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On the Accuracy of the Simplified Bernoulli Trials Collision Algorithm in Treating Flows at Nano Scale and Hypersonic Regime

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Abstract. This paper reviews the accuracy of the Simplified Bernoulli Trial (SBT) algorithm and its variants, i.e., SBT-TAS (SBT on transient adaptive subcells) and ISBT (intelligence SBT) in the simulation of a wide spectrum of rarefied flow problems, including collision frequency ratio evaluation in the equilibrium condition, comparison of the Sonine-polynomial coefficients prediction in the Fourier flow with the theoretical prediction of the Chapman-Enskog expansion, accurate wall heat flux solution for the Fourier flow in the early slip regime, and hypersonic flows over cylinder and biconic geometries. We summarize advantages and requirements that utilization of the SBT collision families brings to a typical DSMC solver.

INTRODUCTION

Direct simulation Monte Carlo (DSMC) is widely utilized for treating either low speed rarefied gas flows at the micro/nano scales or external hypersonic flows at high altitude conditions. Strong physical background and its ability to provide accurate simulation results are of the main advantages of the DSMC algorithm. The original DSMC method is defined as a numerical particle representation of the Boltzmann equation. However, the Kac stochastic equation was also utilized to derive alternative intermolecular collision models in the DSMC algorithm [1]. The collision algorithms play a major role in the DSMC computations and are built on the most sophisticated term of the Boltzmann or Kac stochastic model. The DSMC algorithms are categorized into two main classes concerning the treatment of collisions.

The idea of the first family of DSMC’s collision schemes is based according to the principle of the maximum collision rate per time step. In this group, the “No Time Counter (NTC)” [2] scheme of Bird considers a maximum number of collision rate per time step. The scheme considers the number of randomly selected molecular pairs that should be tested for accepted collisions, while the other methods in this group such as “Time Counter (TC)” [3], “Null Collision (NC)” [4], and “Majorant Frequency Scheme (MFS)” [5] use a time-interval of \( \delta t \) for every accepted collision and a time-step of \( \Delta t \) for the DSMC. The collision procedure is continued until \( \sum_i \delta t_i > \Delta t \).

Considering the fact that a smaller mean collision separation (MCS) of colliding pairs results in more realistic binary collisions, modifications have been proposed to the above-mentioned collision schemes.
LeBeau et al. [6] introduced the virtual sub-cell (VSC) method which performs an \(O(N^2)\) operation to sort all \(N\) particles in a cell to find the nearest-neighbor to any simulator chosen for collision. Bird [7] proposed the transient adaptive sub-cell (TAS) scheme that divides DSMC cells into sub-cells, and collision partners are selected from the same or neighboring sub-cells. To reduce computational costs of VSC model to \(O(N)\), Bird [8] avoided the calculation of all intermolecular distances at the start of the collision procedure and restrict the burden to calculation of intermolecular distances between the randomly selected collision particle and the other particles.

In response to the possibility of the repeated collisions in the first group, which could be avoided only by direct prevention of selecting the same pair, another type of collision schemes, proposed by Belotserkovskii and Yanitskiy [9] and Yanitskiy [1], were developed based on the Kac stochastic equation. Different from previous schemes, this group defines a collision probability function for each particle pair in accordance with the Kac stochastic equation and checks all pair combinations for collision. Yanitskiy’s scheme then led to the introduction of the Bernoulli-Trials (BT) collision scheme. Recently, Stefanov introduced a modified variant of the BT scheme entitled as simplified Bernoulli Trials (SBT) [10]. Unlike the BT scheme, which has a quadratic dependency of the computational cost on the particle number in cells, the latter one (SBT) has a linear dependency and a higher computational efficiency. As an evolution of the SBT scheme to a method which can intelligently prefer collisions for closer pairs, Amiri et al. [11] and Goshayeshi et al. [12] combined SBT with TAS as well as some other auxiliary techniques. Then, Goshayeshi et al. introduced an intelligent variant of the SBT scheme (ISBT) which provides semi-perception of distance for the collision scheme [13]. This semi-cognition reduces approximately 25-32% of the overall MCS in collision cells. Understanding the recent notes of Gallis et al. [14] in the preference of choosing a near neighbor partner rather than the nearest neighbor one, which consequently leads to the saving of the collision scheme from losing some of its probable collisions during the advection phase of particles, the ISBT scheme also follows the same strategy of near neighbor pair-selection.

