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A generalized form of the Bernoulli Trial collision scheme in DSMC: Derivation and evaluation

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ABSTRACT

The impetus of this research is to present a generalized Bernoulli Trial collision scheme in the context of the direct simulation Monte Carlo (DSMC) method. Previously, a subsequent of several collision schemes have been put forward, which were mathematically based on the Kac stochastic model. These include Bernoulli Trial (BT), Ballot Box (BB), Simplified Bernoulli Trial (SBT) and Intelligent Simplified Bernoulli Trial (ISBT) schemes. The number of considered pairs for a possible collision in the above-mentioned schemes varies between $N^{(l)}(N^{(l)}-1)/2$ in BT, 1 in BB, and $(N^{(l)}-1)$ in SBT or ISBT, where $N^{(l)}$ is the instantaneous number of particles in the lth cell. Here, we derive a generalized form of the Bernoulli Trial collision scheme (GBT) where the number of selected pairs is any desired value smaller than $(N^{(l)}-1)$, i.e., $N_{sel} < (N^{(l)}-1)$, keeping the same the collision frequency and accuracy of the solution as the original SBT and BT models. We derive two distinct formulas for the GBT scheme, where both formula recover BB and SBT limits if $N_{\rm sel}$ is set as 1 and $N^{(l)}-1$, respectively, and provide accurate solutions for a wide set of test cases. The present generalization further improves the computational efficiency of the BT-based collision models compared to the standard no time counter (NTC) and nearest neighbor (NN) collision models.

1. Introduction

Direct Simulation Monte Carlo method (DSMC) [1] is the dominant technique for numerical simulation of rarefied flow at the hypersonic regime and at micro/nano scales. The method considers a significant number of simulator particles whose positions and velocities are updated during a consecutive series of ballistic motion and intermolecular binary collisions between particles localized in the neighborhoods of given points in the space, i.e. in cells of a computational grid. Sampling of macroscopic flow field properties is performed for particles positioned inside a cell.

The collision process in DSMC is introduced statistically. During the past decades, various collision algorithms have been suggested. The commonly accepted and widely used No Time Counter (NTC) scheme and its modern variants such as nearest neighbor (NN) are analyzed and discussed widely [2–5]. Majorant Frequency scheme (MFS) is another well-known collision scheme developed by Ivanov [6]. Within a time-step interval of Δt, the method uses a time-interval of δt_i sampled from the Poisson distribution for each accepted collision. The collision process continued until $\sum_i \delta t_i > \Delta t$. In this article, we consider

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the other branch of plausible collision algorithms based on the Kac stochastic equation [7]. The first Bernoulli trials scheme (BT) was put forward by Belotserkovskii and Yanitskiy [8] and Yanitskiy [9]. In accordance with the Kac equation, BT model defines a collision probability function for each particle pair and check all $N^{(l)}(N^{(l)}-1)/2$ pair combinations for a potential collision, where $N^{(l)}$ is the number of particles in the lth cell. Even though the BT scheme avoids the possibility of the repeated collisions, it suffers from high computational costs, i.e., $O(N^2)$. A reduced variant of the BT scheme was developed by Yanitskiy and coworkers, called Ballot Box (BB) [8]. The scheme selects just one pair in random form the whole set of particles available in the cell, but it increased the collision probability of the selected pair by a factor of $N^{(l)}(N^{(l)}-1)/2$. The disadvantage of the Ballot Box scheme is that the scheme required a small collision time step with respect to the optimal time step of the DSMC simulation. In 2011, Stefanov introduced a "simplified" alternative of the Bernoulli Trials scheme called 'SBT' [10,11], with a linear dependency of computational cost on the number of particles per cell, i.e., selecting and checking collision of $N^{(l)}-1$ pairs, with the same level of accuracy as BT. Nevertheless, the computational costs for a larger number of particles per cell are yet significant and numerical efficiency of the SBT is still less than the corresponding characteristics of the standard NTC collision scheme.

The objective of the current work is to derive a generalized form of the Bernoulli Trial collision scheme and reduce further the computational effort of the SBT collision model when the number of particles is comparable with that used in the simulations with the NTC scheme. Here, our starting point is the Kac stochastic model and the derivation of the BT, BB and SBT scheme from the solution operator of the equation considering various levels of mathematical approximations. Then, a general strategy for further simplification of the solution operator is presented, and a general Bernoulli Trials scheme is derived assigned to work with any number of chosen pairs smaller than $N^{(l)}-1$ with no loss of accuracy compared the SBT scheme when the time step and cell size are chosen appropriately. Following Gallis et al. [12] and Taheri et al. [13], the convergence behavior of the new scheme is evaluated in treating one dimensional Fourier problem in slip regime. Furthermore, the accuracy of the GBT scheme in simulating dissociation of gases is considered. The method is then assessed for variety of non-equilibrium gas flow problems such as supersonic steady shock wave, micro/nano cavity flow, and 70-degree blunted cone.

2. Kac master equation

2.1. Principles

Kac stochastic model [7] is a kinetic equation describing the temporal evolution of N-particle velocity distribution function $F_{N^{(l)}}(t, x^{(l)}, c_{N^{(l)}})$ of N-particle system caused by binary collisions. Vectors $x^{(l)} = \{x_1^{(l)}, x_2^{(l)}, \ldots, x_N^{(l)}\}$ and $c^{(l)} = \{c_1^{(l)}, c_2^{(l)}, \ldots, c_N^{(l)}\}$ present particle coordinates $x_i^{(l)} = \{x_i^{(l)}, y_i^{(l)}, z_i^{(l)}\}$ and velocities. $c_i^{(l)} = \{c_{xi}^{(l)}, c_{yi}^{(l)}, c_{zi}^{(l)}\}$ of a set of particles occupying volume $V^{(l)}$ (usually, volume of cell l in a computational grid) at instant t. The Kac stochastic model can be described in the following operator form [9,14]:

$$\frac{\partial}{\partial t}F_{N^{(l)}}\left(t, x^{(l)}, c_{N^{(l)}}\right) = \left[\sum_{1\le i<j\le N^l} w_{ij}(T_{ij}-I)\right]F_{N^{(l)}}\left(t, x^{(l)}, c_{N^{(l)}}\right) = \upsilon(T-I)F_{N^{(l)}}\left(t, x^{(l)}, c_{N^{(l)}}\right), \tag{1}$$

where I is the identity matrix, υ is the collision frequency, and

$$T_{ij} = \int_{4\pi} \psi(c_{ij})B(g_{ij}, \theta)d\Omega(\theta),$$

$$\upsilon = \sum_{1\le i<j\le N^l} w_{ij}; \tag{2}$$

$$T\psi = \sum_{1\le i<j\le N^l} w_{ij}T_{ij}\psi, \quad w_{ij} = \frac{\sigma_{ij}g_{ij}}{V^l}, \tag{3}$$

operator T_{ij} accounts for transformations of particle velocities in results of collisions, $B(g_{ij}, \theta)$ is the collision scattering kernel, $\Omega(\theta)$ is the solid angle, $\psi(c_{ij})$ is a linear normalized space of continuous functions over $\Omega(\theta)$, $g_{ij} = |c_i - c_j|$ and σ_{ij} are the relative velocity and collision cross-section of the colliding pair, respectively. For brevity, in the following consideration we assume by default that all mathematical requirements are fulfilled. The Kac stochastic model is a jump-like strictly Markovian process over the hypersphere $\Omega(N^{(l)}, E, P)$ of $3N^{(l)}-4$ dimensions in Euclidean space $R_{3N}^{(l)}$, where $N^{(l)}$ is the number of particles in the (lth) cell, E is the kinetic energy and P is the momentum of velocity components.

The probability of time interval between two consecutive collisions follows the Poisson distribution:

$$Prob(\delta t > t) = e^{-\upsilon t} \tag{4}$$

Kac equation could be solved at time t with the definition of the transition operator $G(t)$ in the following form:

$$F_{N^{(l)}}\left(t, x^{(l)}, C_{N^{(l)}}\right) = G(t)F_{N^{(l)}}\left(t_0, x^{(l)}, C_{N^{(l)}}\right), \tag{5}$$

where $F_{N^{(l)}}(t_0, x^{(l)},\ C_{N^{(l)}})$ indicates the initial distribution function and the transition operator $G(t)$ could be written as:

$$G(t) = \exp\left[t \sum_{1\le i<j\le N^l} w_{ij}(T_{ij} - I)\right] = \exp\left[t(T - I)\right] \tag{6}$$

2.2. Bernoulli trials

For small interval dt, operator $G(dt)$ given in Eq. (6) can be expanded with respect to degrees of dt and terms of order equal or higher than $O(dt^2)$ be omitted. The approximated transition operator $G(dt)$ is written as [8,9]:

$$G_1(dt) \approx \prod_{1\le i<j\le N^l} \exp\left[(T_{ij} - I)w_{ij}dt\right] = \prod_{i=1}^{N^{(l)}-1} \prod_{j=i+1}^{N^{(l)}} \exp\left[(T_{ij} - I)w_{ij}dt\right] \tag{7}$$

