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A REVIEW OF KAC-BASED COLLISION MODELS: BERNOULLI TRIALS AND ITS SIMPLIFIED AND INTELLIGENT VARIANTS

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KEY WORDS

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ABSTRACT

Graeme Bird developed the Direct Simulation of Monte Carlo (DSMC) in the 1960s, and nowadays this method has gained popularity in simulation of rarefied gas dynamics and micro gas flow problems. In addition to the requirement of employing multidimensional computational mesh, the DSMC method uses a finite set of particles or simulators, denoted by their positions and velocities, to model the advection and collision terms of the Boltzmann equation. The requirement of these large computational resources have been a prohibitive barrier in the DSMC analysis of massive computational two- and three-dimensional problems in rarefied gas dynamics. This work is dedicated to review some recent advancements in reducing the DSMC computational requirements by using Kac model -based collision schemes in the Direct Simulation of Monte Carlo. In general, two major concepts exist for obtaining collision schemes, and here we focus our attention to the one based on the Kac stochastic model. The common advantage of these schemes is that their algorithms avoid the repeat collisions, and can be used to reduce the number of particles as a portion of computational resources. The paper reviews this conception since Yanitiskiy first introduced the Bernoulli Trials collision scheme (BT), to the introduction of Simplified Bernoulli Trials (SBT), proposed by Stefanov. We also present a new intelligent variant of the SBT collision pairs.

1. INTRODUCTION

The Direct Simulation Monte Carlo (DSMC) [1] is a particle-based method commonly used to solve the Boltzmann equation by using stochastic schemes. In the framework of the DSMC method, the real gas dynamics process is discretized in time and space, and two successive split stages of free molecular motion and binary intermolecular collisions are defined in a way directly to simulate the advection and collision terms of the Boltzmann equation. The collision algorithm plays the major role in the DSMC method, and calculates the most sophisticated term of the Boltzmann equation. Theoretical works on the construction of a collision scheme can be categorized in two groups. The concept of the first group is based on the principle of the maximum collision rate per time step, e.g. "No Time Counter (NTC)" [1], "Null-collision" [2], "Majorant Frequency Scheme" [3]. In this group, the Bird's NTC scheme has been widely used as a highly reliable scheme. Since the collision pairs in

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this scheme are merely chosen through random selections, NTC requires a number of particles in the cell that is suitable/high enough to avoid successively repeated collisions.

It should be noted that besides the inherent discretization problems of deterministic numerical approaches, DSMC calculations suffer from two extra problems: (a) the presence of statistical noise in output results, and (b) the dependence of the results on particle number per cell. It has been shown that [4-5] a modified Monte Carlo simulation, which takes into account the asymptotic properties of near continuum low speed regimes, is capable to overcome the first problem. In response to the second problem, other type collision schemes , proposed by Belotserkovskii and Yanitiskiy [6] and Yanitiskiy [7], are constructed on the base of the Kac stochastic model. Contrary to the first group of collision schemes, the latter group in accordance with the Kac stochastic model defines a collision probability function for each particle pair and checks all pair combinations for collision occurrence, hence it avoids at least part of the successively repeated collisions.

In this paper, first we review the Yanitskiy approach to show how the Bernoulli-Trials collision scheme (BT) was derived from the Kac stochastic model to avoid the repeat collisions. Next, we mention how Stefanov introduced a simplified variant of the Bernoulli Trials scheme entitled as 'SBT' [8-9]. Unlike the former scheme (BT), 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. Finally, considering the mean collision separation distance (MCS) as an important parameter of the quality of collisions, we review how it is possible in Bernoulli-Trials collision schemes to reduce MCS and increase the quality of the collision process by using the Transient Adaptive Subcell technique (TAS) [10-12]. A variety of problems ranged from low-speed flows in micro-scale geometries to flows in hypersonic regimes, e.g. the Steady Hypersonic cylinder, were simulated using SBT or its combination with the transient adaptive sub-cell technique (SBT-TAS). These simulations confirm our idea that the SBT/SBT-TAS compared with other methods, i.e. NTC/NTC-TAS, is capable to give an accurate solution by using smaller number of particles per cell or smaller sample-size. Furthermore, in this work as an evolution of the SBT scheme to its intelligent variant, we introduce a new collision scheme entitled as the Intelligent Simplified Bernoulli Trials (ISBT). Benefiting from the procedure of SBT in sorting and choosing collision pairs in an hierarchical order, the ISBT attempts to provide a semi-cognition of distance for the collision scheme. This semi-cognition then will lead to the creation of pseudo-circular subcells that reduce approximately 25-32% of the overall mean collision separation distance (MCS). Understanding the recent notes of Gallis et al. [13-15] 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 policy of near neighbor pair-selection.

2. CONSTRUCTION OF BERNOULLI TRIALS COLLISION SCHEMES

The probability function of the collision pair (i,j) in the Kac stochastic model with a particle evolution system of $\{x^{(l)}, C_{N(l)}\} = \{x_j^{(l)}(t_k), c_j^{(l)}(t_k)\}, j = 1, ..., N^{(l)}$ in cell (*l*) with volume $V^{(l)}$ for time τ , can be constructed as the following:

$$w_{ij}\tau = \frac{\sigma_{ij}g_{ij}\tau}{w^{(l)}},\tag{1}$$

, where σ_{ij} is the product of collision cross-section and $g_{ij} = |c_i - c_j|$ is the particles relative velocities. Considering this equation and the standard kinetic approach, it is possible to derive the Kac master equation of density distribution, denoted by $F_{N(l)}(t, x^{(l)}, C_{N(l)})$, for all possible velocity vectors of $C_{N(l)}$. In case of the given state at 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:

$$F_{N(l)}(t, \boldsymbol{x}^{(l)}, \boldsymbol{C}_{N(l)}) = G(t) F_{N(l)}(t_0, \boldsymbol{x}^{(l)}, \boldsymbol{C}_{N(l)})$$
(2)

