INSTITUTE OF INFORMATION
AND COMMUNICATION TECHNOLOGIES
BULGARIAN ACADEMY OF SCIENCES
CYBERNETICS AND INFORMATION TECHNOLOGIES • Volume **26**, No 2
Sofia • 2026 Print ISSN: 1311-9702; Online ISSN: 1314-4081
DOI: 10.2478/cait-2026-0011

Bernoulli Trial (BT) Collision Operator Scheme Family in the Direct Simulation Monte-Carlo (DSMC): Derivation and Evaluation

Francis Padilla[1], *Ehsan Roohi*[1], *Stefan Stefanov*[2]

[1]*Department of Mechanical and Industrial Engineering, University of Massachusetts Amherst, USA*
[2]*Institute of Mechanics, Bulgarian Academy of Sciences, 1113 Sofia, Bulgaria*
E-mails: francispadilla.career@gmail.com roohie@umass.edu stefanov@inbm.bas.bg

Abstract**:** *The Direct Simulation Monte-Carlo* (*DSMC*) *method is based on splitting the rarefied gas process evolution into two ballistic and collision steps within a time step. The collision step is the more complicated, requiring a rigorous theoretical analysis to discover its relation to the fundamental kinetic equations. In this work, we present a systematic derivation and examination of the Bernoulli-Trial* (*BT*) *family of collision schemes. The master Kac equation describes the binary collision interactions as a stochastic process lying in the background of the DSMC probabilistic rules, and it serves as a starting point for our derivation of the BT family. This study is limited to the analysis of four BT members, including Simplified Bernoulli Trials* (*SBT*)*, Generalized Bernoulli Trials* (*GBT*)*, Symmetrized Simplified Bernoulli Trials* (*SSBT*)*, and Symmetrized Generalized Bernoulli Trials* (*SGBT*)*. These schemes are implemented in the DSMC code, and a simple relaxation problem is simulated to determine optimal values for the pair-selection parameter* N_{sel}.

Keywords**:** *Direct Simulation Monte-Carlo, Collision operators, Mathematical formulation, Rarefied gas dynamics, Kinetic theory of gases, Relaxation processes, Numerical methods, Probability Analysis.*

1. Introduction

Kinetic theory provides the fundamental description of rarefied gas flows, spanning from near-continuum to highly rarefied conditions. The velocity distribution function, being the solution of the well-known Boltzmann equation, provides a connection between microscopic gas properties and macroscopic quantities. The same goal is achieved through the statistical sampling of microscopic particle properties, which is implemented numerically by the Direct Simulation Monte-Carlo (DSMC) technique introduced by Bird [3]. The DSMC algorithm discretizes the time and space into a computational grid and splits the gas-dynamics process over a time step into free-molecular motion and intermolecular collisions

within computational cells. While the particle motion step is relatively straightforward, the collision partner-selection procedure plays a central role in determining both the accuracy and computational cost of the simulation [2].

Through the years since the DSMC was created, many collision algorithms were proposed, and among them, the most popular is the No-Time-Counter (NTC) scheme [3] and the Null-Collision (NC) [4], which selects candidate particle pairs based on a maximum collision rate concept. A similar approach that takes into account the Poissonian character of collision distribution is proposed by the Majorant Collision Scheme (MFS) [5]. Although this approach is computationally efficient, it suffers from some inconsistencies of the stochastic process, such as the non-Markovian character of the collision process [6and repeated collisions between the same particle pairs. The theoretical investigations [7] have shown that repeated collisions between the same particle pairs can occur, especially in low-density simulations or when the number of particles (simulators) per cell is low. Such repeated collisions do not contribute new physical information and may artificially reduce the effective collision rate [7, 8]. These disadvantages reduce accuracy when the number of particles per cell becomes very small.

To avoid these disadvantages, alternative stochastic collision models have been developed to improve statistical consistency. Among these alternatives, the Bernoulli-Trial (BT) family of algorithms [9, 10] provides a rigorous probabilistic framework derived from the Kac stochastic equation [11]. These models determine collision events using Bernoulli trials as probability checks for collisions that avoid repeated collisions over a time step.

The present work deals with a systematic theoretical formulation and derivation of the basic BT collision family schemes from the general transition operator [12] and investigates their efficiency in computational simulations of a relaxation process to equilibrium. The focus of our attention is the determination of pair-selection rules and parameters of the derived approximations and the estimation of their computational cost and statistical accuracy.

In the original BT formulation [12], all possible particle pairs within a cell are evaluated as potential collision partners. While this approach effectively prevents repeated collisions and maintains the approximation accuracy, its computational cost increases with the square of the number of particles in the cell. This makes the method expensive for large-scale simulations. The subsequent several improvements reduce the computational costs of the BT approach. The Simplified Bernoulli Trial (SBT) algorithm [7, 13, 14] reduces the number of candidate pairs by considering only a subset of possible partners for each particle. This significantly lowers computational complexity, making it comparable to the standard NTC scheme while maintaining acceptable accuracy for most non-equilibrium gas flow problems. The next approximation, the Generalized Bernoulli Trial (GBT) scheme, introduced a selection parameter N_{sel}, that allows the user to decrease the number of selected pairs checked for collision [15]. This parameter provides an improved computational efficiency.