The aim of the current paper is to present results of evaluation of the SBT collision family and its variants, i.e., SBT on transient adaptive subcells (SBT-TAS) and intelligent SBT (ISBT) in the treatment of a wide spectrum of rarefied gas flows at micro/nano scales and hypersonic flow regimes [11-13, 15-17]. Accuracy and rigorousness of this collision family will be discussed in details.

SBT COLLISION FAMILIES

The mathematical derivation and details of the derivation of the SBT, SBT-TAS and ISBT collision models have already been reported in Refs. [10-12] and are not repeated here for the sake of brevity. The SBT and ISBT algorithms are depicted in details in Figs. 1-2.

**FIGURE 1. SBT collision procedure per each cell [10]**
The collision probability in the SBT family model is derived from a simplified transition operator of the Kac stochastic model. Using this simplified operator, instead of experiencing all particles located in the index list after the first particle $i$, only one of those particles is randomly selected from the particles located in the list after the $i^{th}$ particle with the probability of $1/k=1/(N_l-i)$, where $N_l$ is the number of particles in the cell. This reduces the level of collision checking to $(N_l-1)$. The collision probability is then multiplied by the factor $k$ to maintain the total probability equal to the theoretical one in the operator. This procedure necessitates small time steps to keep the errors in the truncated parts of the simplified operator small, i.e., $\Delta t < k$. The SBT procedure permits using a few particles per cell, while keeping the accuracy of the DSMC’s solution intact.

In response to recent interests of reducing the MCS of colliding pairs, SBT was implemented on the transient adaptive subcells (SBT-TAS) [12] with supporting techniques: this includes time step control at the subcell level, simplified volume calculation for cut-cell boundaries, and weighted filters for surface properties. As a result, the computational time and accuracy of the SBT-TAS is comparable to the nearest neighbor (NN) method. To decrease the MCS in complex shock-shock interaction problems, other measures can be used; this includes an intelligent variant of SBT, which favors selection of the closer particle to the first one selected [13]. In contrast to SBT, ISBT requires a hierarchical indexing of particles with respect to a random corner of the collision cell, then the selection of the second particle and computations of the collision probability is followed in the same way as the SBT method, but the collision probability is compared with the same random number already used for the selection of the second particle. This indicates that the collision probability is being compared to a smaller random number for closer pairs, and a larger random number for farther pairs (i.e., with a biased acceptance of selection of closer pairs occurring). The combination of ISBT and TAS reduces the MCS for complex problems. In following sections, sample results of the SBT collision family will be presented.

**Collision Frequency Ratio from SBT-TAS and ISBT**

The equilibrium collision frequency ratio of argon gas in the cavity flow at $Kn = 0.005$, $T_w=300$ K, simulated on a 25×25 grid using SBT-TAS technique, is shown in Fig. 1 [13]. VHS collision molecular model is used. Average time step during the simulation is: $2.6\times10^{-12}$. In this state, the theoretical equilibrium collision rate per molecule ($CF_{th}$) is given by [18]:

![FIGURE 2. ISBT collision procedure [13]](image)
where \( n \), \( d \), \( K_B \), \( T_{\text{ref}} \), \( m_s \), and \( \omega \) are number density, gas molecular diameter, Boltzmann constant, reference temperature, molecular mass, and viscosity-temperature exponent, respectively. \( CF_{\text{num}} \) represents the numerical value of this theoretical equilibrium collision rate that is calculated by the division of the number of collisions in each cell \( (N_{\text{coll}}) \) on the execution time \( (\text{Time}) \) and half of the mean particle numbers per cell \( (0.5 N_p) \):

\[
CF_{\text{num}} = \frac{N_{\text{coll}}}{0.5 N_p \text{Time}}
\]