The exponential term in every co-factor in Eq. (7) could be substituted by a linear approximation over dt using Taylor expansion, consequently:

$$G_1(dt) \approx \prod_{i=1}^{N^{(l)}-1} \prod_{j=i+1}^{N^{(l)}} \left[(1 - w_{ij}dt)I + w_{ij}dtT_{ij}\right] = \prod_{i=1}^{N^{(l)}-1} \prod_{j=i+1}^{N^{(l)}} \left[(1 - W_{ij})I + W_{ij}T_{ij}\right], \tag{8}$$

where

$$W_{ij} = \frac{\sigma_{ij}g_{ij}dt}{V^{(l)}} \tag{9}$$

has a meaning of collision probability of pair (i, j) and is normalized in a way to satisfy the condition $prob(W_{ij} > 1) \to 0$. Every co-factor in the right-hand-side of Eq. (8) transforms the velocity distribution function $F_{N^{(l)}}(dt, x^{(l)}, c_{N^{(l)}})$ into $\overline{F_{N^{(l)}}}(dt, x^{(l)}, c_{N^{(l)}})$ over $\Omega(N^{(l)},\ E,\ P)$ according to:

$$\overline{F_{N^{(l)}}}\left(dt, x^{(l)}, c_{N^{(l)}}\right) = (1 - w_{ij}dt)F_{N^{(l)}}\left(dt, x^{(l)}, c_{N^{(l)}}\right) + w_{ij}dt \int_{4\pi} \psi(c_{ij})B(g_{ij}, \theta)d\Omega(\theta), \tag{10}$$

If the time interval dt is considered small such that:

$$W_{ij} = \frac{\sigma_{ij}g_{ij}dt}{V^{(l)}} = w_{ij}dt \le 1 \tag{11}$$

for all possible values of $c_{N^{(l)}}$, Eq. (8) have an apparent algorithmic interpretation. In order to clarify this, we will note two basic probabilistic properties that are used in our further considerations. They concern the probabilistic meanings of product of probabilities $p_A p_B p_c \ldots$. and the second – sum of probabilities $p_A + p_B + p_c \ldots$ of a set of events A, B, C etc. They state that the probability for happening of a set of events $A \cap B \cap C \ldots$. is equal to the product $p_A p_B p_c \ldots$ and the probability of one of all these events $A \cup B \cup C \ldots$. is equal to the sum $p_A + p_B + p_c \ldots$ Using this properties, the probabilistic interpretation is that the collision scheme based on Eq. (8) consists of double product of an operator concerning a pair collision and respectively, must consider the collisions of all $N^{(l)}(N^{(l)} - 1)/2$ pairs of particles $(c_i,\ c_j)$ and with probability p_{ij} accepts the occurrence of the corresponding collision or with probability $(1 - p_{ij})$ rejects it. This scheme is of first order accuracy in terms of time step but its computational costs is of order N^2. The condition given by Eq. (11) could be replaced with a weaker one as follows:

$$P\{w_{ij}dt > 1\} \ll 1 \tag{12}$$

by choosing appropriate time step and cell size. The above procedure states that for all of the possible particle pairs in the collision cell (l), the collision probability should be checked, i.e. the following inequality should be monitored for all available particle pairs $(i,\ j)$ $\{i <\ j = 1, \ldots, N^{(l)}\}$ (before their velocities are changed to post-collision values):

$$W_{ij} = \frac{\sigma_{ij}g_{ij}dt}{V^{(l)}} \ge R_{nf} \tag{13}$$

and accept the collision if $W_{ij} \ge R_{nf}$ and reject it when $W_{ij} < R_{nf}$.

2.3. Ballot Box collision scheme

Consider the transition operator given in Eq. (6) is approximated by cutting the expansion series of operator $G_1(dt)$ (8) to the linear term in terms of dt as:

$$G_2(dt) = I + dt \sum_{1\le i<j\le N^l} w_{ij}(T_{ij} - I). \tag{14}$$

Then, a linearized transition operator should contain a double-sum of probabilities with the number of terms equal to the number of particle pairs denoted by $k = N(N-1)/2$. One probabilistic interpretation suggests choosing only one pair at random from all possible pairs k within a time step instead to check all of them. The probability of to select at random a pair with velocities (c_i, c_j) is constant equal to $1/k$ and must be taken into account in the algorithmic realization. If one introduces constant k inside the summation operator into the operator $G_2(dt)$, replacing $(w_{ij}dt)$ by $\frac{1}{k}(kw_{ij}dt)$, then Eq. (14) could be rewritten as:

$$\begin{aligned} G_2(dt) &= \left[1 - \sum_{1\le i<j\le N^l} \frac{1}{k}(kw_{ij}dt)\right] I + \sum_{1\le i<j\le N^l} \frac{1}{k}(kw_{ij}dt)T_{ij} \\ &= \left(1 - \sum_{1\le i<j\le N^l} s_{ij}p_{ij}\right) I + \sum_{1\le i<j\le N^l} s_{ij}p_{ij}T_{ij} \end{aligned} \tag{15}$$

This form of operator $G_2(dt)$ can be interpreted in a straightforward way that leads to the Ballot Box collision model. In (15), term $s_{ij} = 1/k$ is selection probability of a pair with velocities (c_i, c_j) and $p_{ij} = kw_{ij}dt$ is the collision probability of the selected pair. The weak condition $Prob\{kw_{ij}dt > 1\} \ll 1$ should also be satisfied. In the Ballot Box scheme, the following procedure is performed one time per each cell:

a) At each time step, only a single pair of molecules is randomly selected with probability of $1/k$ from the whole set of particles.
b) The possibility of collision is evaluated with the probability.

$$W_{ij} = kw_{ij}dt = \frac{N(N-1)\sigma_{ij}g_{ij}dt}{2V^{(l)}} > R_{nf} \tag{16}$$

If the collision was accepted, the velocities of the colliding pair are updated to their post-collision values. The computational cost of the scheme depends linearly on the number of particles, i.e., $O(N)$. The problem with the Ballot Box scheme is that $dt \ll \Delta t$ (where Δt is an optimal time step of simulation) in order to fulfill condition $\{Prob(kdtw_{ij)} > 1)\} \ll 1$. The collision algorithm Ballot-Box must be repeated m times per each cell time step Δt, so that $\Delta t = mdt$. In this way, the selection procedure resembles that of the NTC scheme and as a result, the scheme cannot prevent repeated collisions within the time step Δt.

2.4. Simplified Bernoulli-trials

Bernoulli-trials (BT) scheme checks collisions with a given probability for all possible collision pairs. This makes the BT algorithm time-consuming and not suitable for practical applications except when the average number of particles per cell ($\langle N \rangle$) is close to 1. As simplification, Stefanov showed that it is possible to extend the internal product on the right-hand side of the $G_1(dt)$ (Eq. (8)) in a series of j with respect to t and neglect the higher order terms to reach to a new simplified transition operator $G_3(t)$ as follows [10,11]:

$$G_3(dt) = \prod_{i=1}^{N^{(l)}-1} \left[\left(1 - \sum_{j=i+1}^{N^{(l)}} \frac{1}{k}(kw_{ij}dt)\right) I + \sum_{j=i+1}^{N^{(l)}} \frac{1}{k}\left((kw_{ij}dt)T_{ij}\right) \right], \tag{17}$$

where the inner product is replaced by summation and $(k = N^{(l)} - i)$. The algorithmic interpretation of operator $G_3(dt)$ states that instead of checking $N^{(l)}(N^{(l)}-1)/2$ pairs it is possible when pick the first particle i of the next pair in strict order from the particle list, select the second particle at random from $(N^{(l)} - i)$ particles placed after particle i with probability $s_j = 1/(N^{(l)} - i)$ and reduce the number of collision checking to $(N^{(l)} - 1)$. Note that the algorithm covers the whole set of possible collisions. The SBT algorithm permits simulations with far less mean number of particles per cell compared to NTC, $\langle N^{(l)} \rangle \sim 1$–2 and even less than 1 on a finer grid with smaller time step (where $\langle\ \rangle$ means mean value) with reduced computational costs compared to the BT algorithm. The numerical procedure of SBT is as follows: Particles in the lth cell should be locally indexed to produce a particle list numbered as $1 \ldots N^l$. To this aim, the index vectors used in all available DSMC realizations can be used. The first particle of the collision pair (i, j), say i, is selected in sequence from the particle list: $i = 1 \ldots N^l - 1$. The second particle, say j, is chosen randomly with the probability of $1/k$ from $k = N^l - i$ particles taking place in the list after particle i.

$$j = (i+1) + int(k \times R_{nf1}) \tag{18}$$

Each pair is then checked for collision with a corresponding probability, which with taking into account factor F_{num} and time step dt reads

$$W_{ij} = \frac{(N^l - i)F_{num}dt\sigma_{ij}g_{ij}}{V^l} > R_{nf2}. \tag{19}$$

It should be noted that the dt should be adjusted so that in great amount W_{ij} does not exceed unity, say

$$prob\{W_{ij} \geq 1\} \to 0 \tag{20}$$

It is worth noting that the probability for $W_{ij} > 1$ should be kept always close to zero by choosing appropriate cell size and time step. The SBT procedure avoids the production of at least part of the eventually successively repeated collisions which occurs in the NTC scheme when it is applied with a small number of particles. SBT scheme was successfully evaluated for a wide set of rarefied flow test cases [15–20].

2.5. Generalized Bernoulli-trials

The SBT algorithm is more efficient than the original BT scheme, and its efficiency is comparable to the NTC when the number of particles in a cell is small. However, it is still less efficient than the standard NTC in simulations using a relatively larger number of particles per cells and small time step. It is because a fixed number of $N^{(l)} - 1$ pairs should be selected and checked for possible collisions while the NTC usually selects a less number of pairs to check for collision using the estimation of the maximum number of selected pairs for a given time step. The effect in SBT is that most of the selected pairs will not have a significant acceptance chance because their probability W_{ij} is low at a small time step. In this occasion, it is preferred to reduce the number of selected pairs (N_{sel}) to a lower magnitude but increasing the pair weight and respectively the collision probability in such a way that the collision frequency is kept constant. In this regard, a rational option could be considered to reduce the number of selected pairs to $N_{sel} = N^{(l)}/2$ or $N^{(l)}/3$ and even less in order to be of the same number range as the number of selected pairs in the NTC scheme. To start with, the operator form remains the same as given in (17), but the upper bound of the product is reduced to N_{sel}. The new operator reads:

$$G_4(dt) = \prod_{i=1}^{N_{sel}} \left[\left(1 - \sum_{j=i+1}^{N^{(l)}} \frac{1}{k'k} \left(k' k w_{ij} dt \right) \right) I + \sum_{j=i+1}^{N^{(l)}} \frac{1}{k'k} \left(\left(k' k w_{ij} dt \right) T_{ij} \right) \right], \tag{21}$$

where k' is a correction coefficient to compensate the reduction of selected pairs and it must be found. The linearization of the product in (21) with respect to dt gives the following transition operator:

$$G_4'(dt) = \left(1 - \sum_{i=1}^{N_{sel}} \sum_{j=i+1}^{N^{(l)}} \frac{1}{k'k} \left(k' k w_{ij} dt \right) \right) I + \sum_{i=1}^{N_{sel}} \sum_{j=i+1}^{N^{(l)}} \frac{1}{k'k} \left(k' k w_{ij} dt \right) T_{ij}. \tag{22}$$

The operator $G_4'(dt)$ can be realized by selection of one pair similar to the Ballot Box scheme but it here we use it to show how to define the correction coefficient for the selected pairs in the operator with a reduced product.