The development of symmetric collision-selection strategies is a new and subtle improvement. The Symmetrized Simplified Bernoulli Trial (SSBT)

algorithm, following the SBT idea, allows each selected particle to be checked for collision with its neighbours before and after it in the particle list, thereby improving statistical symmetry and physical consistency [16]. The last considered model, the Symmetrized Generalized Bernoulli Trial (SGBT) scheme, incorporates the properties of both GBT and SSBT [17].

These variants of collision models based on rigorous derivation of a series of approximations of the general non-linear transition operator acting over a time step demonstrate that the Bernoulli-Trial framework provides a substantial complement to standard collision algorithms. As discussed in the recent textbook [18], the development of the BT collision approximation family for the modern DSMC method directs researchers' attention to creating flexible hybrid schemes that combine the best qualities of the respective schemes for accurate and efficient modeling of non-equilibrium gas flows in complex domains [19].

Finally, the BT-collision models, the SBT and GBT, and SSBT and SGBT, are tested and their efficiency compared in the benchmarked relaxation process [1, 20].

2. Mathematical formalities

The mathematical formulation used in the derivation of the BT equations is as follows.

Let $A_{ij} \in M_{n\times n}(\mathbb{R})$ be a square matrix. The Taylor expansion of $\exp(A_{ij})$ is

$$\exp(A) = \sum_{n=0}^{\infty} \frac{1}{n!} A_{ij}^{n}. \tag{1}$$

The general form of the exponent sum law $\exp(a+b) = \exp(a) + \exp(b)$ is

$$\exp\left(\sum_n a_n\right) = \prod_n \exp(a_n). \tag{2}$$

Let $N \in \mathbb{N}$ and a_n be a sequence. The expansion over distinct unordered pairs are

$$\begin{aligned} \prod_{1\le i<j\le N} a_n &= \prod_{i=1}^{N-1} \prod_{j=i+1}^{N} a_n, \\ \sum_{1\le i<j\le N} a_n &= \sum_{i=1}^{N-1} \sum_{j=1+1}^{N} a_n. \end{aligned} \tag{3}$$

Let $P(t) = a_0 + a_1 t + a_2 t^2 + \cdots$ be a polynomial with constant or matrix coefficients. Then the collection of terms of degree d or greater using Big-Oh notation is

$$\mathcal{O}\left(t^d\right) = \sum_{n=d}^{\infty} a_n t^n \,. \tag{4}$$

3. Derivation of BT operators

The above mathematical formalities are applied to the Kac master equation. In the operator form, the Kac stochastic model could be written [10] as follows:

$$\begin{aligned} \frac{\partial}{\partial t} F_{N^{(l)}}\left(t, x^{(l)}, c_{N^{(l)}}\right) &= \left[\sum_{1\le i<j\le N^{(l)}} w_{ij}\left(T_{ij} - I\right)\right] F_{N^{(l)}}\left(t, x^{(l)}, c_{N^{(l)}}\right) = \\ &= \upsilon(T - I) F_{N^{(l)}}\left(t, x^{(l)}, c_{N^{(l)}}\right), \end{aligned} \tag{5}$$

where

$$I\psi = \psi, \quad T_{ij} = \int_{4\pi} \psi\left(c_{ij}\right) B\left(g_{ij}, \theta\right) d\Omega(\theta), \quad T\psi = \sum_{1\le i<j\le N^{(l)}} w_{ij} T_{ij} \psi,$$

and $B(g_{ij},\theta)$ is a scattering kernel. The transformation $T_{ij}F_{N^{(l)}}(t,x^{(l)},c_{N^{(l)}})$ results in a probability density distribution of $c_{N^{(l)}}^{ij}$ over $\Omega(N,E,P)$ after the collision of a pair (c_i,c_j) under the condition that before the collision point $c_{N^{(l)}}$ is distributed over $\Omega(N,E,P)$ with the probability density $F_{N^{(l)}}(t,x^{(l)},c_{N^{(l)}})$.

In the Kac model, the probability of the time interval between two successive collisions is distributed according to the exponential distribution of a Poisson process as follows:

(6) $$\text{Prob}(\delta t > t) = e^{-\upsilon t},\ \upsilon = \sum_{1\le i<j\le N^{(l)}} w_{ij}\ ;\ w_{ij} = \frac{\sigma_{ij}g_{ij}}{V^{l}},$$

where the collision probability of pair (i,j) as denoted by (w_{ij}) is a function of σ_{ij}, which is the collision cross-section, and $g_{ij} = |c_i - c_j|$, which is the particles' relative velocities.

In the case of the given state at the time t_0, the operator form of the Kac master equation could be solved at time t with the definition of the transition operator $G(t)$ in the following form:

(7) $$F_{N^{(l)}}(t,x^{(l)},\ C_{N^{(l)}}) = G(t)F_{N^{(l)}}(t_0,\ x^{(l)},\ C_{N^{(l)}}),$$

where the transition operator $G(t)$ could be written as

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

3.1. Bernoulli Trials (BT)

The BT operator [10] is an approximation of (8) considering all pairs of particles (i,j) for collision. The Bernoulli Trial operators are derived from the $G(t)$ by applying equations (2) to (8) as follows:

(9) $$\exp\left(\Delta t\sum_{1\le i<j\le N^{(l)}} w_{ij}\left(T_{ij} - I\right)\right) = \prod_{1\le i<j\le N^{(l)}} \exp\left[\Delta t w_{ij}\left(T_{ij} - I\right)\right].$$

Expand the product of (9) using (3).

