforward consequence from the "*molecular chaos*" hypotheses and explains naturally Boltzmann's statement "*Stosszahlansatz*." The most popular collision schemes NTC,[4] NN,[5] and MCF[6] of the DSMC method use essentially this fact to define the number of collision-partner selections before starting the collision procedure within a time step. However, such a concept works well when the number of particles is large and the system asymptotically approaches a state of local molecular chaos. In the general case, it contradicts to a situation, which is typical when one considers a small bounded domain

with a limited number of particles (typically, a cell of the computational grid used by the DSMC in a calculation). Let us consider the postcollision particle velocities (7) in such a system or more clearly their alternative presentation used in a majority of DSMC collision procedures,

$$\mathbf{c}_1' = \frac{1}{2}[(\mathbf{c}_1 + \mathbf{c}_2) - |\mathbf{g}_{12}|\boldsymbol{\omega}],$$
$$\mathbf{c}_2' = \frac{1}{2}[(\mathbf{c}_1 + \mathbf{c}_2) + |\mathbf{g}_{12}|\boldsymbol{\omega}], \tag{9}$$

where the end of vector $\boldsymbol{\omega}$, replacing $\mathbf{n}_{12}$, realizes a random walk on a sphere of unit radius. If one considers the stochastic properties of velocities, it is obvious that if the velocities $\mathbf{c}_1$, $\mathbf{c}_2$ before a collision are uncorrelated, then their postcollision values $\mathbf{c}_1', \mathbf{c}_2'$ can keep on being uncorrelated depending on the distribution of vector $\boldsymbol{\omega}$ and vice versa, i.e., if $\mathbf{c}_1$, $\mathbf{c}_2$ are correlated, then $\mathbf{c}_1', \mathbf{c}_2'$ remain always correlated. Consequently, the presumption for the existence of "*molecular chaos*" is not generally met in the collision process released by the traditional collision schemes. It is worth noting that an exception is the Nanbu collision scheme,[39] which generates statistically independent velocities in accordance with the Boltzmann collision integral operator. Thus, in the Boltzmann collision operator, the "*molecular chaos*" is imposed *a priori*, and in the DSMC collision procedure, it is not. It means the DSMC mathematical model can describe the phenomena which are a priori excluded from the Boltzmann equation consideration such as macroscopic fluctuations and correlations. As stated in the Introduction, some numerical calculations support this idea and suggest new areas of applications related to the DSMC simulation of the Brownian motion of liquid and solid particles in nonequilibrium fluctuating gas flows (see, for example, Ref. 39). It is clear that the coordinate and velocity reduction process realized by the BBGKY procedure asymptotically leads to the Boltzmann equation only in the Boltzmann-Grad limit ($N \to \infty$, $d_{12} \to 0$, Nd_{12}^2–bounded). It should be noted that the condition $N \to \infty$ must be fulfilled for any small area around any point $\mathbf{r} \in \mathrm{R}^3$. Thus, the Boltzmann expression of collision frequency implemented in the traditional collision DSMC schemes naturally leads to the Boltzmann property for a large enough number of particles in cells of the computational grid.

The homogeneous collision relaxation of Maxwellian molecules is another example showing the difference between the Boltzmann equation and the DSMC model. In this case, an exact solution of the unsteady-state nonlinear Boltzmann equation exists in a closed form, widely known as the Bobylev-Krook-Wu (BKW) solution.[40,41] An important peculiarity of this self-similar solution is related to its validity limited to times $t \geq t_0$, where t_0 is a constant given in mean collision times. For time $t < t_0$, the velocity distribution function is getting nonpositive. The meaning of this limitation in time from below is frequently overlooked and not commented. Namely, it greatly reduces the set of initial states that lead to a perfectly final equilibrium state described by the Maxwellian velocity distribution. A deeper examination shows that the restriction is a consequence of the imposed condition of molecular chaos or statistical independency of molecular velocities. This follows clearly from the exact solution of the two-particle kinetic equation (4) obtained by Sagara and Tsuge[42] for the equilibrium state and generalized by Burenmandula and Zhao[43] for the self-similar relaxation evolution under specific assumptions and neglecting the triple-particle correlation functions in the case of a rarefied gas. These solutions transform into the BKW one only if they are considered in the Boltzmann-Grad limit and molecular chaos is assumed. In the stochastic DSMC model, such conditions are not imposed and could be achieved only asymptotically for $N \to \infty$. It contains correlations (respectively, fluctuations of macroscopic gas properties) naturally. It can start, if not from an arbitrary initial condition, at least from a much wider set of initial states and evolves into an equilibrium state for a large enough but finite number of particles N. The abovementioned arguments suggest that the DSMC model is governed by an N-particle stochastic equation and the mathematical expectation of its empirical velocity distribution approaches the Boltzmann equation solution under given conditions. Section III deals with derivation of its governing equation and the conditions that it must satisfy in order to approach asymptotically the Boltzmann equation solution.

III. SPLITTING SCHEME AND GOVERNING PARTICLE EQUATION OF THE DSMC MODEL

We begin with the Liouville equation (1) and transform it in a form which corresponds in a large account to the DSMC model. The first step is to rewrite Eq. (1) considering a short range potential of binary interactions assumed in a rarefied gas N-particle system. In this situation, it is feasible to separate the binary interaction terms into gain and lost parts as follows:

$$\frac{\partial F_N(t,\mathbb{R},\mathbb{C})}{\partial t} = -\sum_{i=1}^{N} \mathbf{c}_i \frac{\partial F_N(t,\mathbb{R},\mathbb{C})}{\partial \mathbf{r}_i} + \sum_{1\leq i<j\leq N} \left\{ \int d\boldsymbol{\omega}\Phi_{i,j}(g_{i,j},\theta) \times \left[F_N\left(t,\mathbb{R}'_{i,j},\mathbb{C}'_{i,j}\right) - F_N(t,\mathbb{R},\mathbb{C})\right]\right\}, \tag{10}$$

where $\mathbb{R}'_{i,j} = \{\mathbf{r}_1,\ldots,\mathbf{r}'_i,\ldots,\mathbf{r}'_j,\ldots,\mathbf{r}_N\}$, $\mathbb{C}'_{i,j} = \{\mathbf{c}_1,\ldots,\mathbf{c}'_i,\ldots,\mathbf{c}'_j,\ldots,\mathbf{c}_N\}$. In a similar form, the nonhomogeneous and nonlocal N-particle kinetic equation (10) was obtained independently by Leontovich[44] and Prigogine.[45] In order to be maximally close to the DSMC, we will assume that the binary interactions are instantaneous and, correspondingly, $\mathbf{r}'_i = \mathbf{r}_i$, $\mathbf{r}'_j = \mathbf{r}_j$ and $\boldsymbol{\omega} = (\sin\theta\cos\varepsilon, \sin\theta\sin\varepsilon, \cos\theta)$ does not depend on the particle indices. It is convenient to introduce the concept of collision cross section $\sigma(g_{i,j})$ instead of binary interaction function $\Phi_{i,j}$, whereby $d\sigma_{i,j} = \sigma(g_{i,j},\theta)d\theta d\varepsilon$ is the differential collision cross section and, respectively, $d\boldsymbol{\omega}\Phi_{i,j}(g_{i,j},\theta) = g_{i,j}\sigma(g_{i,j},\theta)d\theta d\varepsilon$. After all, Eq. (10) can be rewritten in the form

$$\frac{\partial F_N(t,\mathbb{R},\mathbb{C})}{\partial t} = -\sum_{i=1}^{N} \mathbf{c}_i \frac{\partial F_N(t,\mathbb{R},\mathbb{C})}{\partial \mathbf{r}_i} + \sum_{1\leq i<j\leq N} \left\{ \int g_{i,j}\left[F_N\left(t,\mathbb{R},\mathbb{C}'_{i,j}\right) - F_N(t,\mathbb{R},\mathbb{C})\right]d\sigma_{i,j}\right\}. \tag{11}$$

A next step toward the DSMC model is to apply $N-1$ space variable reduction

$$\tilde{F}_N(t,\mathbf{r}_1,\mathbb{C}) = \int F_N(t,\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N,\mathbb{C}) \prod_{s=2}^{N} d\mathbf{r}_s$$

to Eq. (11) with ($\mathbf{r} = \mathbf{r}_1$) and obtain

$$\frac{\partial \tilde{F}_N(t,\mathbf{r},\mathbb{C})}{\partial t} = -\sum_{i=1}^{N} \mathbf{c}_i \frac{\partial \tilde{F}_N(t,\mathbf{r},\mathbb{C})}{\partial \mathbf{r}} + \sum_{1\le i<j\le N} \left\{ \int g_{i,j} \left[\tilde{F}_N\left(t,\mathbf{r},\mathbb{C}'_{i,j}\right) - \tilde{F}_N(t,\mathbf{r},\mathbb{C}) \right] d\sigma_{i,j} \right\}. \tag{12}$$

Analogous to the DSMC method, Eq. (12) is a nonhomogeneous and local N-particle kinetic equation that describes the time evolution of the N-particle distribution function of particle velocities in vicinity of spatial point $\mathbf{r} \in D \subset R^3$. Since the DSMC method uses a splitting scheme in order to obtain the numerical solution of the mathematical DSMC model at time $t + \Delta t$ if it is known at time t, we apply such a splitting scheme to Eq. (12) assuming that $\tilde{F}_N(t,\mathbf{r},\mathbb{C})$ is known. Then, the solution of Eq. (12) at $t + \Delta t$ is approximated by the first order splitting scheme

$$\frac{\partial \tilde{F}^*_N(t,\mathbf{r},\mathbb{C})}{\partial t} = \sum_{1\le i<j\le N} \left\{ \int g_{i,j} \left[\tilde{F}^*_N\left(t,\mathbf{r},\mathbb{C}'_{i,j}\right) - \tilde{F}^*_N(t,\mathbf{r},\mathbb{C}) \right] d\sigma_{i,j} \right\},$$
$$t < \tau \le t + \Delta t, \quad \tilde{F}^*_N(t+0,\mathbf{r},\mathbb{C}) = \tilde{F}_N(t,\mathbf{r},\mathbb{C}), \quad \mathbf{r} \in D \subset \mathrm{R}^3, \tag{13}$$

$$\frac{\partial \tilde{F}^{**}_N(t,\mathbf{r},\mathbb{C})}{\partial t} = -\sum_{i=1}^{N} \mathbf{c}_i \frac{\partial \tilde{F}^{**}_N(t,\mathbf{r},\mathbb{C})}{\partial \mathbf{r}},$$
$$t < \tau \le t + \Delta t, \quad \tilde{F}^{**}_N(t+0,\mathbf{r},\mathbb{C}) = \tilde{F}^*_N(t+\Delta t,\mathbf{r},\mathbb{C}), \quad \mathbf{r} \in D \subset \mathrm{R}^3, \tag{14}$$

$$\tilde{F}_N(t+\Delta t,\mathbf{r},\mathbb{C}) = \tilde{F}^{**}_N(t+\Delta t,\mathbf{r},\mathbb{C}) + O\left(\Delta t^2\right). \tag{15}$$