The correction coefficient k' is obtained from the equality:

$$k' \sum_{i=1}^{N_{sel}} \sum_{j=i+1}^{N^{(l)}} 1 = \sum_{i=1}^{N^{(l)}-1} \sum_{j=i+1}^{N^{(l)}} 1 \tag{23}$$

$$k' \left[\sum_{i=1}^{N^{(l)}-1} \sum_{j=i+1}^{N^{(l)}} 1 - \sum_{i=1}^{(N^{(l)}-N_{sel})-1} \left(\sum_{j=i+1}^{N^{(l)}-N_{sel}} 1 \right) \right] = \sum_{i=1}^{N^{(l)}-1} \sum_{j=i+1}^{N^{(l)}} 1 \tag{24}$$

$$k' \left[C\left(N^{(l)}, 2\right) - C\left(N^{(l)} - N_{sel}, 2\right) \right] = C\left(N^{(l)}, 2\right) \quad \Rightarrow \quad k' = \frac{C(N^{(l)}, 2)}{C(N^{(l)}, 2) - C(N^{(l)} - N_{sel}, 2)}, \tag{25}$$

where $C(n, m) = (n(n-1)\cdots(n-m)/m!$ is the number of combinations of m from n elements, i.e.

$$C\left(N^{(l)}, 2\right) = N^{(l)}\left(N^{(l)} - 1\right)/2 \quad \text{and} \quad C\left(N^{(l)}, 2\right) - C\left(N^{(l)} - N_{sel}, 2\right) = N_{sel}\left(2N^{(l)} - N_{sel} - 1\right). \tag{26}$$

Finally,

$$k' = \frac{N^{(l)}(N^{(l)} - 1)/2}{N_{sel}(2N^{(l)} - N_{sel} - 1)}. \tag{27}$$

The inverse value of the correction coefficient $1/k'$ has a simple probabilistic meaning of selection probability of N_{sel} pairs from all available pairs in the cell, which total number is $N^{(l)}(N^{(l)} - 1)/2$. Consider the matrix of all collision probabilities

$$\left\{ \begin{array}{cccc|ccc} p_{1N^{(l)}} & p_{2N^{(l)}} & \cdots & p_{sN^{(l)}} & \cdots & p_{(N^{(l)}-1)N^{(l)}} & \iddots \\ p_{1(N^{(l)}-1)} & p_{2(N^{(l)}-1)} & & & & \iddots & \\ & & & p_{s(s+1)} & \iddots & & \\ p_{1s} & & & \iddots & & & \\ & p_{23} & \iddots & & & & \\ p_{12} & \iddots & & & & & \\ \iddots & p_{21} & \cdots & p_{s1} & \cdots & \cdots & p_{N^{(l)}1} \end{array} \right\} \tag{28}$$

They are located in the upper triangle of matrix elements $(p_{12}, \ldots, p_{1,N^{(l)}}, \ldots, p_{N^{(l)}-1\ N^{(l)}})$. In the Bernoulli trials BT scheme all particle pairs are checked for collision sweeping the matrix elements one by one; in SBT only one pair from each column is selected at random with probability $1/k$ to be checked for collision and the corresponding collision probability is corrected by coefficient k. In the transition operator (22), N_{sel} pairs are selected by choosing one pair per column at random from the first N_{sel} columns of the matrix. Thus, N_{sel} pairs are selected from $(C(N^{(l)}, 2) - C(N^{(l)} - N_{sel}, 2))$ pairs and the corresponding selection probability of all N_{sel} pairs from all available pairs is $1/k'$. Respectively, the probability of selection of each pair (i, j) is $(1/k'k)$ and consequently, the total collision probability of each selected pair must be corrected by coefficient $k'k$ in accordance with the transition operator (21).

It is worth noting that in our considerations we assumed that the particle set in each cell within a time step is random. In most cases, the exchange of particles between cells during the free particle motion is enough, and no additional acts are needed. However, the universal algorithm should contain an additional procedure of particle rearrangement. In this regards, the suggested procedure for the generalized form of the BT collision model (GBT) is as follows (depicted in Fig. 1):

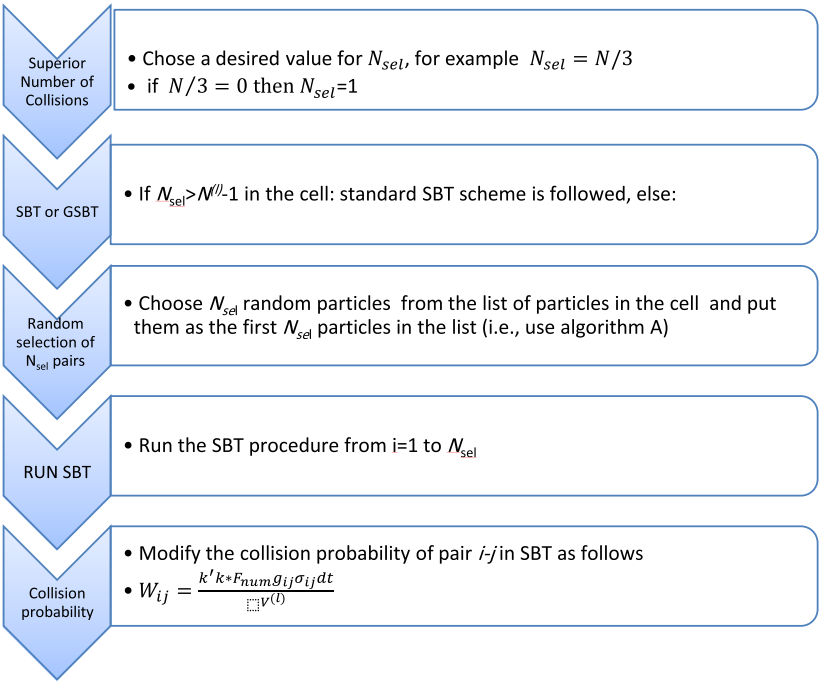


Fig. 1. GBT collision procedure per each cell.

1. Select N_{sel}, i.e., assume N_{sel} is a fraction/function of number of particles in the cell. The following procedure is performed if $N_{sel} < N^{(l)} - 1$ in the cell, otherwise, standard SBT scheme is followed.
2. Algorithm A. Choose N_{sel} random particles from the list of particles in the cell, and reorder the particle list exchanging the positions of the selected particles with those occupying the first N_{sel} positions in the list, i.e., put the N_{sel} selected particles in the index list ordered as first, second, etc. particle in the list. Put the former first, second, etc. particles in their places in the index list.
3. Run the SBT procedure from $i = 1$ to N_{sel}, but modify the collision probability of every pair with the following correction:

$$W_{ij} = \frac{k'k * F_{num} dt \sigma_{ij} g_{ij}}{V^l} \tag{29}$$

where

$$k'k = \frac{C(N^{(l)}, 2)}{N_{sel}(2N^{(l)} - N_{sel} - 1)} \left(N^{(l)} - i\right). \tag{30}$$

Similar to SBT, dt should be adjusted so that W_{ij} in (29) does not exceed unity, i.e., inequality. (20) should be satisfied.

Instead of (30), an alternative collision probability correction in the GBT algorithm is conceivable considering a generalization of the BB and SBT collision formulas, i.e., GBT probability correction should approach to BB and SBT corrections if $N_{sel} = 1$ and $N_{sel} = N - 1$, respectively. To achieve this aim, we slightly modify the BB algorithm to avoid repeated collisions.