(10) $$\prod_{1\le i<j\le N^{(l)}} \exp\left[\Delta t w_{ij}\left(T_{ij} - I\right)\right] = \prod_{i=1}^{N^{(l)}-1}\prod_{j=i+1}^{N^{(l)}} \exp\left[\Delta t w_{ij}\left(T_{ij} - I\right)\right].$$

Taylor expand the product of (10) using (1) is

(11) $$\prod_{i=1}^{N^{(l)}-1}\prod_{j=i+1}^{N^{(l)}} \exp\left[\Delta t w_{ij}\left(T_{ij} - I\right)\right] = \\ = \prod_{i=1}^{N^{(l)}-1}\prod_{j=i+1}^{N^{(l)}}\left[\sum_{n=0}^{\infty}\frac{\left[\Delta t w_{ij}\left(T_{ij}-I\right)\right]^{n}}{n!}\right].$$

Within the inner sum of (11), compute $n = 0$ and $n = 1$. Condense using (4) is

(12) $$\prod_{i=1}^{N^{(l)}-1}\prod_{j=i+1}^{N^{(l)}}\left[\sum_{n=0}^{\infty}\frac{\left[\Delta t w_{ij}\left(T_{ij}-I\right)\right]^{n}}{n!}\right] = \\ = \prod_{i=1}^{N^{(l)}-1}\prod_{j=i+1}^{N^{(l)}}\left[I + \Delta t w_{ij}\left(T_{ij} - I\right) + \sum_{n=2}^{\infty}\frac{\left[\Delta t w_{ij}\left(T_{ij}-I\right)\right]^{n}}{n!}\right] = \\ = \prod_{i=1}^{N^{(l)}-1}\prod_{j=i+1}^{N^{(l)}}\left[I + \Delta t w_{ij}\left(T_{ij} - I\right) + \mathcal{O}\left(\Delta t^{d}\right)\right].$$

For small values of Δt, we approximate for $n \ge 2$ that $\Delta t^{n} \approx 0$. Thus, the remainder $\mathcal{O}(\Delta t^{2}) \approx 0$. Truncate the inner product in (12) to give the BT operator.

(13) $$G_{\text{BT}}(\Delta\text{t}) = \prod_{i=1}^{N^{(l)}-1}\prod_{j=i+1}^{N^{(l)}}\left[I + \Delta t w_{ij}\left(T_{ij} - I\right)\right].$$

An equivalent representation takes the form

(14) $$G_{\text{BT}}(\Delta\text{t}) = \prod_{i=1}^{N^{(l)}-1}\prod_{j=i+1}^{N^{(l)}}\left[(1 - \Delta t w_{ij})I + \left(\Delta t w_{ij}\right)T_{ij}\right].$$

For $w_{ij} \approx 1$ where collision is likely, the operator applies the collision operator T_{ij} and updates velocities. For $w_{ij} \approx 0$ where collision is unlikely, the operator applies the identity operator I and streams the particles without collision.

The computational cost of BT is calculated by counting the number of pairs considered. In this case, BT considers all pairs (i, j),

$$\binom{N^{(l)}}{2} = \frac{N^{(l)}\left(N^{(l)}-1\right)}{2}. \tag{15}$$

Thus, the computational expense of BT is $\mathcal{O}\left(\left(N^{(l)}\right)^2\right)$.

3.3. Simplified Bernoulli Trials (SBT)

The idea of SBT [*7*] is to reduce the computational expenses of BT by limiting the possible collision partners j for each particle i. We begin by linearizing the BT operator. Within the inner product of (14), make the substitution for each fixed i,

$$A_j = w_{ij}\left(T_{ij} - I\right), \tag{16}$$

which yields

$$\prod_{j=i+1}^{N^{(l)}}\left[I + \Delta t w_{ij}\left(T_{ij} - I\right)\right] = \prod_{j=i+1}^{N^{(l)}}\left[I + \Delta t A_{ij}\right]. \tag{17}$$

Expand (17) and distribute the terms, collecting by the power of Δt

$$\begin{aligned}\prod_{j=i+1}^{N^{(l)}}\left[I + \Delta t A_{ij}\right] &= (I + \Delta t A_{i+1})(I + \Delta t A_{i+2}) \cdots \left(I + \Delta t A_{N^{(l)}}\right) = \\ &= (I^2 + \Delta t A_{i+1} + \Delta t A_{i+2} + \Delta t^2 A_{i+1} A_{i+2}) \cdots \left(I + \Delta t A_{N^{(l)}}\right) = \\ &= I^{N^{(l)}} + \Delta t\left(A_{i+1} + \cdots + A_{N^{(l)}}\right) + \Delta t^2(\cdots) + \cdots + \Delta t^{N^{(l)}}(\cdots).\end{aligned} \tag{18}$$

Condense (18) with (4), and further simplify

$$\begin{aligned}&I^{N^{(l)}} + \Delta t\left(A_{i+1} + \cdots + A_{N^{(l)}}\right) + \Delta t^2(\cdots) + \cdots + \Delta t^{N^{(l)}}(\cdots) \; = \\ &= I^{N^{(l)}} + \Delta t\left(A_{i+1} + \cdots + A_{N^{(l)}}\right) + \mathcal{O}(\Delta t^2) \; = I + \Delta t \sum_{j=i+1}^{N^{(l)}} A_j + \mathcal{O}(\Delta t^2).\end{aligned} \tag{19}$$