In this way constructed, the splitting scheme (13) and (14) consists of two consecutive steps considering collision and free-streaming operators within time interval $t < \tau \le t + \Delta t$ in the spatial domain $\mathbf{r} \in D$. It is worth noting that in the DSMC algorithm during the collision step all particle coordinates are kept frozen and are changed only during the ballistic motion within the second step. Here, the meaning of the coordinate vector $\mathbf{r}$ is that the positions of particles are used to determine the distribution function in point $\mathbf{r}$ of the physical space and their mutual dispositions are neglected in accordance with the performed coordinate reduction. On applying the averaging operation

$$\frac{\tilde{F}^*_N(t,\mathbb{C})}{V} = \frac{\int \tilde{F}^*_N(t,\mathbf{r},\mathbb{C}) d\mathbf{r}}{\int d\mathbf{r}}, \quad V = \int d\mathbf{r}, \quad \mathbf{r} \in D, \tag{16}$$

to the right-hand side of Eq. (13) and taking into account that Eq. (14) gives $\partial \tilde{F}^{**}_N(t,\mathbf{r},\mathbb{C})/\partial t = 0$ and, respectively, $\tilde{F}_N(t+\Delta t,\mathbb{C}) = \tilde{F}^*_N(t+\Delta t,\mathbb{C}) + O\left(\Delta t^2\right)$, we obtain a homogeneous equation for the N-particle system in domain D,

$$\frac{\partial \tilde{F}_N(t,\mathbb{C})}{\partial t} = \frac{1}{V} \sum_{1\le i<j\le N} \left\{ \int g_{i,j} \left[\tilde{F}_N\left(t,\mathbb{C}'_{i,j}\right) - \tilde{F}_N(t,\mathbb{C}) \right] d\sigma_{i,j} \right\}. \tag{17}$$

Equation (17) has the same form as the stochastic Kac master equation[22]

$$\frac{\partial \varphi_N(t,\mathbb{C})}{\partial t} = \frac{1}{V} \sum_{1\le i<j\le N} \left\{ \int g_{i,j} \left[\varphi_N\left(t,\mathbb{C}'_{i,j}\right) - \varphi_N(t,\mathbb{C}) \right] d\sigma_{i,j} \right\}. \tag{18}$$

The difference is hidden in the probability interpretation of probability density φ_N and probability interaction terms of the Kac model. The homogeneous equations (17) and (18) describe the evolution of an isolated particle system in domain D with a fixed number of particles N, constant total momentum P, and energy E. The system cannot describe an exchange of particles with other domains of the physical space, and thus, it does not correspond to the general scheme of the DSMC method. In order to overcome this difficulty, one must discretize the spatial domain D and consider the particle motion and interactions in a system of disjoint subdomains covering domain D (an analog of the cells of computational grid in the DSMC), i.e.,

$$D = \bigcup_{l=1}^{M} D^{(l)} \quad \left(D^{(l)} \bigcap_{l\ne m}^{n} D^{(m)} = \varnothing, \quad \int_{D^{(l)}} d\mathbf{r} = V^{(l)}, \quad l = 1, M \right). \tag{19}$$

Correspondingly, in instant t, the particles of the system are distributed over the subdomains $D^{(l)}$,

$$N = \sum_{l=1}^{M} N^{(l)}, \quad \mathbb{R}^{(l)} = \left\{ \mathbf{r}^{(l)}_1, \ldots, \mathbf{r}^{(l)}_{N^{(l)}} \right\} \in D^{(l)},$$
$$\mathbb{C}^{(l)} = \left\{ \mathbf{c}^{(l)}_1, \ldots, \mathbf{c}^{(l)}_{N^{(l)}} \right\}, \; l = 1, M. \tag{20}$$

A size $\Delta r^{(l)}$ and reference point $\mathbf{r}^{(l)}$ are specified for each subdomain $D^{(l)}$. A local $N^{(l)}$–particle distribution function is defined as follows:

$$\tilde{F}_{N^{(l)}}\left(t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right) = \int_{D^{(l)}} \tilde{F}_N(t,\mathbf{r},\mathbb{C}) d\mathbf{r}, \; \mathbf{r} \in D^{(l)}. \tag{21}$$

Then, the splitting scheme (13) and (14) can be presented by the following system of discrete equations:

$$t < \tau \le t + \Delta t, \; l = 1, M,$$
$$\left| \begin{array}{l} \tilde{F}^*_{N^{(l)}}\left(t+0,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right) = \tilde{F}_{N^{(l)}}\left(t,\mathbf{r},\mathbb{C}^{(l)}\right), \quad \mathbf{r} \in D^{(l)} \subset \mathrm{R}^3, \\ \dfrac{\partial \tilde{F}^*_{N^{(l)}}\left(t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right)}{\partial t} = \dfrac{1}{V^{(l)}} \displaystyle\sum_{1\le i<j\le N^{(l)}} \left\{ \int g_{i,j} \left[\tilde{F}^*_{N^{(l)}}\left(t,\mathbf{r}^{(l)},\mathbb{C}'^{(l)}_{i,j}\right) - \tilde{F}^*_{N^{(l)}}\left(t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right) \right] d\sigma_{i,j} \right\}, \end{array} \right. \tag{22}$$

$$\left| \begin{array}{l} \tilde{F}^{**}_{N^{(l)}}\left(t+0,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right) = \tilde{F}^*_{N^{(l)}}\left(t+\Delta t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right), \\ \dfrac{\partial \tilde{F}^{**}_{N^{(l)}}\left(t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right)}{\partial t} = -\displaystyle\sum_{i=1}^{N^{(l)}} \mathbf{c}_i \frac{\partial \tilde{F}^{**}_{N^{(l)}}\left(t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right)}{\partial \mathbf{r}}, \quad \mathbf{r} \in D^{(l)}, \end{array} \right. \tag{23}$$

$$\left| \begin{array}{l} F_N(t+\Delta t,\mathbf{r},\mathbb{C}) = \displaystyle\sum_{l=1}^{M} \tilde{F}^{**}_{N^{(l)}}\left(t+\Delta t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right), \\ \tilde{F}_{N^{(l)}}\left(t+\Delta t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right) = \displaystyle\int_{D^{(l)}} F_N(t+\Delta t,\mathbf{r},\mathbb{C}) d\mathbf{r}, \quad \mathbf{r} \in D \subset \mathrm{R}^3. \end{array} \right. \tag{24}$$

The solution of the deterministic system of Eq. (22) corresponds to the stochastic simulation of particle velocity update in grid cells in the DSMC method during the collision step while the exact coordinates are neglected and are not changed. Within this step, the number of particles $N^{(l)}$, the total energy $E^{(l)}$, and momentum $P^{(l)}$ in subdomain $D^{(l)}$ remain constant. The solution of the deterministic system of Eq. (23) corresponds to the coordinate updates due to ballistic motion of particles within Δt to new positions proportionally to their velocities, which in lack of external forces remain constant within the time step. The equalities (24) of the third step need particular attention. The first constructs a global approximation of the N-particle distribution function from M parts at the end of every time step. The second reconstructs the local $N^{(l)}$–particle distribution functions in all subdomains $D^{(l)}$, (l = 1, M). Combined, they correspond to the indexing operation in the DSMC. These statements capture the effect of exchange of particles between domains $D^{(l)}(l = 1, M)$ on the local $N^{(l)}$-particle distribution functions and, respectively, on the global N-particle distribution function. Mostly, the exchange of particles takes place between adjacent subdomains. It is evident that the number of particles $N^{(l)}$, the total energy $E^{(l)}$, and the momentum $Q^{(l)}$of the particle system in subdomain $D^{(l)}$ are changed every time step. This is a completely different situation compared to the splitting scheme (13) and (14) and Eq. (17) in the homogeneous consideration. They still remain valid only for collision step (22) within interval $t < \tau \le t + \Delta t$ in each subdomain $D^{(l)}$ separately. However, now one should take into account the unknown and irregular variations of $N^{(l)}$, $E^{(l)}$, and $Q^{(l)}$. From a deterministic viewpoint, such a task seems absolutely hopeless and, correspondingly, the above description of the splitting scheme (22) and (23), defined separately in subdomains $D^{(l)}$, looks useless.

To overcome the difficulty mentioned above, one must leave the full deterministic approach and introduce stochastic elements into the particle set description. We will take advantage of the idea of randomized set of particles suggested in Ref. 46. According to this idea, the randomized set of particles can be described by an ensemble of particle sets with a different number of particles by using the $N^{(l)}$-particle distribution function with a random number of particles $N^{(l)}$ distributed with a probability density $P(\mathbf{r}^{(l)}, N^{(l)})$ in a local domain $D^{(l)} \subset D$. Regarding the DSMC method, a randomized set is embodied in the stochastic model by realization of multiple trajectories of the stochastic process from the very beginning to some fixed time instant of the process evolution or by consideration of a large number of time intervals over a single trajectory. The latter approach is used normally for analysis of an established steady state regime of the stochastic process assuming that the system obeys ergodic conditions. Under such conditions, the particle distribution function can be presented by its mathematical expectation. Denoting by $\overline{N}^{(l)} = \sum_{N^{(l)}=0}^{N} P\left(\mathbf{r}^{(l)}, N^{(l)}\right) N^{(l)}$ the average number of particles in domain $D^{(l)}$, the mathematical expectation of the N-particle distribution function obtained from the randomized model with a variable number of particles with expectation $\overline{N}^{(l)}$ reads

$$\tilde{F}_N\left(t, \mathbf{r}^{(l)}, \mathbb{C}\right) = \sum_{N^{(l)}=0}^{N} P\left(\mathbf{r}^{(l)}, N^{(l)}\right) \tilde{F}_{N^{(l)}}\left(t, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right). \tag{25}$$

Now, we are ready to write the governing equation for $\tilde{F}_N\left(t, \mathbf{r}^{(l)}, \mathbb{C}\right)$ in subdomain $D^{(l)}$ based on splitting scheme (22)–(24). It reads as follows:

$$\frac{\partial \tilde{F}_N\left(t, \mathbf{r}^{(l)}, \mathbb{C}\right)}{\partial t} = -\sum_{i=1}^{N} \mathbf{c}_i \frac{\partial \tilde{F}_N\left(t, \mathbf{r}^{(l)}, \mathbb{C}\right)}{\partial \mathbf{r}} + \tilde{J}_N, \tag{26}$$

$$\begin{aligned}
&\tilde{J}_N\left(t, \mathbf{r}^{(l)}, \mathbb{C}\right) \\
&= \frac{1}{V^{(l)}} \sum_{N^{(l)}=0}^{N} P\left(\mathbf{r}^{(l)}, N^{(l)}\right) \left\{ \sum_{1 \le i < j \le N^{(l)}} \left\{ \int g_{i,j} \left[\tilde{F}_{N^{(l)}}\left(t, \mathbf{r}^{(l)}, \mathbb{C}'^{(l)}_{i,j}\right) \right.\right.\right. \\
&\left.\left.\left. - \tilde{F}_{N^{(l)}}\left(t, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right) \right] d\sigma_{i,j} \right\} \right\} \\
&= \frac{1}{V^{(l)}} \sum_{1 \le i < j \le N} \sum_{N^{(l)}=j}^{N} P\left(\mathbf{r}^{(l)}, N^{(l)}\right) \left\{ \int g_{i,j} \left[\tilde{F}_{N^{(l)}}\left(t, \mathbf{r}^{(l)}, \mathbb{C}'^{(l)}_{i,j}\right) \right.\right. \\
&\left.\left. - \tilde{F}_{N^{(l)}}\left(t, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right) \right] d\sigma_{i,j} \right\} \\
&= \frac{1}{V^{(l)}} \sum_{1 \le i < j \le N} \left\{ \int g_{i,j} \left[\tilde{F}_N\left(t, \mathbf{r}^{(l)}, \mathbb{C}'_{i,j}\right) - \tilde{F}_N\left(t, \mathbf{r}^{(l)}, \mathbb{C}\right) \right] d\sigma_{i,j} \right\}.
\end{aligned}$$