The original BB algorithm chooses two particles in random from the whole set of particles in the list. However, we change the particle order and put the first selected particle in the BB procedure as the first particle in the list. The second particle is chosen at random from the particles located after the first one ($i = 1$) in the list of particles. However, the probability correction in the BB scheme, either the original one or the modified version presented here, is $C(N^{(l)}, 2)$, as BB considers only one pair on behalf of all available pairs in the cell. If we pick more pairs out to check their collision possibility, i.e., $N_{sel} > 1$ in GBT, a smaller correction should be introduced, i.e.,

$$\widehat{kk} = \frac{C(N^{(l)}, 2)}{C(N_{sel} + 1, 2)}, \tag{31}$$

where $C(N_{sel} + 1,\ 2)$ stands for the combination of 2 particles from $N_{sel} + 1$ ones. Eq. (31) is the correction incorporating the effects of considering N_{sel} number of selected pairs to be checked for collisions instead of all $N^{(l)}(N^{(l)} - 1)/2$ pairs. The correction given by (31) reduces to $C(N^{(l)}, 2)$ if $N_{sel} = 1$, i.e., BB scheme, and to 1 if $N_{sel} = N^{(l)} - 1$, i.e., SBT scheme. However, the GBT probability correction should include another term compensating the selection of just *one particle* from the particles located after the i-th particle in the list. If SBT with $N_{sel} = N^{(l)} - 1$ is considered, the additional term of the probability correction for the i-th particle should be $(N^l - i)$, while for BB with $N_{sel} = 1$, there is no need for an extra correction in (31). In order to capture both SBT and BB limits, the complementing correction term in (31) should read as: $(N_{sel} + 1 - i)$. Consequently, an alternative GBT collision probability correction instead of (30) reads as:

$$k'k_2 = \frac{C(N^{(l)}, 2)}{C(N_{sel} + 1, 2)}(N_{sel} + 1 - i). \tag{32}$$

In the rest of this paper, we refer to GBT formula with Eq. (30) as Scheme-1 and with Eq. (32) as Scheme-2. We will compare the accuracy of both schemes and show that both algorithms demonstrate the same level of accuracy. Both, Scheme-1 and Scheme-2 give the same collision rate per time step but the difference between them consists of different distributions of the collision probability of the selected pairs – the collision probability in Scheme-1 is more balanced and uniform, while the collision probability in Scheme-2 is linearly changing from a larger collision probability than the average for the first selected pairs to a smaller probability than the average for the last selected pairs. For the limit cases, $N_{sel} = 1$ and $N_{sel} = N - 1$, both algorithms are equivalent with respect to probability distribution. It is worth noting that when we reorder the randomly selected first particles (algorithm A), for appropriately chosen time step and cell size, the results become independent on the collision probability distribution of the selected pairs and depend only on the average collision probability of a pair. Consequently, both algorithms become stochastically equivalent.

3. Results and discussions

3.1. Collision frequency test case

Here, we demonstrate the accuracy of the GBT scheme solution for a series of test cases at rarefied flow conditions. The first test case is the calculation of the equilibrium collision frequency ratio that is the ratio of the numerical collision frequency to that of the theoretical one. The problem considered here is a spatially homogeneous monoatomic gas released from a random state to reach the equilibrium. The gas comprises of molecules with a reference diameter of 0.35 nm at a reference temperature of 300 K. The molecular mass of the gas is assumed to be 5×10^{-26} kg. The initial number density of gas is 1×10^{20} m^{-3} at the reference temperature. The flow field extends in the x-direction from the origin to $x = 1$ m. The cells width changed with the number of cells. The number of simulated particles was also altered to study the validity of the algorithm with different sets of particles per cell (N). The zero-dimensional code of Bird [1] was modified to include the GBT algorithm. In all simulations, the value of $\Delta x/\Delta t$ ($\Delta x = dx/\lambda$ and $\Delta t = dt/t_c$, where λ is the gas mean free path and t_c is the mean collision time) is regulated to be smaller than 2. The number of cells is set at 2000, resulting in $dx = 5 \times 10^{-4}$ m. The time step is fixed to 1×10^{-6} s. These values of dx and dt led to $\Delta x/\Delta t = 1.228$. We compare both probability correction formulas suggested for the GBT scheme by Eqs. (30) and (32). The results are reported for the same initial condition with $N = 10$, while N_{sel} was changed from 1 to $N - 1$. Table 1 shows the results of CF_{ratio} from both GBT formulas as well as the NTC predictions. The equilibrium collision rate per molecule is given theoretically (CF_{th}) by [1]:

$$CF_{th} = 4nd^2\sqrt{\frac{\pi K_B T_{ref}}{m_s}}\left(\frac{T}{T_{ref}}\right)^{1-\omega} \tag{33}$$

where n, d, K_B, T_{ref}, m_s, and ω are number density, gas molecular diameter, Boltzmann constant, reference temperature, molecular mass, and viscosity–temperature exponent, respectively. CF_{num} represents the numerical prediction of the collision frequency that is calculated by the division of the number of collisions in each cell (N_{coll}) to the simulation time ($Time$) and half of the mean particle numbers per cell ($0.5N_p$) as follows:

$$CF_{num} = \frac{N_{coll}}{0.5N_p Time} \tag{34}$$

CF_{ratio} is the ratio of the numerical to the theoretical value, and it must have a magnitude equal to unity at the equilibrium condition. The table shows that solution of both GBT algorithms almost match together and are around unity with a good precision.

Table 1
CF_{ratio} prediction in the 0-D test case from GBT calculations with either of Eq. (30) (Scheme-1) and Eq. (32) (Scheme-2) formulas.

N_{Sel}	1	2	3	4	5	$N-3$	$N-2$	$N-1$	NTC
Scheme-1	1.000128	1.000231	1.000120	1.000131	1.000059	0.999618	1.000004	1.000055	1.000001
Scheme-2	1.000128	1.000120	1.000012	1.000173	0.999277	0.999610	1.000056	1.000055	

3.2. Simple dissociation test case

In order to examine the performance of the GBT scheme to treat chemically reacting flows, we performed a sample test case of dissociation of real gas. For this purpose, zero-dimensional code of Bird (DSMC0D) [1] was modified to include the GBT algorithm. The gas that assumed here is the nitrogen with a reference diameter of 0.417 nm at a reference temperature of 273 K. The molecular mass of the gas is considered to be 4.65×10^{-26} kg. The flow field extends in the x-direction from the origin to $x = 1$ m and the number of cells is assumed to be 1. The total number of particles was set as 10000. The time step for the NTC reference data was 2.5×10^{-11} s, but this value is decreased to 1×10^{-11} s, to avoid the $W_{ij} > 1$ in the GBT simulations. In the general case of 1, 2 and 3 dimensional simulations, the choice of an optimal time step during the simulation can be calculated automatically every time step or time interval consisting of a number of steps by checking equality (20) in each cell for each collision pair and allowing a collision rate with small fixed percent (usually not larger than (2–3)%) of collisions with values of W_{ij} (Eq. (29)) greater than 1. Usually, this limitation is necessary in some local zones of the computational domain but it defines a minimal global time step for the whole computational domain. Thus, in the rest of computational domain the inequality (20) will be almost surely satisfied. Here, the zero-dimensional test case considers the relaxation of nitrogen from an initial excitation vibrational temperature to the chemical equilibrium. Because of dissociation and recombination process, the gas composition is changing toward a chemical equilibrium. When the rate of dissociation and recombination is equal, the gas reaches chemical equilibrium. The following expression gives the equilibrium degree of dissociation (α) as a function of initial number density n_i and the equilibrium temperature T:

$$\alpha^2/(1-\alpha) = \left(0.5047 \times 10^{28}/n_i\right) T^{1/2} \left\{1 - \exp(-3395/T)\right\} \left\{4 + 10\exp(-27658/T) + 6\exp(-41495/T)\right\}^2 \exp(-113200/T) \tag{35}$$

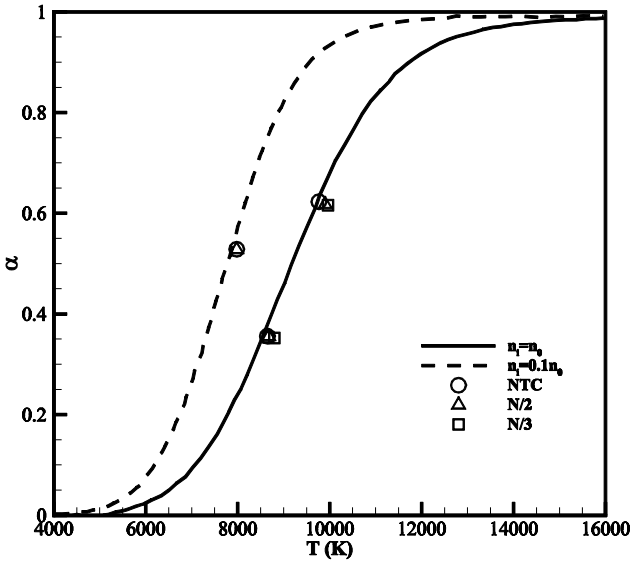


Fig. 2. Equilibrium degree of dissociation in nitrogen.

Fig. 2 shows the equilibrium degree of dissociation as a function of temperature for an initial number density equal to standard number density. Moreover, the results for another initial number density of one-tenth of standard value are reported in this figure. The considered cases repeat the same cases examined by Bird (see Fig. 11–15 of Ref. [1]). The GBT

results from different sets of selecting particles ($N_{sel} = N/2,\ N/3$) are compared with the theoretical data from Eq. (35) and NTC results.

Two cases with different initial temperatures equal to 30000 K and 20000 K but with the same number density equal to the standard number density relax approximately to temperature magnitudes of 9800 K and 8650 K, respectively. Both results are shown together with the theoretical line and corresponding NTC data for $n_i = n_0$ from [1]. The other case is the relaxation from an initial temperature of 25000 K and one-tenth of standard number density that is indicated on the $n_i = 0.1n_0$ line. All cases are in a suitable agreement with the theoretical solution and numerical data obtained by using the standard NTC scheme.

3.3. GBT convergence behavior for the fourier problem

In order to study the convergence behavior of the new scheme, we simulated rarefied Fourier problem in the slip regime. The problem was considered by Gallis et al. [12] and Taheri et al. [13] to investigate the convergence behavior of the NTC and SBT collision schemes, respectively. In the Fourier problem, the gas is confined between two infinite, parallel, fully accommodating walls separated by a distance L, that is shown schematically in Fig. 3. One dimensional code of Bird (DSMC1) is modified to include the new algorithm. Hard-sphere molecules of argon with a reference diameter of $d_{ref} = 3.658 \times 10^{-10}$ m at the reference temperature of 273.15 K are considered. The molecular mass and the reference viscosity of simulated molecules are $m = 6.63 \times 10^{-26}$ kg and $\mu_{ref} = 2.117 \times 10^{-5}$ Pa s, respectively. The simulations were performed at the reference pressure of $P_{init} = P_{ref} = 266.644 \times 10^{-5}$ Pa. Moreover, the Knudsen number was set at 0.0237. The separated distance between the walls was $L = 1$ mm and a modest temperature gradient was applied on the walls, i.e., the walls are kept at the unequal temperature of $T_{hot} = T_{reff} + \Delta T/2$ and $T_{cold} = T_{reff} + \Delta T/2$, where $\Delta T = 100$ K.