\( CF_{\text{ratio}} \) is the ratio of the \( CF_{\text{num}} \) to its theoretical value—given by Eq. (1)—it must have a magnitude close to unity. Using SBT-TAS and setting 2 particles per subcell, i.e., PPSC=2, 16×16 subcells were employed in each cell in average. As Fig. 3-a shows, mean deviation of the equilibrium collision frequency ratio of one is in the order of \( 10^{-4} \) and its maximum is about 0.2%. This proves that number of collisions in SBT-TAS scheme is accurate and coincides with the theory even using small number of particles per subcells (collision cells).

**TABLE 1** Comparison of the \( SOF = \left( \frac{MCS}{2} \right) \) value in the lid-driven cavity flow between NN, ISBT and SBT collision schemes. (Reprinted with permission from B. Goshayeshi, E. Roohi, and S. Stefanov, Phys. Fluids 27, 107104 (2015). Copyright 2015 American Institute of Physics)

<table>
<thead>
<tr>
<th>Collision scheme</th>
<th>Division size in DS2V code</th>
<th>( SOF ) value</th>
<th>( SOF ) normalized by the corresponding NN value</th>
<th>Average ( SOF ) normalized by the corresponding SBT value</th>
</tr>
</thead>
<tbody>
<tr>
<td>NN</td>
<td>100-100</td>
<td>0.0477</td>
<td>1</td>
<td>0.182</td>
</tr>
<tr>
<td>ISBT</td>
<td>100-100</td>
<td>0.1740</td>
<td>3.66</td>
<td>0.666</td>
</tr>
<tr>
<td>SBT</td>
<td>100-100</td>
<td>0.2621</td>
<td>5.49</td>
<td>1</td>
</tr>
</tbody>
</table>

The collision frequency of the ISBT scheme in an equilibrium state, for the argon flow in the cavity test case with \( U_{\text{lid}} = 0 \) m/s, \( Kn=0.01 \) and with surface and fluid temperatures have the same value of 273 K is evaluated using DS2V code with ISBT implemented [13]. VHS collision model of argon is utilized and an average time step of \( 4 \times 10^{-12} \) is utilized in the solver. Fig. 3-b states that the deviation of the \( CF_{\text{ratio}} \) from the unity in the ISBT collision scheme, similar to the SBT scheme, is bounded with acceptable limit of 0.002. As the simulated cavity has diffuse reflecting walls, the eventual correlations cannot propagate at long distances. The dimensionless number, \( SOF \), which is the mean collision separation distance \( (MCS) \) divided by the local mean free path \( (\lambda) \), is selected as a parameter for measuring the quality of collisions.
Table 1 states that the ISBT, compared with the SBT collision scheme, reduced the SOF value quite considerably.

### Fourier Flow: Comparison with Theory

The convergence behavior and accuracy of the DSMC technique Fourier problems for near-continuum conditions was investigated for the NTC scheme [19-20].

![Fourier Flow Diagram](image)

A similar evaluation was made for the SBT method. The hard-sphere argon gas was simulated at the reference pressure and temperature: $P_{\text{init}}=P_{\text{ref}}=266.644 \times 10^{-5}$ Pa and $T_{\text{init}}=T_{\text{ref}}=273.15$ K, and Kn=0.0237. The time step for the SBT results reported in frames of Fig. 4 was set for each case as follows: (a): $3.5 \times 10^{-9}$ s, (b): $7 \times 10^{-9}$ s, (c): $0.625 \times 10^{-9}$ s, (d): $7 \times 10^{-9}$ s. All NTC solutions reported in these figures are extracted from Refs. [19-20]. Fig. 4-a shows that the Sonine-polynomial coefficients $a_k/a_1$ for $k=2,3$ obtained from the DSMC away from walls agree with the theoretical value for NTC and SBT with a few particles per cell. Fig. 4-b compares the heat conductivity ratio (theoretical to DSMC) from NTC and SBT solutions and...
show that both numerical solutions agree with each other. Fig. 4-c compares dependency of the SBT and NTC solutions for the wall heat flux on the number of particles per cell (PPC) and cell size. Both solutions agree with each other, however, SBT used a smaller time step compared to the NTC solution by around one order of magnitude. Fig. 4-d compares the dependency of NTC and SBT solutions for the conductivity ratio on the cell size, for both of the investigated PPC’s, SBT and NTC solutions for the conductivity ratio approach to unity as cell size reduces. But on coarser grid with larger number of particles, i.e. PPC=30, NTC works slightly better because of the random choice of pairs, once we use SBT we cut some possible pairs which could contribute to the solution.