Finally, the system of equations for all subdomains (l = 1, M) of the N-particle distribution function of the randomized model in the corresponding $D^{(l)}$ becomes

$$\begin{aligned}
&\frac{\partial \tilde{F}_N\left(t, \mathbf{r}^{(l)}, \mathbb{C}\right)}{\partial t} + \sum_{i=1}^{N} \mathbf{c}_i \frac{\partial \tilde{F}_N\left(t, \mathbf{r}^{(l)}, \mathbb{C}\right)}{\partial \mathbf{r}} \\
&= \frac{1}{V^{(l)}} \sum_{1 \le i < j \le N} \left\{ \int g_{i,j} \left[\tilde{F}_N\left(t, \mathbf{r}^{(l)}, \mathbb{C}'_{i,j}\right) - \tilde{F}_N\left(t, \mathbf{r}^{(l)}, \mathbb{C}\right) \right] d\sigma_{i,j} \right\}.
\end{aligned} \tag{27}$$

Equation (27) is coupled as a consequence of exchange of particles between the neighboring subdomains during the particle motion. Now, let us consider the limit, when the size of subdomain $\Delta r^{(l)} \to 0$ and correspondingly $V^{(l)} \to 0$, $M \to \infty$, keeping fixed the total number of particles $N < \infty$ in the entire domain D. Evidently, the following relations are valid:

$$\begin{aligned}
&\lim_{V^{(l)} \to 0} \frac{\sum_{N^{(l)}=0}^{N} P\left(\mathbf{r}^{(l)}, N^{(l)}\right) N^{(l)}}{V^{(l)}} = \lim_{V^{(l)} \to 0} \frac{\overline{N}^{(l)}}{V^{(l)}} = n(\mathbf{r}) < \infty, \\
&\lim_{V^{(l)} \to 0} \frac{\sum_{N^{(l)}=0}^{N} P\left(\mathbf{r}^{(l)}, N^{(l)}\right) \tilde{F}_{N^{(l)}}\left(t, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right)}{V^{(l)}} = \overline{F}_N(t, \mathbf{r}, \mathbb{C}) < \infty.
\end{aligned} \tag{28}$$

Applying this limit to Eq. (27) and taking into account (28), we obtain the final form of the N-particle distribution function equation governing the randomized model

$$\begin{aligned}
&\frac{\partial \overline{F}_N(t, \mathbf{r}, \mathbb{C})}{\partial t} + \sum_{i=1}^{N} \mathbf{c}_i \frac{\partial \overline{F}_N(t, \mathbf{r}, \mathbb{C})}{\partial \mathbf{r}} \\
&= \sum_{1 \le i < j \le N} \left\{ \int g_{i,j} \left[\overline{F}_N\left(t, \mathbf{r}, \mathbb{C}'_{i,j}\right) - \overline{F}_N(t, \mathbf{r}, \mathbb{C}) \right] d\sigma_{i,j} \right\}.
\end{aligned} \tag{29}$$

This is a novel nonhomogenous and local equation of the evolution of the randomized N-particle distribution function obtained from

the discretized in time and space splitting scheme (22)–(24). It is similar to Eq. (12) with a key difference that Eq. (29) is applied to the N-particle distribution function (28) randomized over the number of particles with mathematical expectation $s = \overline{N}^{(l)}$ found at instant t in a small volume V in vicinity of point $\mathbf{r}$. The distinction of Eq. (29) from the Leontovich-Prigogine N-particle equation (10) is principle. It is defined in three-dimensional physical space and $3N$-dimensional velocity space and describes the evolution of the local N-particle distribution in vicinity of physical point $\mathbf{r} \in \mathrm{R}^3$, while the Leontovich-Prigogine equation (10) is a nonlocal equation defined in the $6N$-phase-space. The randomized model dynamics described by the splitting scheme (22)–(24) is the fundament of the DSMC method and, respectively, the N-particle nonhomogenous equation (29) is its governing equation. In the discretized splitting scheme, the solution evolution in result of the intermolecular collision process within a time step Δt is described by Eq. (22) obtained on the basis of the stochastic Kac model with a fixed number of particles $N^{(l)}$ in every subdomain $D^{(l)}$, $(l = 1, M)$. The evolution of solution in result of deterministic ballistic motion of the particles in all subdomains is presented by Eq. (23). The equalities (24) describe the redistribution of the particle system among the subdomains in result of particle motion. Thus, the number of particles $N^{(l)}$ and, correspondingly, all properties of the particles system in each subdomain are changed every time step. Altogether, Eqs. (22)–(24) describe the randomized mathematical model, which is the basis of the DSMC method. By now, we have not concerned the issues related to specific numerical schemes and operators realizing the corresponding steps in the splitting scheme. All considerations are general and in a large extend valid for all known schemes of DSMC realization, except Nanbu's method.[10] It should be noted that the important issue of boundary condition realization finds its solution within the framework of the general consideration and, respectively, it is not analyzed here. In order to proceed further, we are going to obtain the equations for the corresponding reduced kinetic N-particle distribution function $f_N^{(s)}(t, \mathbf{r}, \mathbf{c}_1, \ldots, \mathbf{c}_s)$ for the randomized model, considering the set of undistinguishable particles. In this case, any permutation of positions of indices in velocity set $\mathbb{C} = \{\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_N\}$ gives identical states and the reduced kinetic distribution function $\tilde{f}_N^{(s)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_1, \ldots, \mathbf{c}_s\right)$ in subdomain $D^{(l)}$ is defined as follows:

$$\tilde{F}_N^{(s)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_1, \ldots, \mathbf{c}_s\right) = \int \tilde{F}_N\left(t, \mathbf{r}^{(l)}, \mathbb{C}(t)\right) \prod_{i=s+1}^{N} d\mathbf{c}_i,$$

$$\tilde{f}_N^{(s)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_1, \ldots, \mathbf{c}_s\right) = \sum_{N^{(l)}=s}^{N} P\left(\mathbf{r}^{(l)}, N^{(l)}\right)\left(N^{(l)}\right)_s \times \tilde{F}_N^{(s)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_1, \ldots, \mathbf{c}_s\right), \tag{30}$$

where the decreasing factorial $(N^{(l)})_s = N^{(l)}\,(N^{(l)} - 1)\cdots(N^{(l)} - s + 1)$ gives the number of all permutations of the positions of velocity subset $\{\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_s\} \subseteq \mathbb{C}$. Applying the limit $V^{(l)} \to 0$, we obtain

$$f_N^{(s)}(t, \mathbf{r}, \mathbf{c}_1, \ldots, \mathbf{c}_s) = \lim_{V^{(l)} \to 0} \frac{\tilde{f}_N^{(s)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_1, \ldots, \mathbf{c}_s\right)}{V^{(l)}}. \tag{31}$$

Integrating Eq. (27) with respect to velocities of $(N - s)$ particles in subdomain $D^{(l)}$ and randomizing it by applying (30) and limit (31), we obtain similar to the BBGKY[37] kinetic equation system in 3 + $3N$– phase space

$$\frac{\partial f_N^{(s)}}{\partial t} + \sum_{i=1}^{N} \mathbf{c}_i \frac{\partial f_N^{(s)}}{\partial \mathbf{r}} = \sum_{1 \le i < j \le s} J_{i,j}\left[f_N^{(s)}\right] + (N - s) \sum_{i=1}^{s} \int J_{i,s+1}\left[f_N^{s+1}\right] d\mathbf{c}_{s+1}, \tag{32}$$

where the collision integrals are equal to

$$J_{i,j}[f_N^{(s)}] = \int g_{i,j}\Big[f_N^{(s)}\left(t, \mathbf{r}, \ldots, \mathbf{c}_i', \ldots, \mathbf{c}_j' \ldots, \mathbf{c}_s\right) - f_N^{(s)}(t, \mathbf{r}, \mathbf{c}_1, \ldots, \mathbf{c}_s)\Big] d\sigma_{i,j},$$

$$J_{i,s+1}[f_N^{(s+1)}] = \int g_{i,s+1}\Big[f_N^{(s+1)}\left(t, \mathbf{r}, \ldots, \mathbf{c}_i', \ldots, \mathbf{c}_s, \mathbf{c}_{s+1}'\right) - f_N^{(s+1)}(t, \mathbf{r}, \mathbf{c}_1, \ldots, \mathbf{c}_s, \mathbf{c}_{s+1})\Big] d\sigma_{i,s+1}. \tag{33}$$

Previously, a similar kinetic equation system was obtained by Nurlybaev and Yanitskii[46] for the randomized Kac model of a homogeneous particle system.

Equations (29) and (32) are obtained from the discretized splitting scheme (22)–(24) by a limit transition to $\Delta t \to 0$, $\Delta r^{(l)} \to 0$ $(V^{(l)} \to 0, M \to \infty)$ and the total number of particles $N = \sum_{l=1}^{M} N^{(l)}$ kept bounded in the considered domain D. It is worth noting that the number density $n(\mathbf{r}^{(l)}) = \overline{N}^{(l)}/V^{(l)}$ is bounded in each subdomain $D^{(l)}$, $l = 1, M$, when $M \to \infty$. This limit is essentially different from the Boltzmann-Grad limit ($\Delta t \to 0$, $\Delta r^{(l)} \to 0$, $N^{(l)} \to \infty$, $\sigma_{i,j} \to 0$, $N^{(l)}\sigma_{i,j}^2$–bounded), leading to the Boltzmann equation under the assumption of molecular chaos. Besides the total number of particles in the entire domain D being bounded, it does not require assumption of molecular chaos. At the same time, similar to the Boltzmann-Grad limit, the stochastic nature of the Kac collision model described by Eq. (21) sets up a condition of coupling the decrease in volume $V^{(l)}$ and time step Δt with a decrease in so called "collision cylinder" $(g_{i,j}\sigma_{i,j}\Delta t)$ of a particle pair $(i, j) \in D^{(l)}$ so that $(g_{i,j}\sigma_{i,j}\Delta t/V^{(l)}) \le 1$, where the total collision cross section is equal to $\sigma_{i,j} = \int d\sigma_{i,j}$. It should be added that this condition is also physically reasonable for the molecules of a rarefied gas.