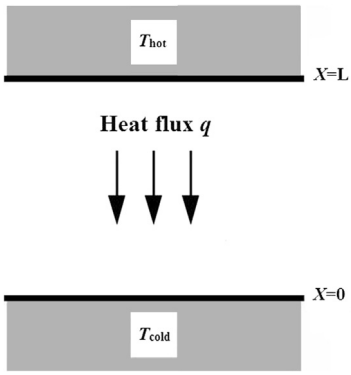


Fig. 3. Schematic of the Fourier problem.

We followed the strategy suggested in [13] to study the convergence behavior of the GBT scheme. For more details, we address the readers to this paper. The GBT convergence behavior for the heat flux is investigated over a range of discretization parameters and N_{sel}. Firstly; we study the effect of number of simulated particles per cell on the convergence behavior. For this purpose, simulations results reported in Table 2 are performed with a fixed number of cells, i.e., 400 cells, and time step is set constant at 0.625 ns, while the number of simulated particles is increased from 10 to 60, and moreover for each value of particle per cell (PPC), the number of selected particles for collisions (N_{sel}) is changed. In the limiting conditions of PPC and dx parameters (PPC $\to \infty$ and $dx \to 0$), according to Gallis et al. [12] the wall heat flux converges to a value $q = 1512$ W/m^2 that could be accepted close enough to the mathematically expected one for this problem. The results of these simulations are presented in Table 2. The results indicate that as the number of particles per cells was increased from 10 to 60, the heat flux magnitude approaches to the mathematically expected value. A slight dependency on N_{sel} is detectable from the data in the table.

Table 2
Heat flux dependence on PPC at various N_{sel}.

N_{sel}	q (W/m^2) (PPC = 10)	q (W/m^2) (PPC = 60)
$N-1$	1525	1513
$N/2$	1526	1515
$N/3$	1531	1515
$N/4$	1531	1513
BB	1536	1519

Considering the general recommendations for the cell size and time step in DSMC, i.e., $\Delta x = dx/\lambda \approx 0.33$ and $\Delta t = dt/t_c \approx 0.25$, where t_c is the mean collision time, it is reported that the SBT solution needs a $1 < \Delta x/\Delta t < 2$ in addition to

keeping both of cell size and time step small to provide a converged solution [13]. In other words, the ratio $\Delta x/\Delta t$ should be chosen in a way to fulfill the molecular analog of the well-known Courant–Levy–Friedrich (CFL) condition. Since the GBT is an extended variant of the SBT algorithm, it is expected to need the same requirement for its convergence, i.e., the cell size and time step are coupled and should be chosen in such a way that $1 < \Delta x/\Delta t < 2$. In order to study the effect of cell size and time step effect on convergence behavior, we performed a set of simulations with two different values of $\Delta x/\Delta t$ ratios. For the set of run that $\Delta x/\Delta t$ is equal to 1.469, number of cells was 2424 and the time step was set to 0.832 ns. Moreover, another test was performed with 400 cells and time step of 0.625 ns, i.e., $\Delta x/\Delta t = 11.859$. All simulations are performed with fixed particles per cell number of 10. Table 3 shows the simulation results. The results in the table indicate a suitable agreement with the mathematical expectation value of heat flux magnitude for $\Delta x/\Delta t = 1.469$. This implies that if the appropriate combination of cell size and time step be employed, the GBT scheme could predict heat flux with a high accuracy.

Table 3
Heat flux dependence on dt/dx at various N_{sel}.

N_{sel}	q (W/m^2) ($\Delta x/\Delta t = 1.469$)	q (W/m^2) ($\Delta x/\Delta t = 11.859$)
NTC	1509	–
$N-1$	1512	1527
$N/2$	1514	1526
BB	1518	1536

It is worth noting that in Taheri et al. [13] the heat flux analysis was performed in the limit ($dx \to 0$ and $dt \to 0$) by using the SBT algorithm keeping the total number of particles same for a wide range of the number of particles per cell including such with much less than $N = 10$ down to $N = 1$ and $N = 0.5$. It was done by refining the grid appropriately with a decrease of the time step and cell size according to the condition used also here ($\Delta x/\Delta t = 1.469$). It was shown that the SBT scheme retains the same accuracy with respect to the heat flux for all cases with different number of particles per cell down to $N = 0.5$ (see Fig. 15 in [13]).

3.4. The lid-driven cavity

The other problem considered is the lid driven microcavity with a 1×10^{-6} m length containing the argon gas at Kn = 0.01, with the molecular mass and molecular diameter of 6.64×10^{-26} kg and 4.092×10^{-10} m, respectively; see Fig. 4. The lid velocity is set at 100 m/s, and all walls are diffuse reflectors at a constant temperature of 273 K. The GBT scheme was implemented in the DS2V code released with the Bird last monograph [5].

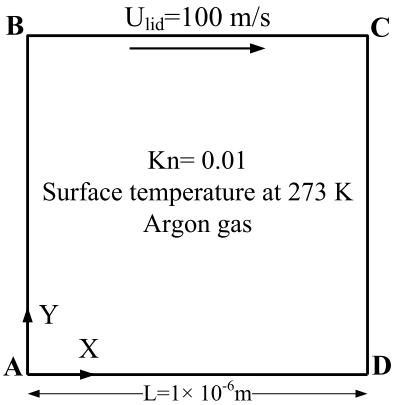


Fig. 4. Geometry and boundary condition of the cavity test case.

The GBT solution for the collision frequency and other flow field properties is compared with the prediction of other collision schemes. Data in Table 4 report the average value of CF_{ratio} calculated at the horizontal centerline of the cavity from the nearest neighbor (NN), SBT and GBT collision schemes. GBT results are reported with various N_{sel} magnitudes, i.e., $N_{sel} = N - 4$, $N - 6$ and $0.5N$, where $N = 10$ particles per cell is set in the initial condition. The table shows a suitable agreement between the SBT and GBT results.

Flow field properties including velocity components, pressure distribution and temperature jump on the moving lid from NN, SBT, and GBT with various N_{sel} are reported in Fig. 5. An excellent agreement is observed between GBT solutions and SBT and NN solutions.

Table 4
Comparison of the CF_{ratio} from various collision schemes.

NN	SBT	GBT ($N_{sel} = N - 4$)	GBT ($N_{sel} = N - 6$)	GBT ($N_{sel} = 0.5 \times N$)
0.9985934	0.9993474	0.9988435	0.9985452	0.9991280

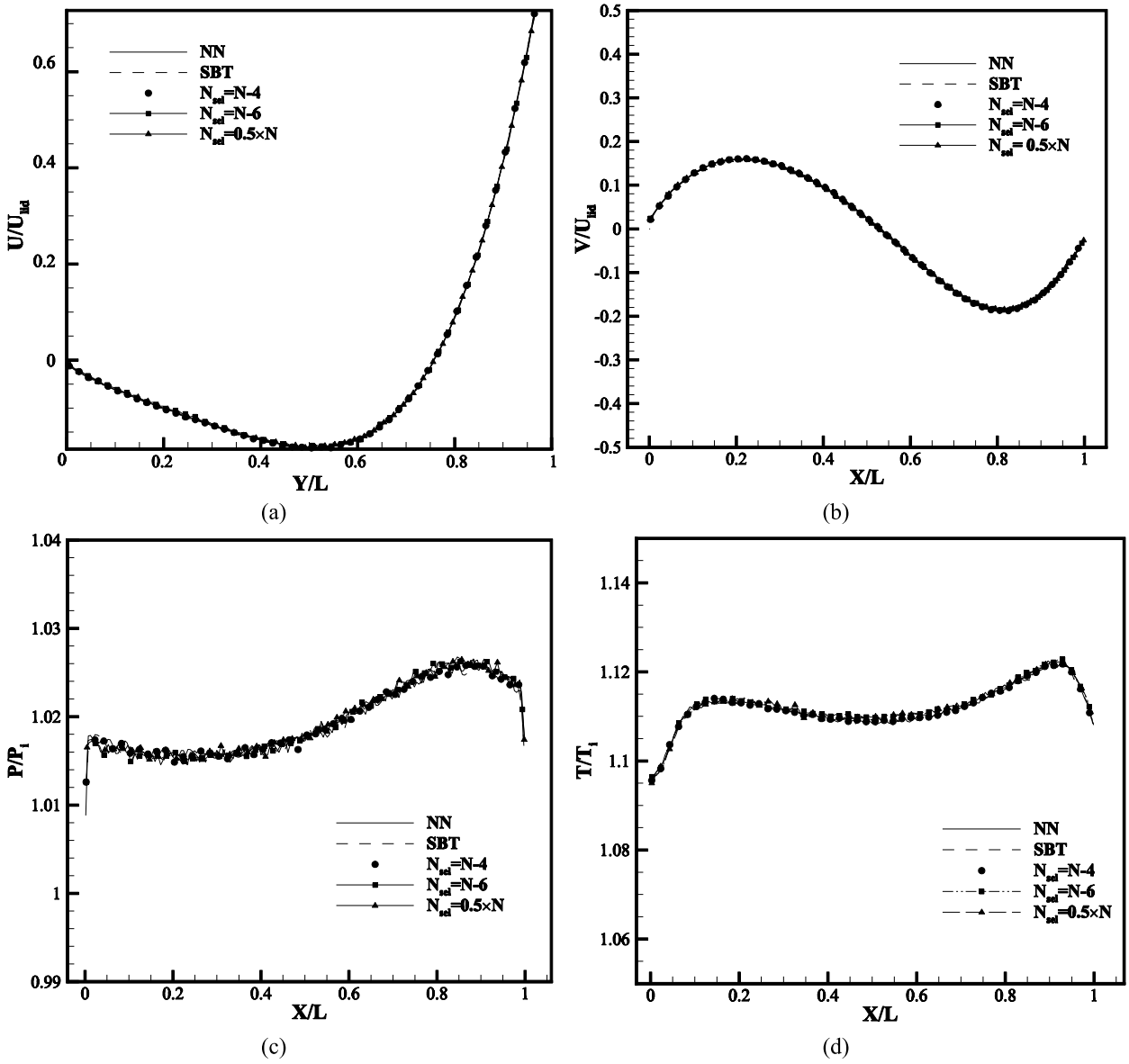


Fig. 5. (a)–(b) Velocity components along the cavity horizontal centerline. (c) Pressure distribution at centerline. (d) Temperature jump on the moving lid.