**Hypersonic Flow over Cylinder and Biconic Geometry**

Hypersonic flows over the cylinder and biconic geometry are famous test cases in rarefied gas dynamics considered by various researchers to evaluate their DSMC solvers and algorithms.

Goshayeshi et al. [12, 13] evaluated the performance of the SBT, SBT-TAS and ISBT techniques in treating rarefied hypersonic flows. For the hypersonic cylinder case, Mach 10 (2634.1 m/s) flow of argon at T=200 K passing over a 12 inch circular cylinder with a fully diffusive surface at Ts=500 K and a nominal free-stream Knudsen number of 0.01 is considered. The average time step of the DSMC solver for this test case is \(6.41 \times 10^{-7}\). Fig. 5-a shows a comparison of temperature contour around the cylinder from NN, ISBT-TAS, and SBT-TAS techniques. All SBT solutions match NN solution; however, ISBT matches the NN
solution in the wake region much better. Figs. 5-b-c compares surface properties (heat flux, shear stress, pressure, slip velocity) over the cylinder. For all investigated properties, there is an excellent agreement between the SBT family results and those of NN.

Hypersonic nitrogen flow of Mach 15.6 passing over a 25°-55° degree biconic geometry is a quite complex test case for numerical schemes as it consists of a laminar recirculation zone, laminar expanding zone, high-speed low-density region, and low-speed high-density region. DSMC simulation of this case is performed using VHS collision model in the DS2V code. The average time step of the DSMC solver for this test case is $3.9 \times 10^{-8}$. A comparison of the heat flux and pressure distribution over the biconic geometry, from SBT-TAS, ISBT-TAS, NN and experimental data is shown in Fig. 6. Fig. 7 shows contour of temperature and SOF from ISBT-TAS and NN over the biconic surface. All numerical solutions show almost a suitable match between ISBT-TAS and NN.

![Graph](image1)

**FIGURE 6.** Comparison of heat flux and pressure distribution around the biconic geometry from different DSMC models: B1, C1 and C2 stand for different test cases using different total number of particles (Both frames are reprinted with permission from B. Goshayeshi, E. Roohi, and S. Stefanov, Phys. Fluids 27, 107104 (2015). Copyright 2015 American Institute of Physics)

![Graph](image2)

**FIGURE 7.** a) Comparison of ISBT-TAS and NN collision schemes in treating hypersonic external flow over biconic, a) temperature contours, b) contours of SOF (Both frames are reprinted with permission from B. Goshayeshi, E. Roohi, and S. Stefanov, Phys. Fluids 27, 107104 (2015). Copyright 2015 American Institute of Physics)
CONCLUDING REMARKS

The current paper provides a review of the previous works demonstrating the performance of the SBT collision families. The early Kac-based models, such as the original BT model, suffered from high computational costs, while the SBT collision families have comparable computational costs to the standard models based on the Boltzmann equation such as NTC and NN schemes. A wide spectrum of rarefied flow test cases, ranging from simple equilibrium collision frequency to complicated shock-shock interactions, was simulated using the SBT collision family models and it was shown that SBT collision families could provide accurate solutions using small particles per cell. The benefit of the SBT collision model will be more clearly pronounced in complex 3D simulations, where a large number of particles is required if one relies on the standard schemes. A hybrid NTC-SBT scheme could be also utilized for these complex 3D cases.

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REFERENCES