Truncate $\mathcal{O}(\Delta t^2)$ with the same assumption that $\Delta t^2 \approx 0$

$$I + \Delta t \sum_{j=i+1}^{N^{(l)}} A_j + \mathcal{O}(\Delta t^2) \approx I + \Delta t \sum_{j=i+1}^{N^{(l)}} A_j. \tag{20}$$

Back-substitute (16) into (20) and rearrange:

$$\begin{aligned}I + \sum_{j=i+1}^{N^{(l)}} A_j &= I + \Delta t \sum_{j=i+1}^{N^{(l)}} w_{ij}\left(T_{ij} - I\right) = I - \sum_{j=i+1}^{N^{(l)}} \Delta t w_{ij} + \\ &+ \sum_{j=i+1}^{N^{(l)}}\left(\Delta t w_{ij}\right) T_{ij} \; = \left(1 - \sum_{j=i+1}^{N^{(l)}} \Delta t w_{ij}\right) I + \sum_{j=i+1}^{N^{(l)}}\left(\Delta t w_{ij}\right) T_{ij}.\end{aligned} \tag{21}$$

Replacing the inner sum of (14) with (21) returns the linearized BT operator

$$G'_{\mathrm{BT}}(\Delta \mathrm{t}) = \prod_{i=1}^{N^{(l)}-1}\left[\left(1 - \sum_{j=i+1}^{N^{(l)}} \Delta t w_{ij}\right) I + \sum_{j=i+1}^{N^{(l)}}\left(\Delta t w_{ij}\right) T_{ij}\right]. \tag{22}$$

Here, for each particle i, the possible collision partners j are those occurring after particle i. As represented by the bounds of the sum,

$$i \in \left\{1, \cdots, N^{(l)} - 1\right\}, \tag{23}$$

$$j \in \left\{i + 1, \cdots, N^{(l)}\right\}. \tag{24}$$

The adjustments to partner selection probability require the introduction of a correction factor (the selection scaling factor). Similarly, the collision action requires a statistical weight to account for the particles that are disregarded. By (24), for a given particle i, there are $N^{(l)} - i$ possible collision partners j. Thus, the correction coefficient and statistical weight are

(25) $$k = N^{(l)} - i,$$

(26) $$\frac{1}{k} = \frac{1}{N^{(l)} - i}. .$$

The key assumption is that

(27) $$w_{ij}^{(\text{exact})} \approx \frac{1}{k}\left(kw_{ij}\right).$$

Substituting (27) into (22) gives the Simplified Bernoulli Trial operator

(28) $$G_{\text{SBT}}(\Delta\text{t}) = \prod_{i=1}^{N^{(l)}-1}\left[\left(1 - \sum_{j=i+1}^{N^{(l)}}\frac{1}{k}\left(\Delta tkw_{ij}\right)\right)I + \sum_{j=i+1}^{N^{(l)}}\frac{1}{k}\left(\Delta tkw_{ij}\right)T_{ij}\right],$$

$$G_{\text{SBT}}(\Delta\text{t}) = \prod_{i=1}^{N^{(l)}-1}\left[\left(1 - \sum_{j=i+1}^{N^{(l)}}\frac{1}{k}\left(\Delta tkw_{ij}\right)\right)I + \sum_{j=i+1}^{N^{(l)}}\frac{1}{k}\left(\Delta tkw_{ij}\right)T_{ij}\right].$$

SBT considers $i = 1$ to $i = N^{(l)} - 1$ pairs. Thus, SBT has a computation expense of $\mathcal{O}\left(N^{(l)} - 1\right)$

3.4. Generalized Bernoulli Trials (GBT)

The reduction in particle-pair considerations provided by SBT motivates generalizing the controlled number of pair considerations. Call this parameter N_{sel}. This number is manually chosen and can be fine-tuned to run faster solutions with relatively similar accuracy. The reduction of particle-pair considerations will require an additional correction coefficient k', which is obtained by setting the relation

(29) $$k'\sum_{i=1}^{N_{\text{sel}}}\sum_{j=i+1}^{N^{(l)}} 1 = \sum_{1\le i<j\le N^{(l)}} 1,$$

which implies, without loss of generality, the unitless effect of k' of N_{sel} pairs with $j \in \left\{i+1, \cdots, N^{(l)}\right\}$ is identical to the effect of considering all pairs. The left-hand side deals with the desired pairs, N_{sel}. Consider the complement $N^{(l)} - N_{\text{sel}}$, which are the undesired pairs. Then, the desired pairs are identical to the total pairs minus the undesired pairs. Substituting into the left-hand side of (29) results in

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

Expand the right-hand side of (30) by (3)

(31) $$\sum_{1\le i<j\le N^{(l)}} 1 = \sum_{i=1}^{N^{(l)}-1}\sum_{j=i+1}^{N^{(l)}} 1.$$

Substituting (29) and (31) into (30) yields

(32) $$k'\left[\sum_{i=1}^{N^{(l)}-1}\sum_{j=i+1}^{N^{(l)}} 1 - \sum_{i=1}^{\left(\text{N}^{(\text{l})}-\text{N}_{\text{sel}}\right)-1}\left(\sum_{j=i+1}^{\text{N}^{(\text{l})}-\text{N}_{\text{sel}}} 1\right)\right]\sum_{i=1}^{N^{(l)}-1}\sum_{j=i+1}^{N^{(l)}} 1.$$