3.5. Steady strong shock-wave

The next problem examined here is the one-dimensional stationary normal shock wave [1]. For this purpose, the Bird's original one-dimensional code (DSMC-1S) is modified to include the SBT and GBT collision schemes.

The calculations are performed with a uniform grid of 600 cells without subcells. The stationary shock wave has a Mach number, defined as the ratio of shock wave velocity to the upstream speed of sound, of 8. The working fluid considered here is the argon gas at a reference temperature of 293 K. The variable soft sphere (VSS) model was used with scattering parameter of $\alpha = 1.6625$, and the viscosity–temperature index is set at $\omega = 0.81$. The upstream flow conditions are set as $U_1 = 2549.19$ m/s, $T_1 = 293$ K and number density of $n_1 = 1 \times 10^{20}$ m^{-3}. With this setting for temperature and molecular mass, the speed of sound at the upstream of the shock is calculated as $a_1 = 318.63$ m/s. By using of suit-

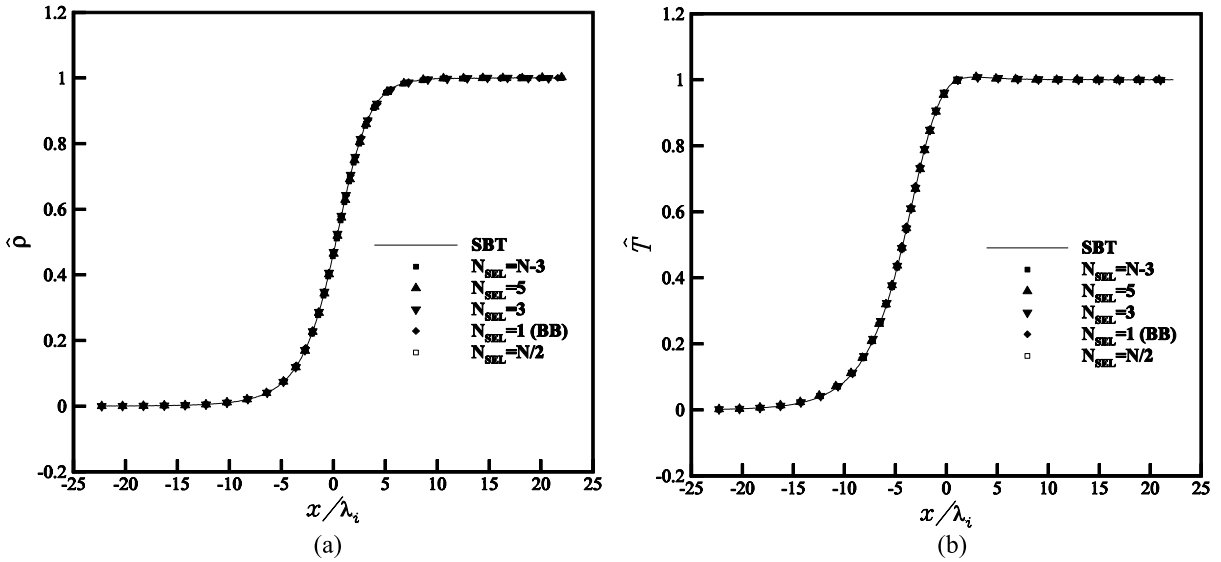


Fig. 6. Normalized density (a) and temperature (b) for different value of N_{sel} in normal shock.

able Rankine–Huguenot relation for the stationary normal shock wave, the downstream flow properties are computed as $U_2 = 667.17$ m/s, $T_2 = 6115.52$ K, $n_2 = 3.821 \times 10^{20}$ m^{-3}. The density and temperature are reported in the normalized form, i.e.: $\hat{\rho} = \frac{\rho - \rho_1}{\rho_2 - \rho_1}$, $\hat{T} = \frac{T - T_1}{T_2 - T_1}$. Fig. 6 shows the normalized density and temperature for the considered steady normal shock wave problem. The results obtained from GBT calculations with various N_{sel} are compared with the SBT solution. The figure shows an excellent agreement between the SBT and all GBT solutions for every used N_{sel}.

The BT collision family are able to perform accurate simulations with a small number of particles per cells [10,11]. To test the performance of the GBT scheme, the comparison is made with the solution of other collision schemes such as NTC and SBT. The stationary shock wave problem was simulated with a small number of particles per cell with SBT and GBT schemes. To reproduce the reference profile of density and temperature for a strong normal shock wave, we run the original DSMC1S.FOR code using NTC collision scheme with an average number of 50 simulator particles per cell. Fig. 7-a shows the normalized profiles obtained from both GBT formulas with PPC = 5 and two N_{sel} values, i.e., 2 and 3, completely match together. The NTC scheme was also run with PPC = 2. Fig. 7-b compares the solutions obtained from these schemes. Similar to SBT, GBT scheme could simulate the normal shock accurately with quite a low number of particles per cell. Fig. 7-c indicates that GBT scheme could keep the accuracy even with an average PPC = 0.5 with $N_{sel} = 0.5 \times N$.

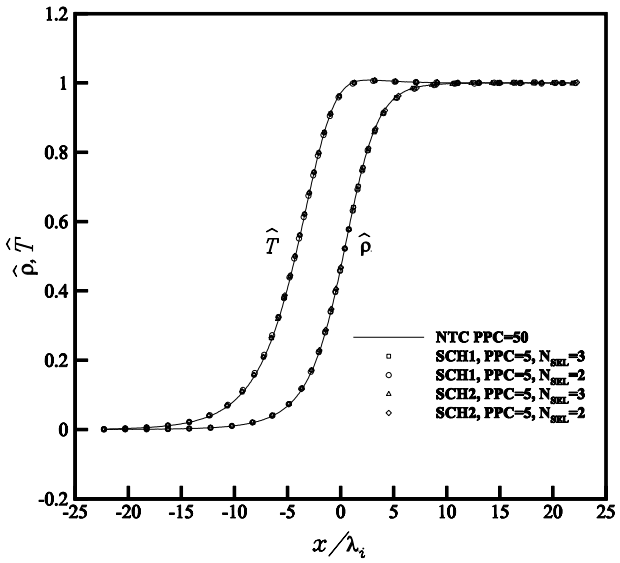
3.6. 70-degree blunted cone

The last test case considers the accuracy of the GBT scheme implemented on transient adaptive subcells (GBT-TAS) for treating hypersonic nitrogen flow over a 70-degree blunted cone, a simplified model but identical in geometric proportions to the Mars pathfinder probe. The same case was considered by Moss et al. [21] and recently by Palharini et al. [22]. Geometry, boundary condition and details of the computational domains of the geometry are demonstrated in Fig. 8. Table 5 presents freestream parameters used in the numerical simulation of the problem.

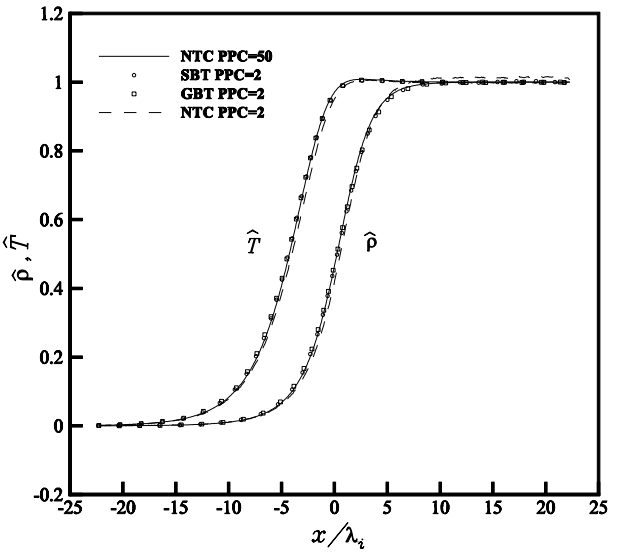
Table 5
Freestream values used in simulation.