IV. MOLECULAR CHAOS AND THE RANDOMIZED PARTICLE MODEL

In general, Eqs. (29) and (32) describe the evolution of an open N-particle system with binary collision dynamics in vicinity of each point $\mathbf{r} \in D$ in the general case of particle number variations and possible correlations between particle velocities. The equations are consistent with the generic structure of the DSMC method without entering into the details of specific numerical techniques realizing the corresponding steps of the splitting scheme. With a view to their subsequent consideration, we will explore the randomized model, described by Eqs. (29) and (32), with respect to molecular chaos assumption and conditions of convergence to the Boltzmann equation. Equation (32) with reduced kinetic distributed function $f_N^{(s)}$ gives different levels of detailed description. For $s = 1$, it leads to the last equation of the Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchy,

$$\frac{\partial f_N^{(1)}}{\partial t} + \sum_{i=1}^{N} \mathbf{c}_i \frac{\partial f_N^{(1)}}{\partial \mathbf{r}} = (N-1) \int g_{1,2} \left[f_N^{(2)}\left(t, \mathbf{r}, \mathbf{c}_1', \mathbf{c}_2'\right) - f_N^{(2)}\left(t, \mathbf{r}, \mathbf{c}_1, \mathbf{c}_2\right) \right] d\sigma_{1,2}, \tag{34}$$

which transforms into the Boltzmann equation under the assumption of molecular chaos and $N \to \infty$. In order to determine conditions that the randomized model has to satisfy or at least has to approach to the state of molecular chaos, we will consider the homogeneous Kac equation (23) of the splitting scheme in the subdomain $D^{(l)}$ with $V^{(l)}$, $N^{(l)} \to \infty$. In his famous lectures,[22] Kac has showed that the Boltzmann property of molecular chaos has propagated in time if the particle system started from an initial state of molecular chaos, i.e.,

$$\lim_{N^{(l)}, V^{(l)} \to \infty} \tilde{F}_N^{(s)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_1, \ldots, \mathbf{c}_s\right) = \prod_{i=1}^{s} \tilde{F}_N^{(1)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_i\right), \quad N^{(l)}/V^{(l)} \approx n < \infty. \tag{35}$$

However, our goal is to find conditions, when the Boltzmann property is fair for the randomized model described with the splitting scheme (22)–(24) with bounded $N^{(l)}$ and $V^{(l)}$. The following statement proposed by Nurlybaev and Yanitskii[46] contains the items we are searching for. Reformulated in terms of our task, it reads as follows:

The sequence of reduced kinetic distribution functions $f_N^{(s)}(t, \mathbf{r}, \mathbf{c}_1, \ldots, \mathbf{c}_s)$, which are solutions of equation system (32), meets the property of molecular chaos in a randomized particle set, defined in vicinity of $\mathbf{r} \in D^{(l)} \subset D$ with bounded $N^{(l)}$ and $V^{(l)}$, if and only if the following two conditions are observed:

1. The velocities are statistically independent, i.e., for any $1 \le N^{(l)} \le N$ and $s \le N$ (N is the total number of particles in domain D),

$$\tilde{F}_N^{(s)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_1, \ldots, \mathbf{c}_s\right) = \prod_{i=1}^{s} \tilde{F}_N^{(1)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_i\right), \; N^{(l)}/V^{(l)} \approx n < \infty. \tag{36}$$

2. The number of particles in the subdomain $D^{(l)}$ is distributed according to the Poisson law,

$$P(\mathbf{r}^{(l)}, N^{(l)}) = \frac{\left(\overline{N}^{(l)}\right)^{N^{(l)}}}{\left(N^{(l)}\right)!} e^{-\overline{N}^{(l)}}. \tag{37}$$

The sufficiency can be verified directly from (36) and (37). The following relation for $s = 1$ is obvious:

$$\begin{aligned} \tilde{f}_N^{(1)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_1\right) &= \sum_{N^{(l)}=0}^{N} \frac{\left(\overline{N}^{(l)}\right)^{N^{(l)}}}{\left(N^{(l)}\right)!} e^{-\overline{N}^{(l)}} N^{(l)} \tilde{F}_N^{(1)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_1\right) \\ &= \overline{N}^{(l)} \tilde{F}_N^{(1)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_1\right) e^{-\overline{N}^{(l)}} \sum_{N^{(l)}=0}^{N} \frac{\left(\overline{N}^{(l)}\right)^{N^{(l)}-1}}{\left(N^{(l)}-1\right)!} \\ &= \overline{N}^{(l)} \tilde{F}_N^{(1)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_1\right) e^{-\overline{N}^{(l)}} e^{-\overline{N}^{(l)}} = \overline{N}^{(l)} \tilde{F}_N^{(1)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_1\right). \end{aligned}$$

In the above expression, $N \to \infty$ was assumed, which is reasonable for the large number of particles in the entire domain D. Then, substituting (36) and (37) into the expression for $f^{(s)}$ gives

$$\begin{aligned} &\tilde{f}_N^{(s)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_1, \ldots, \mathbf{c}_s\right) \\ &= \sum_{N^{(l)}=0}^{N} \frac{\left(\overline{N}^{(l)}\right)^{N^{(l)}}}{N^{(l)}!} e^{-\overline{N}^{(l)}} N^{(l)} \prod_{i=1}^{s} \tilde{F}_N^{(1)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_i\right) \\ &= \left(\overline{N}^{(l)}\right)^{s} \prod_{i=1}^{s} \tilde{F}_N^{(1)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_i\right) \left(e^{-\overline{N}^{(l)}} \sum_{N^{(l)}=0}^{N} \frac{\left(\overline{N}^{(l)}\right)^{\left(N^{(l)}-s\right)}}{\left(N^{(l)}-s\right)!} \right) \\ &= \prod_{i=1}^{s} \overline{N}^{(l)} \tilde{F}_N^{(1)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_i\right) = \prod_{i=1}^{s} \overline{N}^{(l)} \tilde{F}_N^{(1)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_i\right) \\ &= \prod_{i=1}^{s} \tilde{f}_N^{(1)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_1\right). \end{aligned} \tag{38}$$

Applying the limit (31)–(38), we obtain

$$f_N^{(s)}(t, \mathbf{r}, \mathbf{c}_1, \ldots, \mathbf{c}_s) = \lim_{V^{(l)} \to 0} \frac{\prod_{i=1}^{s} \tilde{f}_N^{(1)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_1\right)}{V^{(l)}} = \prod_{i=1}^{s} f_N^{(1)}(t, \mathbf{r}, \mathbf{c}_i). \tag{39}$$

This proves the sufficiency. The consideration of the necessity is much longer and complicated, and we refer to the paper by Nurlybaev and Yanitskii,[46] where the proof is given for the case of a homogeneous particle system. If conditions (36) and (37) are fulfilled and also equality (39) is valid, then Eq. (34) asymptotically tends to the Boltzmann equation (6) in all subdomains $D^{(l)}$, $l = 1, M$. From the more general conditions of equation validity, it follows that the new N-particle nonhomogenous equations (29) and (32) are valid for the more general case of state with possible correlations between particle velocities. However, if the Boltzmann property is fulfilled in a domain D, one could reasonably assume that it would asymptotically approximate the Boltzmann equation in its subdomains $D^{(l)}$. In the later assumption, we make a proviso of excluding boundary areas and domains with eventually strong nonequilibrium (shock waves), which might be sources of particle velocity correlations.

By now, we have considered the randomized model of particle system in subdomain $D^{(l)}$ with a variable number of particles $N^{(l)}$ having unknown probability distribution $P(r^{(l)}, N^{(l)})$. Conditions (36) and (37), which are necessary for the existence of molecular chaos in the randomized model, require not only statistical independence of molecular velocities following from condition (36) but also specify the Poisson distribution law (37) for the particle number variations. Both conditions are valid for an arbitrary average number of particles $\overline{N}^{(l)}$ in the open subdomain $D^{(l)}$. At the same time, the total number of particles N in the entire domain D must be large enough in order to ensure a correct determination of N-particle distribution functions $\tilde{f}_N^{(s)}\left(t, \mathbf{r}^{(l)}, \mathbf{c}_1, \ldots, \mathbf{c}_s\right)$ in an arbitrary subdomain $D^{(l)} \subset D$. The general definition of functions $\tilde{f}_N^{(s)}$ by relations (30) takes into account all possible particle subsets with $(0 \le N^{(l)} \le N)$ although subsets with very large $N^{(l)} \to N$ are extremely unlikely. In the limit $\Delta r^{(l)} \to 0$ ($V^{(l)} \to 0$), the average number of particles

in subdomain $D^{(l)}$ is very small $\overline{N}^{(l)} \to 0$ but always larger than zero because of relation ($\sum_{l=1}^{M} N^{(l)} = N$). When the domain resolution is very fine, the subdomains mostly are empty and rarely contain more than one particle so that a binary collision is to be realized. In view of this remark, the limit ($\Delta t \to 0$, $\Delta r^{(l)} \to 0$ and the total number of particles N bounded) approaches the exact binary collision molecular dynamics rather than satisfying the Boltzmann equation (6), which requires the conditions of the Boltzmann-Grad limit.

Bearing in mind the above remarks, an important question is how one has to interpret the asymptotic approximation of the Boltzmann equation and existence of molecular chaos in the randomized model with a variable number of particles $0 \le N^{(l)} \le N$ in subdomain $D^{(l)} \subset D$ and how to relate them to the particle-based DSMC method. First of all, one should assume statistical independence of molecular velocities in domain D with a large enough number of particles N in order to employ the Boltzmann-Grad limit. Second, one should neglect any short-range correlations arising due to binary collisions, a presumption reasonable for a rarefied gas, and assume as well that the statistical independence of particle velocities is spread throughout all subdomains $D^{(l)}$, $l = 1, M$. Then, conditions (36) and (37) guaranty the statistical independence of molecular velocities (39) in the randomized model with an arbitrary average number of particles $0 < \overline{N}^{(l)} \le N$ in subdomain $D^{(l)}$. Along with this, it would be worth noting that the discretization of space and time and the implementation of splitting scheme (22)–(24) exploit implicitly another assumption for the randomized model, namely, that the binary collisions are to be considered as indistinguishable events within a time step $\tau \in (t, t + \Delta t)$ and subdomain $\mathbf{r} \in D^{(l)}$.

Another important issue is the determination of the total number of particles (simulators) N in the whole computational domain D. Traditionally, it is calculated as a sum of particles occupying all subdomains (cells of the computational grid), and thus, the average number of particles $\overline{N}^{(l)}$ in a subdomain $D^{(l)}$ depends on it. There are many empirical assessments of the minimum number of particles per cell necessary to obtain accurate DSMC results. The theoretical analysis presented in this paper offers another insight into the problem. Bird, when proposing originally the DSMC method, with genius intuition had captured a universal property of rarefied gas dynamics: the evolution in time of a particle system with binary interactions between particles is self-similar for a large number of particles $N \to \infty$. The fundamental idea to simulate accurately a rarefied gas flow by using a large enough but finite number of particles at appropriate physical scales paves a path between the microscopic and the macroscopic physical description. Thus, the choice of an optimal total number of particles N to describe accurately the flow behavior and flow properties in the computational domain D is a physical rather than a mathematical problem. From theoretical viewpoint, the problem is open, but its validity has been supported by numerous DSMC calculations. However, the other issue related to discretization of particle set and choice of optimal average number of particles per cell is definitely a subject of method accuracy. The latter is often wrongly mixed with the requirement for a minimum total number of particles necessary for simulation of correct physical behavior.