Simplifying gives

(33) $$k'\left[\binom{N^{(l)}}{2} - \binom{N^{(l)}-N_{\text{sel}}}{2}\right] = \binom{N^{(l)}}{2}.$$

Thus, the correction coefficient for GBT is

(34) $$k' = \frac{N^{(l)}\left(N^{(l)}-1\right)}{N_{\text{sel}}\left(2N^{(l)}-N_{\text{sel}}-1\right)}.$$

With the identical idea of (27)

(35) $$w_{ij}^{(\text{exact})} \approx \frac{1}{k'k}\left(k'kw_{ij}\right).$$

Finally, the GBT operator by using (35) in (22)

(36) $$G_{\text{GBT}}(\Delta t) =$$
$$=\prod_{i=1}^{N_{\text{sel}}}\left[\left(1 - \Delta t\sum_{j=i+1}^{N^{(l)}}\frac{1}{k'k}\left(k'kw_{ij}\right)\right)I + \Delta t\sum_{j=i+1}^{N^{(l)}}\frac{1}{k'k}\left(k'kw_{ij}\right)T_{ij}\right].$$

3.5. Symmetrized Simplified Bernoulli Trials (SSBT)

Both SBT and GBT consider collision partner candidates "after" particle i. The idea of symmetry and the consideration of particles "before" provides a more consistent model by giving equal selection chances.

Symmetric inclusion can be applied because of the commutativity of particle collision probabilities: $w_{ij} = w_{ji}$. Meaning, probability can be equivalently represented by

$$w_{ij} = \frac{w_{ij}+w_{ji}}{2}. \tag{37}$$

The transposition in the indices allows the operator to sum over all $j \neq i$. This further implies the correction coefficient for SSBT is

$$k_{\mathrm{SS}} = N^{(l)} - 1. \tag{38}$$

From (37), the probability of collision is approximately

$$w_{ij}^{(\mathrm{exact})} \approx \frac{1}{k_{\mathrm{SS}}}\left(\frac{k_{\mathrm{SS}}}{2}\left(w_{ij} + w_{ji}\right)\right). \tag{39}$$

Over all particles i with all possible partner candidates a distinct j, the SSBT operator takes the form

$$G_{\mathrm{SSBT}}(\Delta t) = \prod_{i=1}^{N^{(l)}}\left[\left[1 - \sum_{j=1,j\neq i}^{N^{(l)}} \frac{1}{k_{\mathrm{SS}}}\left(\frac{k_{\mathrm{SS}}}{2}\left(p_{ij} + p_{ji}\right)\right)\right] I + \right. \\ \left. + \sum_{j=1,j\neq i}^{N^{(l)}} \frac{1}{k_{\mathrm{SS}}}\left(\frac{k_{\mathrm{SS}}}{2}\left(p_{ij} + p_{ji}\right)\right) T_{ij}\right]. \tag{40}$$

3.6. Symmetrized Generalized Bernoulli Trials (SGBT)

SSBT may also be generalized by setting a number N_{sel} for the limit of total pair considerations. To find the correction coefficient, employ the idea of (29)

$$k_{\mathrm{SG}} \sum_{i=1}^{N_{\mathrm{sel}}} \sum_{j=1,j\neq i}^{N^{(l)}} 1 = \sum_{i=1}^{N^{(l)}} \sum_{j=1,j\neq i}^{N^{(l)}} 1. \tag{41}$$

Whose relation implies

$$k_{\mathrm{SG}} = \frac{N^{(l)}}{N_{\mathrm{sel}}}. \tag{42}$$

Treating the appropriate bounds and plugging (42) with (40) admits

$$G_{\mathrm{SGBT}}(\Delta t) = \prod_{i=1}^{N_{\mathrm{sel}}}\left[\left[1 - \sum_{j=1,j\neq i}^{N^{(l)}} \frac{1}{k_{\mathrm{SG}}k_{\mathrm{SS}}}\left(\frac{k_{\mathrm{SG}}k_{\mathrm{SS}}}{2}\left(p_{ij} + p_{ji}\right)\right)\right] I + \right. \\ \left. + \sum_{j=1,j\neq i}^{N^{(l)}} \frac{1}{k_{\mathrm{SG}}k_{\mathrm{SS}}}\left(\frac{k_{\mathrm{SG}}k_{\mathrm{SS}}}{2}\left(p_{ij} + p_{ji}\right)\right) T_{ij}\right]. \tag{43}$$

4. Results and discussion

4.1. Validation of GBT and SGBT for low Particles Per Cell simulations

The following results were obtained with a particle-per-cell (PPC or $N^{(l)}$) of 10 for GBT and SGBT. Relaxation from initially non-equilibrium [1] to the equilibrium of argon gas was considered. For various N_{sel} ranging from 2 to $N^{(l)} - 1 = 9$, the

simulation time was normalized by SBT and SSBT times at $N_{\mathrm{sel}} = 9$, respectively. To ensure accuracy, each simulation was conducted with a time step fitted to maintain Probability Exceed Ratio (WER) [δ] within a specified tolerance.