Velocity (V_∞)	1503.1 m/s
Temperature (T_∞)	13.316 K
Number density (n_∞)	3.717×10^{20} m^{-3}
Density (ρ_∞)	1.730×10^{-5} kg/m^3
Pressure (P_∞)	6.833×10^{-2} Pa
Dynamic viscosity (μ_∞)	7.279×10^{-6} N s/m^2
Mean free path (λ_∞)	1.691×10^{-3} m
Knudsen (Kn_∞)	0.034
Reynolds (Re_∞)	178.6

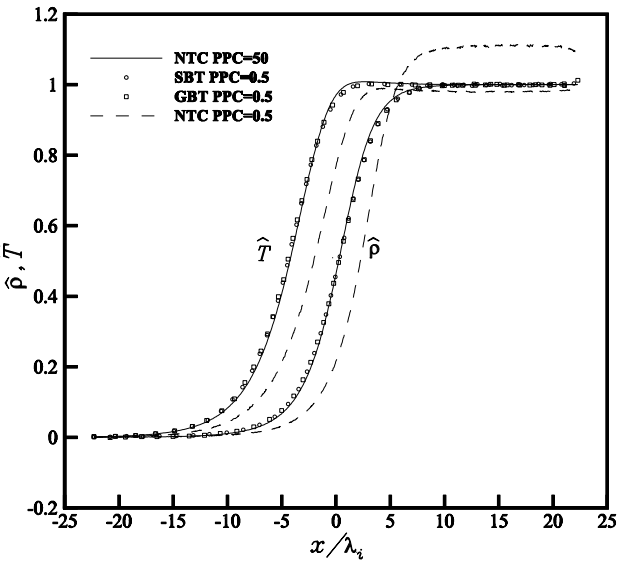
Nitrogen at $T_{ref} = 300$ K, with the molecular mass of 4.65×10^{-26} kg, molecular diameter of 4.17×10^{-10} m, the value of rotational collision number ($Z_{rot} = 5$), and viscosity–temperature index of $\omega = 0.75$, was considered. In the code, the vibrational mode was deactivated. The results reported here were obtained using a 200 × 200 grid adapted



a) Both GBT schemes with PPC=5



b) PPC=2



c) PPC=0.5

Fig. 7. Comparison of different scheme for small number of particles per cell.

to PPC = 9.5 and subcells with an average number of particle per subcell of PPSC = 3 for SBT-TAS and GBT-TAS collision algorithms. The algorithms were implemented in DS2V code of Bird. TAS technique is used to provide an adequate number of subcells compatible with the instantaneous number of particles per each collision cell in hypersonic flow with significant variations of the collision frequency and gas mean free path [23,24]. Fig. 9 shows streamlines and the formed vortex behind the probe from the NN, the default scheme in DS2V, SBT-TAS, and GBT-TAS schemes. An excellent agreement is observed among all the schemes. Fig. 10 shows the surface properties of the probe obtained from the NN, SBT-TAS, and GBT-TAS with different numbers of collisions in subcell, i.e., $N_{sel} = 0.5 \times N$, $N_{sel} = 0.7 \times N$, $N_{sel} = N - 2$, where N is the instantaneous number of particles in each subcell. All results agree suitably with each other.

The computational performance of GBT-TAS with an average PPSC = 3 and $N_{sel} = N - 2$ is compared with SBT-TAS in Table 6. The required time and required number of iterations to achieve a converged heat flux distribution are reported. In this regard, the normalized difference between two consecutive outputs of the heat flux is considered, if this normalized difference is less than 0.0006, the solution is assumed to be reached a converged heat flux solution. The employed hardware is a Core-i7-3770 K CPU with 24 GB RAM. The table shows that computational cost of the GBT-TAS is lower than SBT-TAS

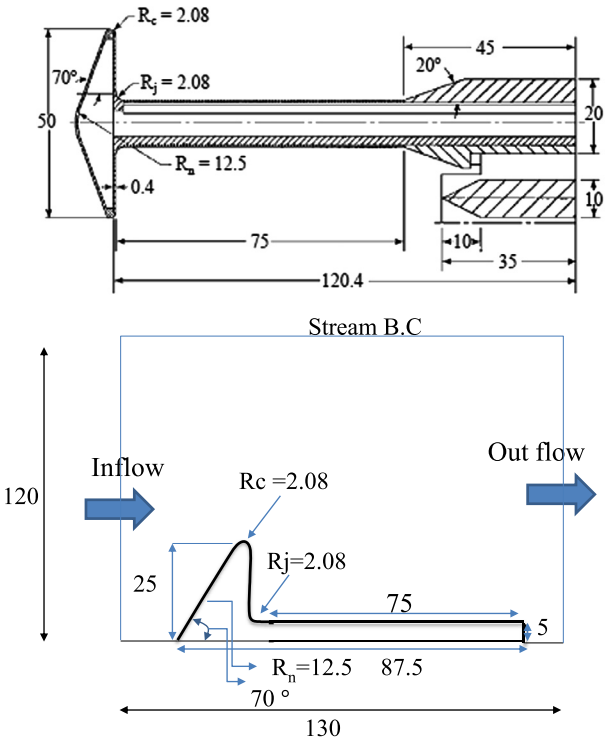


Fig. 8. Top: Mars pathfinder probe geometry, bottom: Geometry and boundary condition of the 70-degree blunted cone test case (units are in mm, R_c: corner radius, R_j: cone base radius, R_n: nose radius).

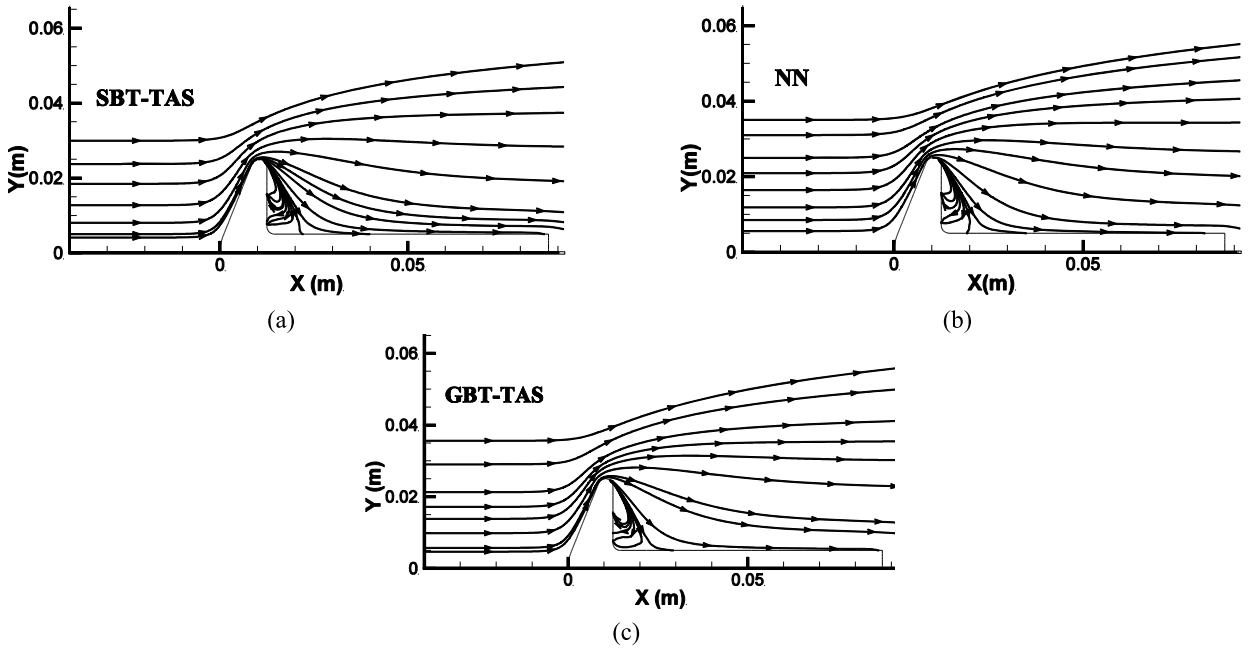


Fig. 9. Streamlines and vortexes over the probe (a) SBT-TAS, (b) NN and (c) GBT-TAS.

if $N_{sel} = N - 2$. The table shows that even though the average number of selections per cell is higher for the SBT scheme, it has a relatively reduced rate of accepted collisions compared to the GBT, i.e., acceptance to selection ratio ($\langle N_c \rangle / \langle N_{sel} \rangle$) is around 30% for the SBT-TAS, while it is around 50% for the GBT-TAS with $N_{sel} = N - 2$.