V. DERIVATION OF DSMC COLLISION SCHEMES FROM THE GENERAL TRANSITION OPERATOR

In the DSMC method, the splitting scheme (22)–(24) is realized by applying three successive procedures within each time step, as described in Sec. III. The ballistic motion (23) and indexation (24) of the particles are realized by standard well-known deterministic procedures and are not considered here. The particle interactions with the boundaries, requiring a special analysis, are also beyond the scope of the present study. The last, most complex, and influential collision relaxation procedure (22) can be accomplished by different collision schemes, and it is a subject of the following assessment.

The current analysis is focused on the binary collision model (22), which is realized by a stochastic collision procedure applied separately in each subdomain $D^{(l)}$, $(l = 1, M)$. Each collision scheme consists of two intrinsic parts: selection of collision partners and realization of collisions of selected pairs. The second part refers to replacement of precollision with postcollision velocities depending on the binary interaction model, which could be realized by using random impact parameters (in most of the collision schemes) or by using the "*ab initio*" approach (see, for example, Ref. 47). Since the statistical properties of the collision relaxation procedure (22) are not affected notably by velocity update, it is not discussed here. The selection of collision partners is a procedure of critical importance for accuracy of any collision scheme. Since a comprehensive analysis of the mostly used collision-partner selection schemes is given in the review paper of Roohi and Stefanov,[8] we will consider only the essential items in the light of statements obtained for the randomized model in Sec. IV.

The collision-partner selection scheme is a core element of the DSMC method and determines its accuracy along with the time and space discretization. The effect of average particle number $\overline{N}^{(l)}$ in cells on the accuracy of the collision scheme is a particularly important issue, and furthermore, we will analyze it using the operator approach proposed by Yanitskii,[25,26] which was used by Stefanov and Roohi *et al.* in Refs. 27, 28, and 30 for derivation of new approximations of the collision process.

Equation (22) describing the evolution of the collision process of the Kac model in time interval $\tau \in (t, t + \Delta t)$ can be presented[22] in the following operator form:

$$\frac{\partial \tilde{F}^{*}_{N^{(l)}}\left(t, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right)}{\partial t} = \Omega \tilde{F}^{*}_{N^{(l)}}\left(t, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right), \tag{40}$$

where

$$\Omega \tilde{F}^{*}_{N^{(l)}}\left(t, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right) = \frac{1}{V^{(l)}} \sum_{1 \le i < j \le N^{(l)}} \left\{ \int g_{ij} \left[\tilde{F}^{*}_{N^{(l)}}\left(t, \mathbf{r}^{(l)}, \mathbb{C}^{\prime(l)}_{i,j}\right) - \tilde{F}^{*}_{N^{(l)}}\left(t, \mathbf{r}^{(l)}, \mathbb{C}^{(l)}\right) \right] d\sigma_{ij} \right\}. \tag{41}$$

Operator Ω generates a change in $\tilde{F}^{*}_{N^{(l)}}$ for infinitesimally small $\Delta t \to 0$, corresponding to a change in result of a single collision (defined as instantaneous event). Furthermore, we assume all conditions[22] for the existence of operator Ω fulfilled. Then, the solution of Eq. (40) at time $(t + \Delta t)$ can be expanded into the following series

of the solution at time t with regard to the number of collisions k:

$$\tilde{F}^{*}_{N^{(l)}}\left(t+\Delta t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right)=\sum_{k=0}^{\infty}\frac{\Omega^{k}\tilde{F}^{*}_{N^{(l)}}\left(t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right)}{k!}(\nu\Delta t)^{k}, \quad (42)$$

where ν is the binary collision frequency, which, in general case, depends on the solution and, respectively, is unknown. Yanitskii[25,26] has transformed (42) in the following compact form:

$$\tilde{F}^{*}_{N^{(l)}}\left(t+\Delta t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right)=G(\Delta t)\tilde{F}^{*}_{N^{(l)}}\left(t,\mathbf{r}^{(l)},\mathbb{C}^{(l)}\right), \quad (43)$$

where the transition operator $G(\Delta t)$ is given by

$$\mathrm{G}(\Delta t)=\sum_{k=0}^{\infty}\frac{\Omega^{k}}{k!}(\nu\Delta t)^{k}=\exp[\Delta t\nu(\mathrm{T}-\mathrm{I})]. \quad (44)$$

The new operators I and T, introduced in (44), decompose operator Ω into identity and 3D-velocity rotation operators,

$$\begin{aligned}&\mathrm{I}\psi=\psi,\quad \mathrm{T}_{i,j}\psi=\frac{1}{\sigma_{i,j}}\int_{4\pi}\psi(\mathbf{c}_i,\mathbf{c}_j)\sigma(g_{i,j},\theta)d\theta d\varepsilon,\\ &\mathrm{T}\psi=\sum_{1\le i<j\le N^{(l)}}\omega_{i,j}\mathrm{T}_{i,j}\psi.\end{aligned} \quad (45)$$

The unknown binary collision frequency ν is given by

$$\nu=\sum_{1\le i<j\le N^{(l)}}\omega_{i,j};\quad \omega_{i,j}=\frac{\sigma_{i,j}g_{i,j}}{V^{(l)}}. \quad (46)$$

Thus, the final form of $G(\Delta t)$ could be written as

$$\mathrm{G}(\Delta t)=\exp\left[\Delta t\sum_{1\le i<j\le N^{(l)}}\omega_{ij}(\mathrm{T}_{ij}-\mathrm{I})\right]. \quad (47)$$

Yanitskii[26] has showed that the stochastic interpretation of the transition operator (47) gives a general scheme of collision process in each cell (l) with a collision probability of any randomly chosen particle pair (i,j) in (l) equal to

$$W_{i,j}=\frac{\omega_{i,j}}{\nu}=\frac{\omega_{i,j}}{\sum_{1\le i<j\le N^{(l)}}\omega_{ij}}. \quad (48)$$

From the exponential form of operator (47), it follows that the random distribution of the time intervals δt_k between two consecutive collisions $(k,k+1)$ is equal to

$$Prob(\delta t_k\le\Delta t)=1-e^{-\nu\Delta t} \quad (49)$$

and the number of collisions K in cell (l) within a time step Δt is defined by the condition

$$\sum_{k=1}^{K}\delta t_k\le\Delta t<\sum_{k=1}^{K+1}\delta t_k. \quad (50)$$

The high computational costs of the general algorithm equal to $O[(N^{(l)})^3]$ make it inappropriate for practical use. However, its importance is determined by the revelation[26] that almost all known collision schemes appeared to be somewhat approximations of the general scheme realizing the transition between states in the Kac model. We will illustrate this statement showing that Bird's NTC collision scheme[4] can be derived from the transition operator (47) under assumptions of the Boltzmann-Grad limit and molecular chaos when $\Delta t\to 0$, $\Delta r^{(l)}\to 0$, $N^{(l)}\to\infty$. In the case, one can define a constant equal to an upper estimation of the Boltzmann binary collision frequency that serves for selection of a number of particle pairs—candidates for potential collisions in subdomain (cell) $D^{(l)}$. It gives

$$\nu_{\max}=\frac{N^{(l)}\left(N^{(l)}-1\right)}{2}\frac{(\sigma g)_{\max}}{V^{(l)}}=\frac{N^{(l)}\left(N^{(l)}-1\right)}{2}\omega_{\max}. \quad (51)$$

Here, the property $\left\langle N^{(l)}\left(N^{(l)}-1\right)\right\rangle=\left(\overline{N}^{(l)}\right)^2$ of Poisson distribution (37) is taken into account. It is worth noting that the collision frequency, which is an integral characteristic, can be expressed explicitly in form (51) only if the final kinetic equation has form (8) and $\nu_{\max}=C_{\max}\left(\overline{N}^{(l)}/2V^{(l)}\right)\nu_c$, $(C_{\max}>1)$. Thus, the Boltzmann-Grad limit validity is assumed by default, i.e., the large number of particles in an arbitrary small subdomain (computational cell) is assumed as an intrinsic property of the considered particle system in any subdomain. In this case, a new transition operator $\mathrm{G}_{\max}(\Delta t)$, which corresponds to $\nu_{\max}$, can be defined as follows:

$$\begin{aligned}&\mathrm{G}_{\max}(\Delta t)=\mathrm{G}(\Delta t),\\ &\exp[\Delta t\nu_{\max}(\mathrm{T}_{\max}-\mathrm{I})]=\exp\left[\Delta t\sum_{1\le i<j\le N^{(l)}}\omega_{i,j}(\mathrm{T}_{i,j}-\mathrm{I})\right],\\ &\frac{N^{(l)}\left(N^{(l)}-1\right)}{2}\omega_{\max}(\mathrm{T}_{\max}-\mathrm{I})=\sum_{1\le i<j\le N^{(l)}}\omega_{i,j}(\mathrm{T}_{i,j}-\mathrm{I}),\\ &\sum_{1\le i<j\le N^{(l)}}\omega_{\max}(\mathrm{T}_{\max,i,j}-\mathrm{I})=\sum_{1\le i<j\le N^{(l)}}\omega_{i,j}(\mathrm{T}_{i,j}-\mathrm{I}).\end{aligned} \quad (52)$$

The resulting new velocity rotation operator giving the postcollision velocities of a selected pair (i,j) is equal to

$$\mathrm{T}_{\max,i,j}=\left(1-\frac{\omega_{i,j}}{\omega_{\max}}\right)\mathrm{I}+\frac{\omega_{i,j}}{\omega_{\max}}\mathrm{T}_{i,j}. \quad (53)$$

The probability interpretation of (53) describes exactly the acceptance-rejection procedure with collision probability

$$w_{i,j}=\frac{\omega_{i,j}}{\omega_{\max}}=\frac{\sigma_{i,j}g_{i,j}}{(\sigma g)_{\max}}. \quad (54)$$

By applying operator $\mathrm{T}_{\max,i,j}$, the collision event of pair (i,j) is accepted with probability $w_{i,j}$ and rejected with probability $1-w_{i,j}$. In NTC, selected pairs are chosen at random and the number of selected pairs is equal to the integer part of $\Delta t\nu_{\max}$,

$$N_{sel}=\lfloor\Delta t\nu_{\max}\rfloor=\max\{i\in\mathbb{N}|i\le\Delta t\nu_{\max}\}, \quad (55)$$

where $\mathbb{N}=\{0,1,2,\ldots\}$. The fractional part

$$\mathrm{frac}(\Delta t\nu_{\max})=\Delta t\nu_{\max}-\lfloor\Delta t\nu_{\max}\rfloor \quad (56)$$

is a remainder, which is added to the number of selected pairs at the next time step. This completes the proof of the statement that the NTC collision scheme follows from the randomized model description and the general transition operator (47) if conditions (36) and

(37) are observed. The same proof is valid for the other popular collision scheme MCF.[48] The difference between NTC and MCF is the way how the number of selected pairs per time step is counted up. Instead, using the explicit formulas (55) and (56) as done in NTC, in MCF, the sum of exponentially distributed random time intervals between consecutive collisions is repeatedly compared to the time step and the collision procedure is stopped in conformity with conditions (49) and (50). As shown in the following, this approach avoids one of the sources of systematic errors, which is linked to the use of remainder (56), when the number of particles in cells is getting small.