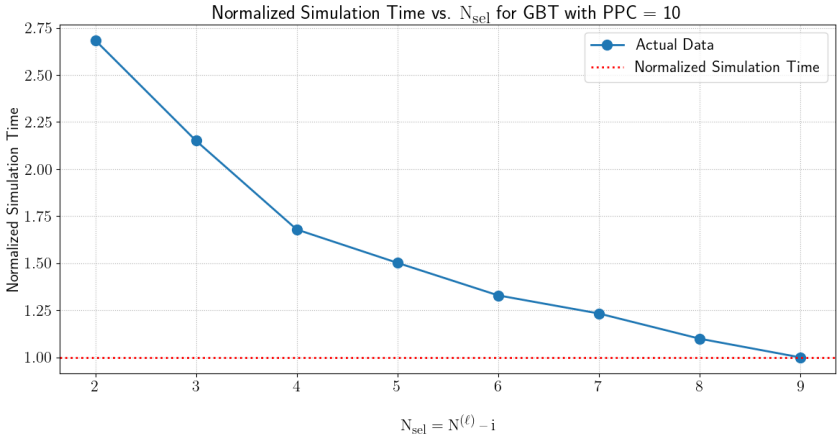

Fig. 1. Generalized Bernoulli trials for $2 \leq N_{\mathrm{sel}} \leq 9$

For the GBT simulations, WER was constrained to 0.0015 ± 0.0005. GBT at 10 PPC obtained an optimal value at $N_{\mathrm{sel}} = 9$, which defaulted to SBT. The maximum obtained value at $N_{\mathrm{sel}} = 2$ yielded a normalized simulation time of ≈ 2.683, as shown in Fig. 1.

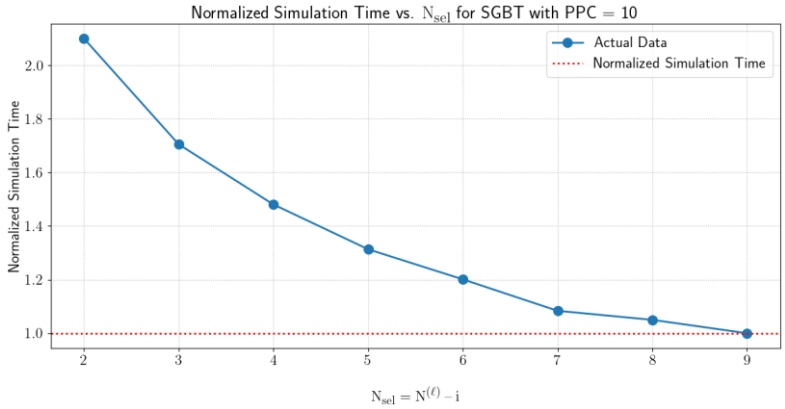

Fig. 2. SGBT for $2 \leq N_{\mathrm{sel}} \leq 9$

For the SGBT simulations, WER was constrained to 0.0175 ± 0.025. GBT at 10 PPC obtained an optimal value at $N_{\mathrm{sel}} = 9$, which also defaulted to SSBT. The maximum obtained value at $N_{\mathrm{sel}} = 2$ resulted in a normalized simulation time of ≈ 2.099 (Fig. 2).

4.2. Validation of GBT and SGBT for higher Particles Per Cell simulations

The following results were obtained with PPC = 20 for GBT and SGBT. For various N_{sel} ranging from 2 to $N^{(l)} - 1 = 19$, the simulation time was normalized

by SBT and SSBT times at $N_{\mathrm{sel}} = 19$, respectively. We continue to withhold accuracy by constraining WER to specified tolerances.

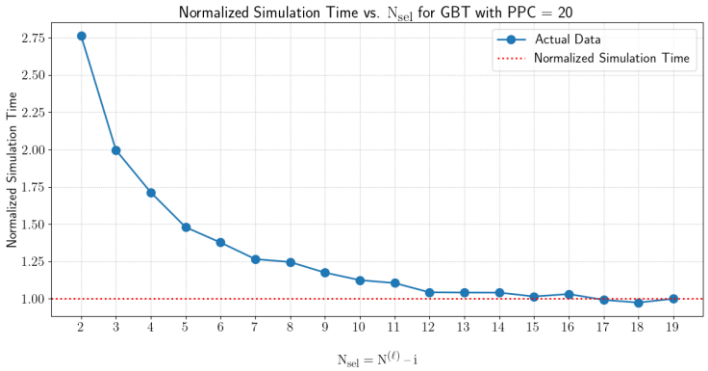

Fig. 3. GBT for $2 \leq N_{\mathrm{sel}} \leq 19$

For the GBT simulations, WER was constrained to 0.0015 ± 0.0005. Both $N_{\mathrm{sel}} = 17$ and $N_{\mathrm{sel}} = 18$ resulted in faster normalized simulation time to SSBT. In this case, $N_{\mathrm{sel}} = 18$ yielded the optimal value, resulting in a normalized simulation time of ≈ 0.974. The simulations achieved a maximum normalized time at $N_{\mathrm{sel}} = 2$ with a value of ≈ 2.763 (Fig. 3).