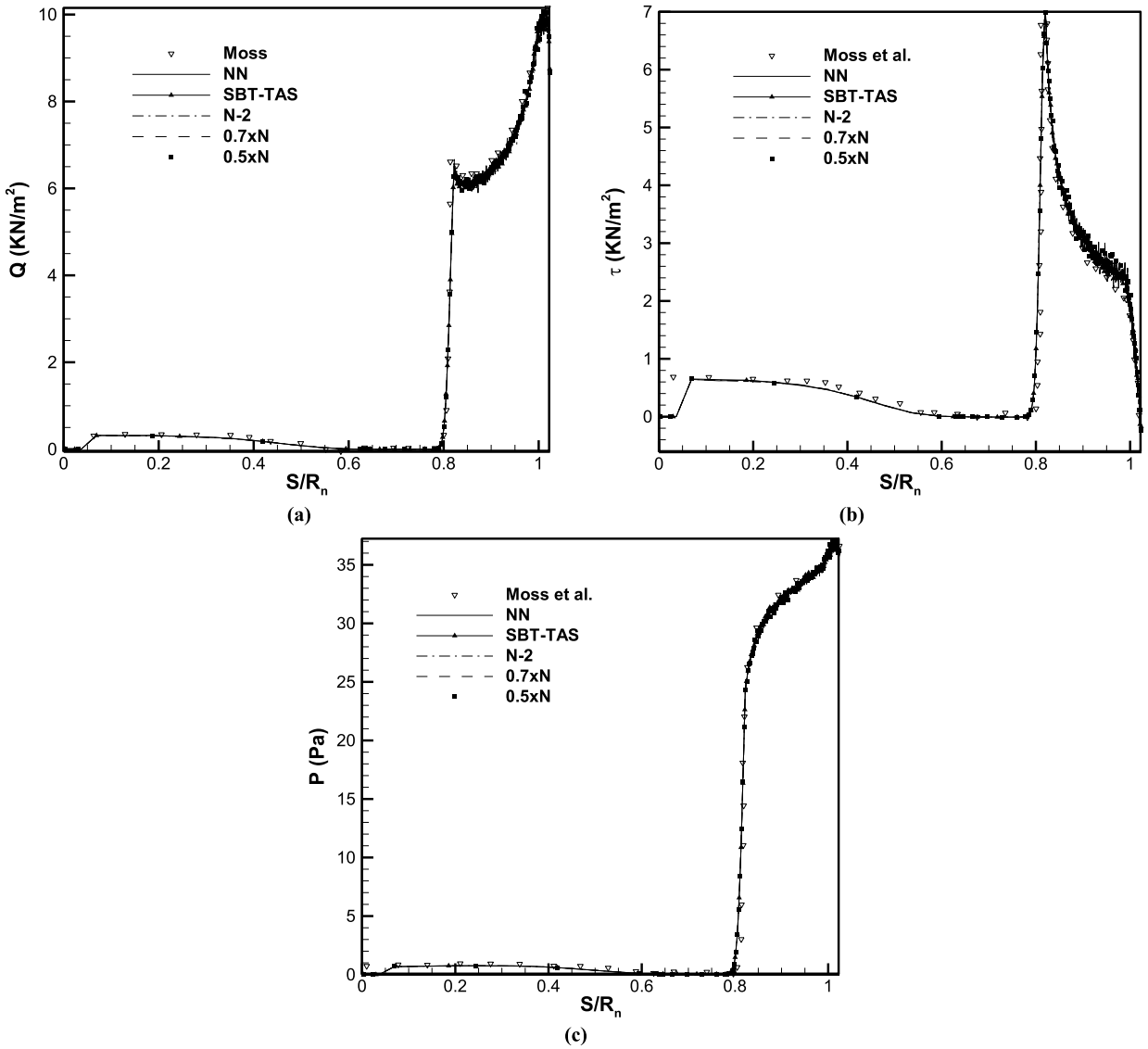


Fig. 10. Surface properties distribution (a), heat flux (b), shear stress (c). Pressure obtained from GBT-TAS at various N_{sel} compared with NN and SBT-TAS solutions.

Table 6
Comparison of computational performance of SBT-TAS and GBT-TAS.

Collision scheme	CPU-time (min)	Number of sampling before heat flux convergence	Solution time (s)	$\langle N_{sel}\rangle$ at $t = 3849.5$ (s)	$\langle N_{sel}\rangle$ at heat flux convergence time	$\langle N_c\rangle$ at $t = 3849.5$ (s)	Accept to select ratio at $t = 3849$
SBT-TAS, $N_{sel} = N - 1$	51.91	868	4745.531	2.36	2.39	0.73	30%
GBT-TAS, $N_{sel} = N - 2$	35.92	308	3849.500	1.59	1.59	0.85	53%

Concluding remarks

Here, a generalized Bernoulli Trial (GBT) collision is derived from the Kac stochastic equation. The GBT technique reduces the number of selected pairs for a possible binary collision while it ensures a correct collision frequency using a modified collision probability formula. The scheme is able to work with any desired number of collision pairs N_{sel}, selected from number of particles N occupied a considered cell within time step, e.g., $N_{sel} < N-1$, by using suitable time step and cell size. The derivation of two different GBT schemes was achieved considering two different points of views; one is a mathematical derivation and simplification of the solution operator of the Kac stochastic model and another is a generalization of the

Ballot Box (BB) and simplified Bernoulli Trial (SBT) correction formulas. Even though two different formulas were derived for GBT, solutions of both schemes completely agreed with each other. As the introduced correction in GBT formula increases the collision probability, further limitation in time step size should be set to avoid $W_{ij} > 1$, where W_{ij} is the collision probability. Both derived formulas were evaluated for various test cases, i.e., relaxation to equilibrium, dissociation of real gas, Fourier problem, cavity flow, steady shock wave and a blunted cone. In all occasions, GBT solution agreed well with the solution of the NTC, SBT and NN schemes while the computational performance of the GBT is reduced compared to the SBT scheme if a proper N_{sel} is chosen.

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Appendix A. A GBT pseudo algorithm

In GBT, the following pseudo algorithm for particle selection is running for each cell l.

1. Compute $k' = \frac{N^{(l)}(N^{(l)}-1)/2}{N_{sel}(2N^{(l)}-N_{sel}-1)}$
2. Choose N_{sel} from $N^{(l)}$ particles at random
3. Exchange their positions in the particle list (algorithm A).
4. For $i = 1,\ N_{sel}$
   Compute $k = (N^{(l)} - i)$
   Compute index of second particle $j = i + rand * k + 1$
   Compute probability $W_{ij} = \frac{k'k * F_{num} dt \sigma_{ij} g_{ij}}{V^l}$. If rand $< W_{ij}$ the collision of particle pair (i, j) is accepted and new particle velocities are computed
   Proceed to next i
1. End

References

[1] G.A. Bird, Molecular Gas Dynamics and the Direct Simulation of Gas Flows, Clarendon Press, Oxford, 1994.
[2] M.A. Gallis, J.R. Torczynski, D.J. Rader, G.A. Bird, Convergence behavior of a new DSMC algorithm, J. Comput. Phys. 228 (12) (2009) 4532–4548.
[3] G.A. Bird, M.A. Gallis, J.R. Torczynski, D.J. Rader, Accuracy and efficiency of the sophisticated direct simulation Monte Carlo algorithm for simulating noncontinuum gas flows, Phys. Fluids 21 (2009) 017103.
[4] M.A. Gallis, J.R. Torczynski, Effect of collision-partner selection schemes on the accuracy and efficiency of the direct simulation Monte Carlo method, Int. J. Numer. Methods Fluids 67 (8) (2011) 1057–1072.
[5] G.A. Bird, The DSMC Method, CreateSpace Independent Publishing Platform, USA, 2013.
[6] M.S. Ivanov, S.V. Rogasinskii, Theoretical analysis of traditional and modern schemes of the DSMC method, in: A. Beylich (Ed.), Proc. 17th Symposiums on Rarefied Gas Dynamics, VCH, Weinheim, 1990, pp. 629–642.
[7] M. Kac, Probability and Related Topics in Physical Sciences, Interscience Publishers Ltd., London, 1959.
[8] O.M. Belotserkovskii, V.E. Yanitskiy, The statistical particles-in-cells method for solving rarefied gas dynamics problems, USSR Comput. Math. Math. Phys. 15 (1975) 101–114.
[9] V. Yanitskiy, Operator approach to Direct Simulation Monte Carlo theory in rarefied gas dynamics, in: A. Beylich (Ed.), Proc. 17th Symposiums on Rarefied Gas Dynamics, VCH, Weinheim, 1990, pp. 770–777.
[10] S.K. Stefanov, Particle Monte Carlo algorithms with small number of particles in grid cells, in: Numerical Methods and Applications, Springer, 2011, pp. 110–117.
[11] S.K. Stefanov, On DSMC calculations of rarefied gas flows with small number of particles in cells, SIAM J. Sci. Comput. 33 (2011) 677–702.
[12] M.A. Gallis, J.R. Torczynski, D.J. Rader, M. Tij, A. Santos, Normal solutions of the Boltzmann equation for highly nonequilibrium Fourier flow and Couette flow, Phys. Fluids 18 (2006) 017104.
[13] E. Taheri, E. Roohi, S. Stefanov, On the convergence of the simplified Bernoulli trial collision scheme in rarefied Fourier flow, Phys. Fluids 29 (6) (2017) 062003.
[14] E. Roohi, S. Stefanov, Collision Partner Selection Schemes in DSMC: from micro/nano flows to hypersonic flows, Phys. Rep. 656 (C) (2016) 1–38.
[15] A. Amiri-Jaghargh, E. Roohi, H. Niazmand, S. Stefanov, DSMC simulation of low Knudsen micro/nanoflows using small number of particles per cells, J. Heat Transf. 135 (10) (2013) 101008.
[16] A. Amiri-Jaghargh, E. Roohi, S. Stefanov, H. Nami, H. Niazmand, DSMC simulation of micro/nano flows using SBT–TAS technique, Comput. Fluids 102 (2014) 266–276.
[17] A. Shoja-Sani, E. Roohi, M. Kahrom, S. Stefanov, Investigation of aerodynamic characteristics of rarefied flow around NACA 0012 airfoil using DSMC and NS solvers, Eur. J. Mech. B, Fluids 48 (2014) 59–74.
[18] S.A. Saadati, E. Roohi, Detailed investigation of flow and thermal field in micro/nano nozzles using Simplified Bernoulli Trial (SBT) collision scheme in DSMC, Aerosp. Sci. Technol. 46 (2015) 236–255.
[19] S.M. Madani, E. Roohi, Evaluation of the SBT-TAS collision scheme on treating unsteady flows, Eur. J. Mech. B, Fluids 64 (2017) 17–29.
[20] A. Ebrahimi, E. Roohi, DSMC investigation of rarefied gas flow through diverging micro- and nanochannels, Microfluid. Nanofluid. 21 (2) (2017) 18.
[21] J.N. Moss, V.K. Dogra, R.G. Wilmoth, DSMC Simulations of Mach 20 Nitrogen Flows About a 70 Degree Blunted Cone and Its Wake, Technical Report, NASA-TM-107762, NAS 1.15:107762, 1993.

[22] R.C. Palharini, C. White, T.J. Scanlon, R.E. Brown, M.K. Borg, J.M. Reese, Benchmark numerical simulations of rarefied non-reacting gas flows using an open-source DSMC code, Comput. Fluids 120 (2015) 140–157.
[23] B. Goshayeshi, E. Roohi, S. Stefanov, A novel Simplified Bernoulli Trials collision scheme in the DSMC with intelligence over particle distances, Phys. Fluids 27 (10) (2015) 107104.
[24] B. Goshayeshi, E. Roohi, S. Stefanov, DSMC simulation of hypersonic flows using an improved SBT-TAS technique, J. Comput. Phys. 303 (C) (2015) 28–44.