An alternative approximation approach to the general transition operator (47) is developed by Yanitskii[25,26] and used by Stefanov, Roohi, and collaborators in Refs. 27, 28, and 30 to derive a group of Bernoulli-trials schemes on the basis of the randomized particle model without using the Boltzmann-Grad limit properties. It consists of a sequence of simplifying approximations over time step Δt of the general transition operator (47) defined on the particle set in each subdomain $D^{(l)}$ under conditions of the limit ($\Delta t \to 0$, $\Delta r^{(l)} \to 0$, $V^{(l)} \to 0$, $N^{(l)}/V^{(l)}$ is bounded, and $N = \sum_{l=1}^{M} N^{(l)}$ is bounded). As described in Sec. III, this limit leads to the governing N-particle equations (29) and (32). The approach of successive approximation of (47) is outlined in detail in the review paper.[8]

The operator (47) can be written in the following form:

$$\mathrm{G}(\Delta t) = \prod_{i=1}^{N^{(l)}-1} \prod_{j=i+1}^{N^{(l)}} \exp[\Delta t \omega_{i,j}(\mathrm{T}_{i,j} - \mathrm{I})], \tag{57}$$

and each cofactor in this presentation is replaced by an approximation linear in Δt. This gives

$$\mathrm{G}_{BT}(\Delta t) = \prod_{i=1}^{N^{(l)}-1} \prod_{j=i+1}^{N^{(l)}} [(1 - \Delta t \omega_{i,j})\mathrm{I} + \Delta t \omega_{i,j}\mathrm{T}_{i,j}]. \tag{58}$$

The approximation operator $\mathrm{G}_{BT}(\Delta t)$ has a probability interpretation, which gives the Bernoulli-trials (BT) scheme[25,26] if

$$w_{i,j} = \Delta t \omega_{i,j}, \; w_{i,j} \le 1. \tag{59}$$

The quadratic dependence of operator (58) on the number of particles $N^{(l)}$ determines computational costs equal to $O[(N^{(l)})^2]$.

The "Ballot-box" (BB) collision scheme[26] can be obtained from (58) if the term linear in Δt is isolated,

$$\mathrm{G}_{BB}(\Delta t) = \mathrm{I} + \Delta t \sum_{1 \le i < j \le N^{(l)}} \omega_{i,j}(\mathrm{T}_{i,j} - \mathrm{I}), \tag{60}$$

and (60) is transformed into the form

$$\mathrm{G}_{BB}(\Delta t) = \left[1 - \sum_{1 \le i < j \le N^{(l)}} \frac{1}{k}(k\omega_{i,j}\Delta t)\right]\mathrm{I} + \sum_{1 \le i < j \le N^{(l)}} \frac{1}{k}(k\omega_{i,j}\Delta t)\mathrm{T}_{i,j}, \tag{61}$$

where the number of particle pairs is denoted by $k = N^{(l)}(N^{(l)} - 1)/2$. The computational costs of the BB scheme are equal to $O[(N^{(l)})]$. However, the probability interpretation of (61) determines one collision per time step, which must be very small in order to fulfill the condition $(k\omega_{i,j}\Delta t) \le 1$.

Instead proceeding directly to operator (61), Stefanov[27] showed that it is possible to extend the internal product in (58) in a series of j with respect to Δt in order to obtain a new simplified transition operator

$$\mathrm{G}_{SBT}(\Delta t) = \prod_{i=1}^{N^{(l)}-1} \left\{\left[1 - \sum_{j=1}^{N^{(l)}} \frac{1}{k}(k\omega_{i,j}\Delta t)\right]\mathrm{I} + \sum_{j=1}^{N^{(l)}} \frac{1}{k}(k\omega_{i,j}\Delta t)\mathrm{T}_{i,j}\right\}, \tag{62}$$

where $k = N^{(l)} - i$. The algorithmic interpretation of operator $\mathrm{G}_{SBT}(\Delta t)$ determines the Simplified Bernoulli trials (SBT) scheme. The computational costs of the SBT are equal to $O[(N^{(l)})]$. The number of selected pairs per time step is equal to $N^{(l)} - 1$ with a requirement for eventual overruns of condition $(k\omega_{i,j}\Delta t) \le 1$ to be very rare.

An additional partial linearization of operator (62) with regard to Δt, which is proposed in Ref. 30, gives a generalized form of the approximation operator,

$$\mathrm{G}_{GBT}(\Delta t) = \prod_{i=1}^{N_{sel}} \left\{\left[1 - \sum_{j=1}^{N^{(l)}} \frac{1}{k'k}\left(k'k\omega_{i,j}\Delta t\right)\right]\mathrm{I} + \sum_{j=1}^{N^{(l)}} \frac{1}{k'k}\left(k'k\omega_{i,j}\Delta t\right)\mathrm{T}_{i,j}\right\}, \tag{63}$$

where the number of selected pair N_{sel} can vary in the range $1 \le N_{sel} \le N^{(l)} - 1$ and $k'k$ is equal to

$$\begin{aligned} k' &= \frac{\mathrm{C}\left(N^{(l)}, 2\right)}{\mathrm{C}\left(N^{(l)}, 2\right) - \mathrm{C}\left(N^{(l)} - N_{sel,2)}\right)}, \\ \mathrm{C}\left(N^{(l)}, 2\right) &= N^{(l)}\left(N^{(l)} - 1\right)/2, \\ \mathrm{C}\left(N^{(l)}, 2\right) - \mathrm{C}\left(N^{(l)} - N_{sel,2)}\right) &= N_{sel}\left(2N^{(l)} - N_{sel} - 1\right)/2, \\ k &= N^{(l)} - i, \\ k'k &= \frac{N^{(l)}\left(N^{(l)} - 1\right)}{N_{sel}\left(2N^{(l)} - N_{sel} - 1\right)}\left(N^{(l)} - i\right), \end{aligned} \tag{64}$$

where $\mathrm{C}(m, n) = n(n-1)\cdots(n-m+1)/m!$ is the number of combinations of m from n elements.

The generalized Bernoulli-trials (GBT) scheme transforms into SBT for $N_{sel} = N^{(l)} - 1$ and reduces to BB for $N_{sel} = 1$. Again the probability of overruns has to tend to zero, i.e., $prob(k'k\omega_{i,j}\Delta t > 1) \to 0$.

The difference in the derivation of the standard NTC and MCF collision schemes and the group of Bernoulli-trials schemes from the general operator (47) determines their different properties. The most important distinction is set in the conditions of the corresponding mathematical limits used in the approximations, respectively, the Boltzmann-Grad limit for NTC and MCF leading for $N \to \infty$ to the Boltzmann equation (8) and the limit $\Delta t \to 0$, $\Delta r^{(l)} \to 0$, $N = \sum_{l=1}^{M} N^{(l)}$ bounded, leading to the governing N-particle Eqs. (29) and (32). The analysis of a collision scheme with respect to these limits helps reveal the sources of systematic errors.

VI. SOURCES OF SYSTEMATIC ERRORS IN THE DSMC METHOD

The discretization in time and space and splitting the governing equation (29) into a sequence of Eqs. (22) and (23), considered in each subdomain $D^{(l)}(l = 1, M)$, gives an approximation $O(\Delta t, \Delta r)$ of Eq. (29), which requires the coordinate distribution of $N^{(l)}$ particles in each subdomain to be considered as homogeneous within a time step m and the instant of any collision to be associated with the discrete time t_m of the current time step. It is worth noting that the Strang splitting scheme[49,50] gives a higher order approximation with respect to time step $O(\Delta t^2)$.

The average number of particles per cell $\overline{N}^{(l)}$ is another inherent parameter of any collision scheme with crucial impact on its accuracy. In the following, we focus on the effect of the average number of particles per cell on the accuracy of collision schemes examining them with respect to the limit conditions, assumed in the derivation of both standard and Bernoulli-trial type collision schemes. In our analysis, both groups are represented by No-Time-Counter NTC and Generalized Bernoulli-trials GBT,[30] respectively. Actually, the numerical results presented in this section were obtained by using GBT with a number of selected pairs set to $N_{sel} = N^{(l)} - 1$ in all simulations what in practice transformed GBT into Simplified Bernoulli-trials SBT.

The flowcharts of both schemes are given in Fig. 1. The factor F_{num} relates the number of simulated molecules (simulators) to the real number of gas molecules at given physical conditions. It must be given when the equations are presented in dimensional form. In Secs. III–V, $F_{num} = 1$ was assumed.

The first step in the NTC procedure is the calculation of the number of collision-partner selections by using an upper estimation of binary collision frequency (51). As discussed in Sec. V, it assumes implicitly the Boltzmann-Grad limit validity leading to the Boltzmann equation (8). Therefore, the use of estimation (55) requires a large number of particles in cells in order to be consistent with the Boltzmann collision frequency. Thus, the NTC and MFC collision schemes are accurate when they are applied with a large enough number of particles per cell. If the computational grid is refined keeping fixed the total number of particles N in the computational domain D, then the conditions of the second limit ($\Delta t \to 0$, $\Delta r^{(l)} \to 0$, $N = \sum_{l=1}^{M} N^{(l)}$ bounded) are applied and the average number of particles per cell $\overline{N}^{(l)}$ is decreased. With a decrease in the average number of particles per cell, several negative effects of inconsistency of the NTC with the Boltzmann-Grad limit are observed, which are sources of systematic errors.

First, the instantaneous values of integral estimation (51) have larger relative deviations from the mathematical expectation of the collision frequency for small $\overline{N}^{(l)}$ compared to the cases with large $\overline{N}^{(l)}$. The larger variance transforms into a larger systematic error of the computed collision frequency, and this effect was demonstrated in Ref. 51 for both NTC and MFC collision schemes by analyzing the exponential distribution function of the time intervals between successive collisions (49).