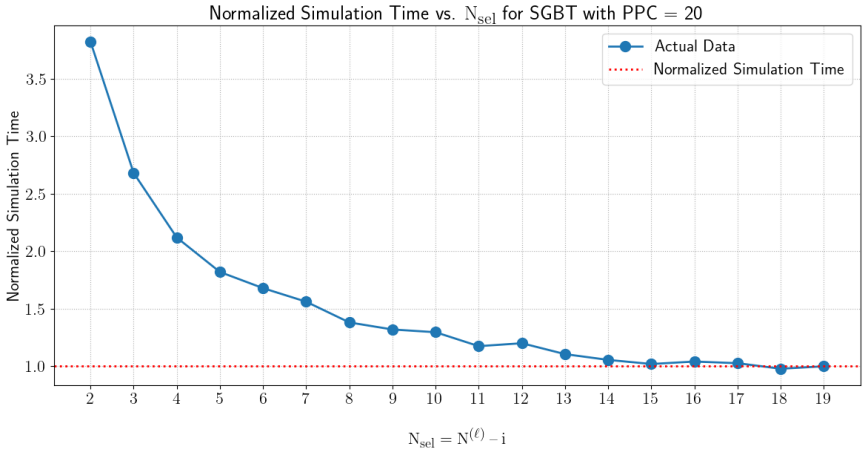

Fig. 4. SGBT for $2 \leq N_{\mathrm{sel}} \leq 19$

For the SGBT simulations, WER was also constrained to 0.0015 ± 0.0005. SGBT returned parallel results with the existence of a nontrivial optimal value of $N_{\mathrm{sel}} = 18$, which resulted in the minimum normalized computational time of ≈ 0.978. The maximum normalized time resulted from $N_{\mathrm{sel}} = 2$, which yielded a value of ≈ 3.822 (Fig. 4).

4.3. Influence of PPC by comparison of methods

The data suggest that a higher PPC makes GBT and SGBT more effective. This can be seen visually: the PPC = 20 plots shown in Figs 1-4 show the normalized

simulation time axis for a longer period and converge faster than the PPC = 10 plots. This implies that a higher value indicates a lower value for N_{sel} can yield results comparably fast while maintaining accuracy.

The contrapositive also suggests a noticeable inefficiency for lower values of N_{sel} with a higher PPC value. The maximum values for PPC = 20 are consistently greater than those of PPC = 10. For instance, SGBT with $N_{\mathrm{sel}} = 2$ obtained a maximum value of 2.099 for PPC = 10, but a lesser result of 2.763 for PPC = 20.

Intuitively, this is consistent with the fact that more particles tend to allow for greater approximations in the form of a lesser N_{sel}. This may be visually illustrated by the range of minima and maxima for lower PPC and higher PPC.

4.4. Comparison of optimal N_{sel}

For GBT and SGBT at PPC = 10, the optimal value for N_{sel} was 9. This implies that for lower PPC values, SBT is the more efficient collision-pairing algorithm. For PPC = 20, GBT and SGBT have an optimal time for $N_{\mathrm{sel}} = 18$. In line with the plots, GBT and SGBT become more efficient at higher PPC values.

For GBT, both $N_{\mathrm{sel}} = 17$ and $N_{\mathrm{sel}} = 17$ achieved a faster time than SBT. While SGBT had only its optimal N_{sel} faster than SSBT, the plots show a greater proportion of cap N_{sel} values with normalized simulation times closer to the normalization line, with cap N_{sel} equal to 19 (SSBT).

5. Conclusion

This work is a sequential presentation of the formulation, derivation, and evaluation of the Bernoulli-Trial (BT) family of collision operator schemes within the Direct Simulation Monte Carlo (DSMC) framework. The BT approximations, derived from the general transition operator of the Kac Master equation, provide a rigorous probabilistic description of a series of collision partner selection schemes that significantly complement the group of collision algorithms used in DSMC simulations. The present study was limited to several members of the BT family, including the Simplified Bernoulli Trials (SBT), Generalized Bernoulli Trials (GBT), Symmetrized Simplified Bernoulli Trials (SSBT), and Symmetrized Generalized Bernoulli Trials (SGBT) schemes.

The mathematical derivation is based on the sequential linearization of parts of the general transition operator, presenting a solution of the Kac Master equation over a small discrete time step. One important consequence of these approximations is the creation of collision algorithms that keep the solution accuracy when working with a small number of particles in cells. In particular, the introduction of the pair-selection parameter N_{sel} in the generalized formulations allows for decreasing N_{sel} and balancing computational efficiency and statistical accuracy while preserving the statistical consistency of the collision process.

Benchmarked relaxation to equilibrium problem was used to evaluate the performance of the BT-based algorithms under different Particle-Per-Cell (PPC) conditions. For low PPC values, the SBT scheme is more efficient than the other considered algorithms because it minimizes the number of pair evaluations while

maintaining sufficient accuracy. For higher PPC values, however, the generalized algorithms – particularly GBT and SGBT – become more preferable because an appropriate selection of N_{sel} significantly reduces computational cost without loss of physical fidelity.

The symmetric collision selection improves the statistical consistency of the algorithm by allowing particles to interact with neighbours both before and after their index positions.

The development of the BT family of collision approximating algorithms gives rise to creating flexible hybrid schemes that combine the best qualities of the respective schemes for accurate and efficient modeling in time and space of non-equilibrium gas flows in complex domains. The hybrid approach, combined with an adaptive computational grid, may expand DSMC applications to a broader range of large-scale rarefied gas flows without requiring a prohibitively large number of simulators or computational resources.

***Acknowledgement*s:** Stefan Stefanov acknowledges the support provided by the MES under the Grant No D01-325/01.12.2023 for NCDSC – part of the Bulgarian National Roadmap on RIs.