No-time-counter NTC	**Generalized Bernoulli-trials with**
applied to a cell (l)	$N_{sel} = N^{(l)} - 1$
	(SBT) applied to a cell (l)
Compute	Compute
$A_{sel} = \frac{N^{(l)}\left(N^{(l)}-1\right)}{2}\frac{F_{num}\left(\sigma g\right)_{\max}}{V^{(l)}}\Delta t + \Delta A'_{sel}$	$N_{sel} = N^{(l)} - 1$
$N_{sel} = \lfloor A_{sel} \rfloor$	
$\Delta A'_{sel} = A_{sel} - N_{sel}$	
1. Select a pair (i, j) at random from $N^{(l)}$ particles	1. Select first particle in order from the list $i = 1, \ldots, N_{sel}$; select the second particle (j) at random from $\left(N^{(l)} - i\right)$ particles after i_{th} particle in the list $j \in \left\{i+1, \ldots, N^{(l)}\right\}$
2. Accept collision of (i, j) with probability $w_{i,j} = \frac{\sigma_{i,j} g_{i,j}}{\left(\sigma g\right)_{\max}}$ and change $(\mathbf{c}_i, \mathbf{c}_j)$ to post-collision $(\mathbf{c}'_i, \mathbf{c}'_j)$	2. Accept collision (i, j) with probability $w_{i,j} = k'k\frac{F_{num}\sigma_{i,j} g_{i,j}}{V^{(l)}}\Delta t$ and change $(\mathbf{c}_i, \mathbf{c}_j)$ to postcollision $(\mathbf{c}'_i, \mathbf{c}'_j)$
Repeat 1and 2 for N_{sel} collision pairs	Repeat 1and 2 for N_{sel} collision pairs

FIG. 1. Flowcharts of NTC and GBT collision schemes.

A second source of systematic error of the collision frequency, which is not negligible for small $\overline{N}^{(l)}$, is introduced in NTC by using remainders (56). The time intervals between successive collisions of pair in a homogeneous particle system have an exponential distribution so that the number of collisions obeys the Poisson law. The remainder is a cut-off computational operation that gives uniformly distributed fraction $\mathrm{frac}(\Delta t v_{\max}) \in (0, 1)$. For large $\overline{N}^{(l)}$, the fraction added to the number of collisions in each time step is small compared to the number of collisions realized in the cell. In this case, the effect of adding a random fraction distributed uniformly in the interval (0, 1) to the sum of exponentially distributed intervals (50) is negligible. For small $\overline{N}^{(l)}$, the number of collisions per time step is small ($K = 0, 1, 2$) and the effect of this adding violates significantly the correct estimation of the collision rate. In the MCF scheme, the use of a remainder is avoided by applying conditions (49) and (50), which give a correct integer number of collision-partner selections, distributed in accordance with Poisson's law.

The third source of systematic errors, perhaps the most significant for small $\overline{N}^{(l)}$, concerns the realization of duplicate collisions (successively repeated collisions of the same pair). It was shown[27] that the duplicate (repeated) collisions effectively reduce the collision rate. The intuitive decision to avoid a duplicate collision by choosing a new partner does not solve successfully the problem. Excluding a particle from the process of selection decreases effectively the set of particles by 1. This introduces a systematic error in the collision frequency, which is negligible for large $\overline{N}^{(l)}$ but becomes notable for small $\overline{N}^{(l)}$.[52]

The Bernoulli-trials schemes are approximations of the general operator (47) under conditions of the second limit ($\Delta t \to 0$, $\Delta r^{(l)} \to 0$, $N = \sum_{l=1}^{M} N^{(l)}$ bounded), leading to the governing N-particle equations (29) and (32). This approach extends the features and accuracy of the DSMC method toward a more precise consideration of nonequilibrium gas phenomena including ones which are beyond the Boltzmann equation validity such as nonequilibrium molecular fluctuations and velocity correlations. The main numerical benefit is that the computational grid can be refined keeping the total number of particles N constant or bounded in a computational domain D without introducing sources of systematic errors, which are intrinsic for the standard schemes. The number of collisions in a cell is determined by realization of collisions of the selected individual pairs (i, j) with given probability $w_{i,j}$ without using knowledge about the collision frequency in the considered cell. The corresponding approximation of the general operator (47) chosen among (60)–(63) defines a number of selected pairs and a restrictive condition of the time step ensuring approximation accuracy. The sources of systematic errors are limited mainly to a correct choice of space and time resolution. The other parameter, the total number of simulators, should be determined from a viewpoint of correct simulation of the studied phenomenon. In each cell, the particles are considered as indistinguishable and randomly distributed. Usually, it is ensured by the natural exchange of particles between cells during the step of ballistic motion. In order to ensure an efficient exchange of particles, the time step and cell size are to be coupled with an optimal relation. The violation of some of these conditions and assumptions leads to systematic errors.

The first source of systematic error is an inappropriate discretization in space and time. The violation of the basic condition $prob(k' k\omega_{i,j}\Delta t > 1) \to 0$ is a consequence of this. It must be coupled by a condition for an efficient exchange of particles, which states that the mean transition distance passed by a particle should be approximately equal or less (if needed) to the cell size $\Delta \mathbf{r}^{(l)}$. Both conditions define an optimal relation between time step and cell size,

$$\begin{vmatrix} prob\left(k' k\omega_{i,j}\Delta t > 1\right) \to 0, \ 1 \le i < j \le N^{(l)} \\ \dfrac{\left|\left(c'_m + \mathbf{c}_0\right)\Delta t\right|}{\Delta \mathbf{r}^{(l)}} \sim 1 \end{vmatrix}, \tag{65}$$

where c'_m is the molecular thermal velocity and $\mathbf{c}_0$ is the mean flow velocity.

The ordered selection of the first particle $1 \le i \le N_{sel}$ of each pair is a second source of eventual systematic error if the exchange of particles between cells is small and some particles may hold on in the same cell several time steps. Then, the first N_{sel} particles in this cell are checked for collision more often than the rest of them and some nonphysical velocity correlations may appear. In practice, the natural exchange of particles during the simulation is enough to randomize the set of particles of each cell. However, in case of need, a randomizing procedure is proposed in Ref. 30 that eliminates potential undesired velocity correlations.

The limit $\Delta t \to 0$, $\Delta r^{(l)} \to 0$, while N is fixed, leads to a very precise detection of place and instant of every collision, and only the impact parameters of each collision remain to be chosen at random from probability distributions. It means that under these conditions the DSMC approaches the behavior of the molecular dynamic method. Thus, there is a principal difference between both groups of collision schemes (standard NTC or MCF on one side and Bernoulli-trials on the other side), which is defined by the limit underlying them. The limited number of particles in cells generates systematic errors in the standard collision schemes for reasons related to the Boltzmann-Grad limit conditions, while the basis of the Bernoulli-trials schemes allows the use a small number of particles in cells without introducing typical NTC errors. However, this property requires a more fine resolution in time and space in order to obtain a more accurate solution with a small number of particles per cell. In this situation, the Boltzmann equation solution is also achieved if the local gas flow satisfies the Boltzmann gas properties.

In the final part of this study, the different limit behavior of both groups of collision-partner selection schemes is illustrated by DSMC calculations of the near-continuum, one-dimensional heat conduction flow between two parallel infinite plates.[53] The convergence of the standard NTC scheme (denoted as DSMC94) and its sophisticated modification—Nearest-neighbor NN scheme (denoted as DSMC07)—has been studied on this problem systematically by Gallis *et al.*[54,55] Later analogous calculations by using the Simplified Bernoulli-trials (SBT) scheme have been performed by Taheri *et al.*[36] The convergence analysis in these papers has been performed for different time steps Δt, cell sizes $\Delta \mathbf{r}^{(l)}$, and average numbers of particles per cell $\overline{N}^{(l)}$ by varying them independently within a range of interest.

All numerical results presented in the current study are obtained for the same basic parameters of the Fourier flow, given in the work of Rader *et al.*[53] and Taheri *et al.*[36] The test case is pure heat conduction between two diffusively reflecting walls with different temperatures $T_1 = 223.15$ K at $x = 0$ and $T_2 = 323.15$ K

TABLE I. Heat flux Q (computed at walls) with constant number of cells $M = 400$ between walls and various total number of simulators N in domain D (a test with respect to the Boltzmann-Grad limit with various $\overline{N}^{(l)}$ of simulators per cell).

M (cells)	$\overline{N}^{(l)}$ (simulators)	$\lvert c'_m \Delta t\rvert / \Delta \mathbf{r}^{(l)}$	Q_{SBT}	Q_{NTC}	Q_{NN}	Samples
400	200	0.5	1511	1512	1513	500 000
400	30	1.0	1514	1514	1515	1 000 000
400	10	1.0	1522	1501	1487	1 500 000
400	5	1.0	1536	1439	1430	3 000 000

TABLE II. Heat flux Q (computed at walls) with various number of cells M between walls and constant total number of simulators $N = 12\,000$ (a test with respect to the limit $\Delta t \to 0$, $\Delta r^{(l)} \to 0$ and $N = \sum_{l=1}^{M} N^{(l)}$ fixed).

M (cells)	$\overline{N}^{(l)}$ (simulators)	$\frac{\lvert c'_m \Delta t\rvert}{\Delta \mathbf{r}^{(l)}}$	Q_{SBT}	Q_{NTC}	Q_{NN}	$\frac{t_{SBT}}{t_{ref}}$	$\frac{t_{NTC}}{t_{ref}}$	$\frac{t_{NN}}{t_{ref}}$	Samples
400	30.0	1.0	1514	1514	1515	1.3	1.0	1.7	1 000 000
1 200	10.0	1.0	1513	1504	1462	1.5	1.2	1.8	1 000 000
2 400	5.0	1.0	1512	1501	1423	1.6	1.4	1.9	1 000 000
12 000	1.0	1.0	1514	1265	1403	2.0	2.0	2.5	1 000 000
24 000	0.5	1.0	1514			2.7			1 000 000
120 000	0.1	1.0	1514			5.6			1 000 000

at $x = L$. The distance between the walls is equal to $L = 0.001$ m, and initially, the gap is filled with motionless gas at the reference pressure and temperature: $P_{init} = P_{ref} = 266.644$ Pa (2 Torr) and $T_{init} = T_{ref} = 273.15$ K. Simulations were performed using the hard-sphere argon with molecular mass $m = 6.63 \times 10^{-26}$ kg and reference viscosity $\mu_{\text{ref}} = 2.117 \times 10^{-5}$ Pa s at reference temperature. The employed value for the argon molecular diameter is $d_{\text{ref}} = 3.658 \times 10^{-10}$ m. Bird's one-dimensional code DSMC1[4] is modified to include the Generalized Bernoulli-trials (GBT) scheme. All variables and functions of the code are converted to double precision. The modified DSMC1 code has been employed to perform all calculations with the GBT scheme with a number of particle pair selections $N_{sel} = N^{(l)} - 1$ (equivalent to the use of the SBT scheme). The numerical results for the standard NTC and the nearest-neighbor NN schemes have been obtained by employing Bird's sophisticated one-dimensional executable code DS1, available on Bird's website. The calculations have been performed on a uniform grid with a uniform time step.

In order to approach the limit behavior of the studied collision-partner selection schemes, computations have been performed for a set of parameters varying toward the corresponding limit. The heat flux is chosen to illustrate the DSMC calculations as the most sensitive macroscopic parameter of the studied pure conduction heat transfer problem. The starting point for the analysis is the case calculated by the NTC scheme with the number of cells $M = 400$ and average number of particles per cell $\overline{N}^{(l)} = 200$, which gives heat flux at walls $Q = 1512$ w/m^2, determined in the previous studies[54,55] as close enough to the exact solution. This case was calculated again by using three different collision schemes SBT (presenting the Bernoulli-trials group), NTC, and NN (presenting the standard schemes) with different numbers of particles per cell $\overline{N}^{(l)}$ keeping constant the cell size and time step. The results are summarized in Table I. The statistical sample size is collected over a number of time steps given in the last column of the table identical for all three schemes. One can see that for $\overline{N}^{(l)} = 200$ all SBT, NTC, and NN give an established heat flux very close to the exact solution with small deviations less than 0.2%. These deviations are assumed to be within the range of approximation error of the method and are beyond the aims of our analysis. Decreasing the number of particles, the heat flux obtained by the

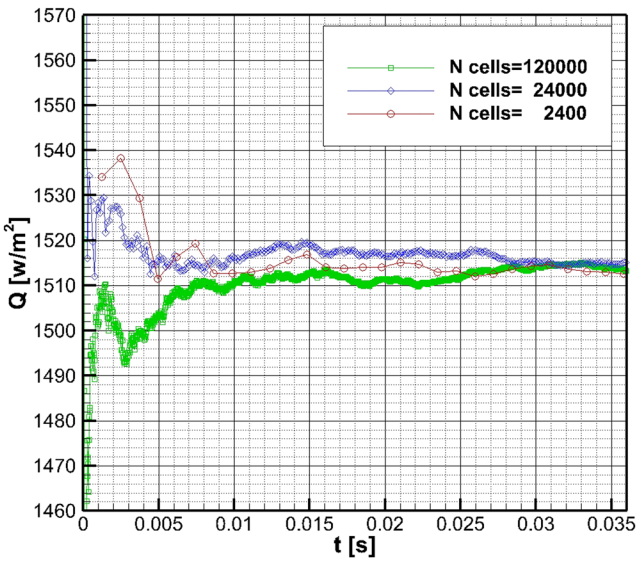

FIG. 2. Heat flux time evolution for three SBT simulations (see Table II).

standard collision schemes NTC and NN deviates notably from the exact solution. According to the error source analysis above, this is due to the violation of the Boltzmann-Grad limit conditions (assuming a large number of particles in cells), required for using the estimation of collision frequency (51). The heat flux obtained by SBT also deviates slightly. The reason is different. According to the second limit, the time and space resolution is not fine enough to keep accuracy of the approximating solution with the employed number of particles within a given range.

The effect of time and mesh refining in agreement with the second limit conditions is shown in Table II for the same three collision-collision selection schemes. The mesh refinement is coupled with a decrease in time step so that the mean transition time for passing a cell satisfies the condition $|c'_m \Delta t|/\Delta \mathbf{r}^{(l)} = 1$. The relative computational time t/t_{ref} for passing a number of time steps given in the last column is also presented in the table. It is clearly seen that with the time and mesh refining the standard NTC and NN quickly failed to keep the accuracy of the solution due to violation

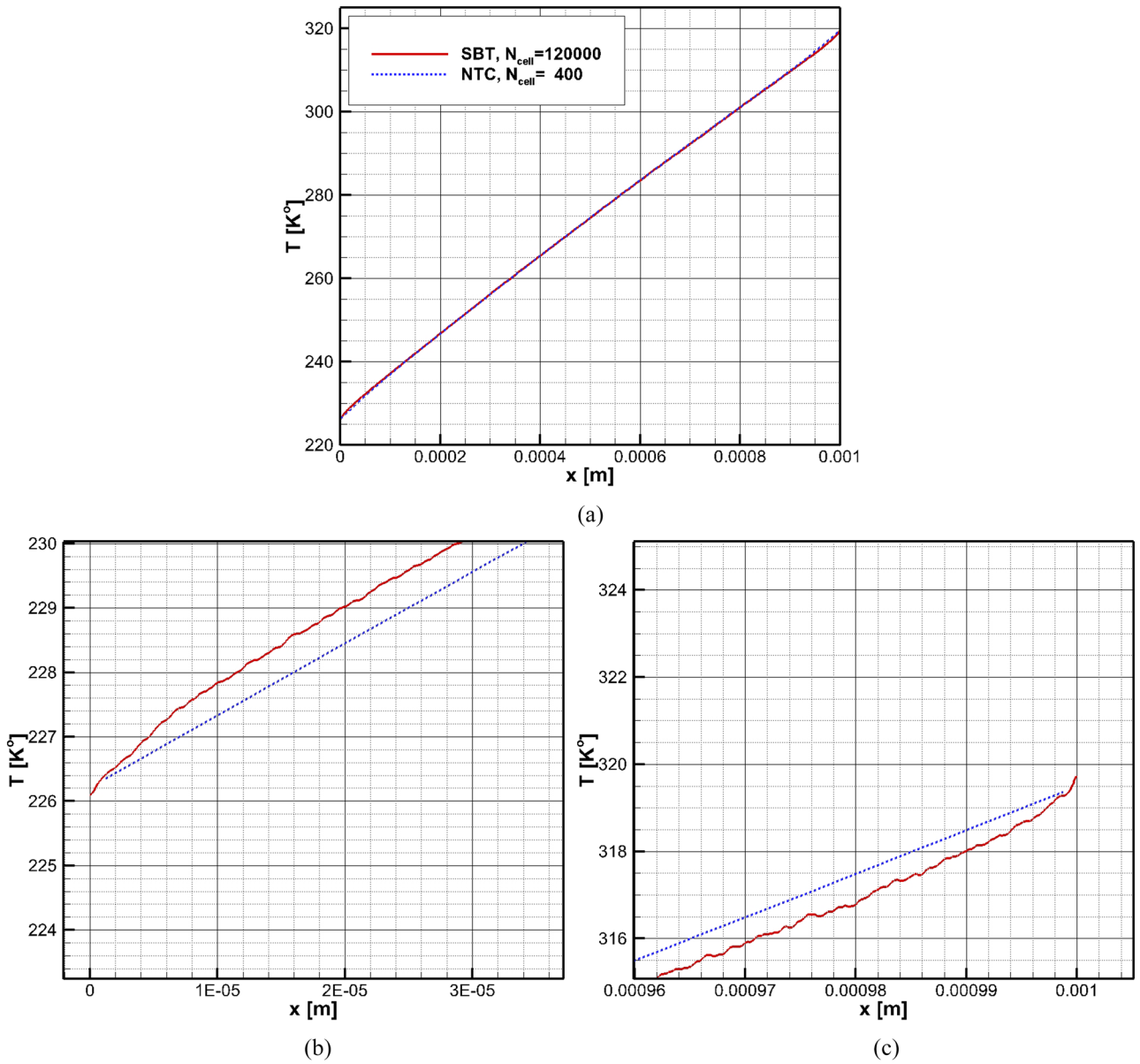

FIG. 3. Comparison of temperature profiles, obtained with NTC (M = 400 cells and $\overline{N}^{(l)} = 30.0$) and SBT ($M$ = 120 000 cells and $\overline{N}^{(l)} = 0.1$). Temperature profiles (a) in the entire domain and the zoomed (b) left boundary part and (c) right boundary part of profiles, showing details of temperature jumps and different nonlinear behavior of both solutions.

of the basic requirement of the Boltzmann-Grad limit for keeping a large number of particles in arbitrary small cells. The behavior of the SBT solution is quite different. In spite of the decrease in the average number of simulators down to $\overline{N}^{(l)} = 0.1$, with coupled refining of time and mesh, the SBT scheme continues keeping a high approximation accuracy and the systematic error remains very small.

The convergence history of the heat flux time evolution is shown in Fig. 2. One can see that the coupled refinement of time step and mesh increases the number of time steps to reach the steady state regime and, respectively, the computational time needed to obtain an accurate solution. This should be taken into account when choosing a strategy for optimal calculations.

Temperature profiles between the two walls, obtained by using the NTC scheme with $M = 400$ cells and the SBT scheme with $M = 120\,000$ when keeping identical the total number of simulators $N = 12\,000$, are compared in Fig. 3. The agreement is excellent in a larger part of the distance between walls. Differences are observed in the areas near the walls. The parts are zoomed and the details of the temperature profile and temperature jump are shown in Fig. 3: (b) in the left area near the cold wall and (c) in the right area near the hot wall. It is clearly seen that near the walls both solutions differ from each other remarkably and the nonlinear character of the temperature profile is better pronounced in the SBT solution. The other important observation is that the temperature jump at walls can be calculated with high accuracy by using SBT (respectively, GBT) on a fine grid. This example demonstrates the capability of the SBT (respectively, GBT) solution on a fine grid with a small number of particles in cells to capture precisely near-wall nonequilibrium effects of a rarefied gas flow.

The analysis of the local governing equation and general transition operator shows that any modifications of the collision-partner selection scheme, taking into account the details of particle location distribution in cells, such as the separation distance in NN scheme,[5] intelligent particle choice,[34] and collision probability modification[56] in a cell, may destroy the basic assumption for local homogeneity and introduce new systematic errors. The results obtained by the nearest-neighbor (NN) collision scheme with a small number of particles in cells in this section demonstrate this negative effect on the heat flux estimation.

VII. CONCLUSIONS

The analysis in this paper has shown that, by starting from the basic principles which lay in the fundament of the Direct Simulation Monte Carlo (DSMC) method, a novel nonhomogeneous N-particle kinetic equation has been derived. Its local 3D-character in physical space and 3N-dimensions in velocity space have required introduction of a randomized model of particle sets in cells of the mesh covering the computational domain. It has been found that the randomized model asymptotically approximated the Boltzmann equation properties under specific conditions.

The general transition operator describing the evolution of the randomized model during the collision process has been used to proof the derivation of all known DSMC collision schemes, including the standard NTC, from the collision operator of the randomized model.

The popular collision-partner selection schemes, represented by the standard NTC and Bernoulli-trials approximations of the general transition operator, represented by Simplified Bernoulli-trials (SBT) as a particular case of the Generalized Bernoulli-trials (GBT) scheme, have been tested against conditions of two approximation limits: first, leading to the Boltzmann equation and, second, leading to the novel N-particle kinetic one. The main sources of systematic errors have been revealed by analysis of the behavior of the collision schemes with regard to both the limits.

The numerical results presented in Sec. VI in the tables and figures suggest some general conclusions regarding the quality of the analyzed collision-partner selection schemes that could be useful for optimal application of the DSMC method.

If the studied problem permits the use of a coarser mesh with a large number of simulators in cells, the standard NTC or MFC schemes are preferable due to their slightly better efficiency. If the problem requires the use of fine or transient adaptive grid with fine sub-cell resolution, then the Bernoulli-trials schemes GBT or SBT should be applied in the areas with a small number of simulators. Moreover, the use of GBT or SBT must be accompanied with coupling of time step and cell size.

Preferably, GBT or SBT should be applied on a fine grid in areas with strong nonequilibrium or in zones with potential velocity correlations. The near-wall or shock wave layers might be such areas.[57,58]

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