References

1. B i r d, G. A. Approach to Translational Equilibrium in a Rigid Sphere Gas. – Phys. Fluids, Vol. **6**, 1963, No 10, pp. 1518-1519.
2. R o o h i, E., S. S t e f a n o v. Collision Partner Selection Schemes in DSMC: From Micro/Nano Flows to Hypersonic Flows. – Physics Reports, Vol. **656**, 2016, pp. 1-38.
3. B i r d, G. A. Molecular Gas Dynamics and the Direct Simulation of Gas Flows. Oxford, Oxford University Press, 1994.
4. K o u r a, K. Null-Collision Technique in the Direct-Simulation Monte-Carlo Method. – Physics of Fluids, Vol. **29**, 1986, No 11, pp. 3509-3511.
5. I v a n o v, M. S., S. V. R o g a s i n s k y. Theoretical Analysis of Traditional and Modern Schemes of the DSMC Method. – In: A. E. Beylich, Ed. Rarefied Gas Dynamics, Proc. 17th Symp. Rarefied Gas Dynamics, VCH, Aachen, Germany, 1991, pp. 629-642.
6. S h o j a-S a n i, A., E. R o o h i, M. J a v a n i, H. A k h l a g h i, S. S t e f a n o v. Efficient Collision Algorithms in DSMC for Rarefied Gas Dynamics: Markovian NTC-Pre-Scan and Bernoulli-Trial Schemes. –Vacuum, Vol. **247**, 2026, 115138.
7. S t e f a n o v, S. K. On DSMC Calculations of Rarefied Gas Flows with a Small Number of Particles in Cells. – SIAM J. Sci. Comput., Vol. **33**, 2011, No 2, pp. 677-702.
8. A k h l a g h i, H., E. R o o h i, S. S t e f a n o v. On the Consequences of Successively Repeated Collisions in a No-Time-Counter Collision Scheme in DSMC. – Computers & Fluids, Vol. **161**, 2018, No 1, pp. 23-32.
9. B e l o t s e r k o v s k i i, O. M., V. E. Y a n i t s k i i. The Statistical Particles-In-Cells Method for Solving Rarefied Gas Dynamics Problems. – USSR Comput. Math. Math. Phys, Vol. **15**, 1975, No 5, pp. 101-114.
10. Y a n i t s k i y, V. E. Operator Approach to Direct Simulation Monte-Carlo Theory in Rarefied Gas Dynamics. – In: A. E. Beylich, Ed. Rarefied Gas Dynamics: Proc. 17th Symp. Rarefied Gas Dynamics, VCH, Aachen, Germany, 1991, pp. 770-777.
11. K a c, M. Probability and Related Topics in Physical Sciences. New York, Interscience Publishers, 1959.
12. Y a n i t s k i i, V. E. Stochastic Model of a Boltzmann Gas and Its Numerical Realization. ─ In: A. A. Dorodnicyn, Ed. Modern Problems in Computational Aerohydrodynamics. Boca Raton, CRC Press, London, Ann Arbor, 1992, pp. 339-355

13. S t e f a n o v, S. K. Particle Monte-Carlo Algorithms with Small Number of Particles in Grid Cells. – In: I. Dimov, S. Dimova, N. Kolkovska, Eds. Numer. Methods Appl, Berlin, Heidelberg, Springer, 2011, pp. 110-117.
14. S t e f a n o v, S. DSMC Collision Algorithms Based on Kac Stochastic Model. – In: M. Mareschal, A. Santos, Eds. Rarefied Gas Dynamics 28, AIP Conference Proceedings, Zaragoza, Spain, Vol. **1501**, 2012, pp. 609-614.
15. R o o h i, E., S. S t e f a n o v, A. A. S h o a-S a n i, H. E j r a e i. A Generalized Form of the Bernoulli Trial Collision Scheme in DSMC: Derivation and Evaluation. – J. Comput. Phys., Vol. **354**, 2018 (Supplement C), No 2, pp. 476-492.
16. T a h e r i, E., E. R o o h i, S. S t e f a n o v. A Symmetrized and Simplified Bernoulli Trial Collision Scheme in Direct Simulation Monte Carlo. – Phys. Fluids, Vol. **34**, 2022, No 1, 012010.
17. J a v a n i, M., E. R o o h i, S. S t e f a n o v. Symmetrized Generalized and Simplified Bernoulli-Trial Collision Schemes in DSMC. – Comput.&Fluids, Vol. **272**, 2024, No 10, 106188.
18. R o o h i, E., H. A k h l a g h i, S. S t e f a n o v. Advances in Direct Simulation Monte-Carlo: From Micro-Scale to Rarefied Flow Phenomena. – Singapore, Springer Nature, 2025.
19. S t e f a n o v, S., E. R o o h i, A. S h o j a-S a n i. A Novel Transient-Adaptive Subcell Algorithm with a Hybrid Application of Different Collision Techniques in Direct Simulation Monte-Carlo (DSMC). – Phys. Fluids, Vol. **34**, 2022, No 9, 092003.
20. M e t r o p o l i s, N., A. W. R o s e n b l u t h, M. N. R o s e n b l u t h, A. H. T e l l e r, E. T e l l e r. Equation of State Calculations by Fast Computing Machines. – The Journal of Chemical Physics, Vol. **21**, 1953, No 6, pp. 1087-1092.

Received: 08.03.2026, Accepted: 20.04.2026