, and G(t) is defined as follows: $G(t) = \left[t \sum_{1 \le i \le N^{(l)}} w_{ii}(T_{ii} - I)\right] =$

$$G(t) = \left[t \sum_{1 \le i < j \le N^{(l)}} w_{ij}(T_{ij} - I)\right] = exp[t(T - I)],$$
(3)



, where

$$I\psi \equiv \psi, \qquad T_{ij} = \int_0^{4\pi} \psi(\boldsymbol{C}_{ij}) \, d\sigma_{ij}(\boldsymbol{\Omega}) \tag{4}$$

are operators, acting on a linear normal space of continues functions $\psi(C)$ over Ω , $d\sigma_{ij}(\Omega)$ is a differential cross section (see [16]). For small interval τ each term of the equation (3) can be extended to turn G(t) into the following form $G_1(\tau)$ (while terms of order equal or higher than $O(\tau^2)$ are neglected):

$$G_{1}(\boldsymbol{\tau}) = \prod_{i=1}^{N^{(l)}-1} \prod_{j=i+1}^{N^{(l)}} [(1 - \boldsymbol{\tau} w_{ij})I + \boldsymbol{\tau} w_{ij}T_{ij}]$$

=
$$\prod_{i=1}^{N^{(l)}-1} \prod_{j=i+1}^{N^{(l)}} [(1 - W_{ij})I + W_{ij}T_{ij}], \qquad (5)$$

2.1 The BT algorithm

The Bernoulli trials (BT) collision algorithm proposed by Yanitskiy [7] implements the W_{ij} in the right hand side of the equation (5) as the probability function for collision of the pair(*i*,*j*) within time interval of τ . The BT algorithm states that for all of the available particle pairs in the collision cell (*l*), the acceptance/rejection should be checked, i.e. the following inequality should be checked for all available particle pairs(*i*,*j*) { $i < j = 1, ..., N^{(l)}$ } (before their velocities are changed to post collision values):

$$W_{ij} = \frac{\sigma_{ij}g_{ij}\tau}{V^{(l)}} > Ranf, \tag{6}$$

, and the probability for $W_{ij} > 1$ should be kept always close to zero, by choosing appropriate time step and cell size.

2.2 The SBT algorithm

The computational cost of the BT algorithm has a quadratic dependency with the number of particles in a cell. Stefanov [8-9] extended the internal product in the right hand side of the equation (5) in a series of j with respect to τ to reach to a new simplified transition operator $G_2(\tau)$ (where terms of order equal or higher than $O(\tau)$ are neglected):

$$G_{2}(\tau) = \prod_{i=1}^{N^{(l)}-1} \left[\left(1 - \sum_{j=i+1}^{N^{(l)}-1} \frac{1}{k} (k\tau w_{ij}) \right) I + \sum_{j=i+1}^{N^{(l)}-1} \frac{1}{k} ((k\tau w_{ij})T_{ij}) \right]$$
(7)

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

The algorithmic interpretation of operator $G_2(\tau)$ states that the SBT procedure starts with a locally indexing of particles in the l^{th} cell from 1 till $N^{(l)}$. The first particle, say *i*, is sequentially selected from 1 to $N^{(l)}$, while its pair, say *j*, at each sequent is randomly selected among the further available particles, by considering this approach:

$$j = (i+1) + int \left(Ranf \times \left(N^{(l)} - i \right) \right)$$
(8)

, where $Ranf \in [0, 1)$. Eventually, the collision is accepted if the SBT probability function of W_{ij} fulfills the following inequality:

$$W_{ij} = kF_n \frac{\sigma_{ij}g_{ij}\tau}{v^{(l)}} > Ranf$$
(9)

, where F_n is the ratio of the number of real molecules to the simulated particles. Similar to BT algorithm, the probability for $W_{ij} > 1$, should be kept always close to zero by choosing appropriate time step and cell size.

2.3 Comparison of BT and SBT collision algorithms

Previous studies on the BT and SBT algorithms revealed that in general both schemes have the same behavior pattern. For instance, in relative to other collision schemes, e.g. the NTC scheme, Stefanov [9] demonstrated that the BT and SBT schemes could employ much smaller number of particles in rarefied or in micro gas flow problems. However, the performance studies indicated that in case of employing the same number of particles, the computational costs of BT and SBT schemes are larger



than the NTC, and the SBT scheme obtains a much lower computational costs than the BT scheme (see Ref. [9]).

3. EXTENSION OF THE SBT-TAS ALGORITHM TO CURVED BOUNDARY GEOMETRIES

3.1 Transient Adaptive Sub-Cell Technique (TAS)

In DSMC, the mean collision separation distance (MCS) is a critical parameter that is used as a quality-meter of accepted collisions. It is said that, a good collision is a one, which its MCS is smaller than one-third of the local mean free path. Subcell is an aided tool for collision schemes that provides a closer look upon cell space. It means subcells help the collision operations to work in smaller frameworks. However, as the numerical simulation goes by and the number density variation increases among cells, the idea of using a constant number of subcells for all cells might look inefficient. Transient adaptive subcell technique (TAS) is a response to the desire of dynamically adapting collision cell space in accordance with the instantaneous available particle numbers in that cell. It is while that subcell generation in the TAS technique has only transient burden on memory allocation of numerical simulation. In other words, the adaptation will dynamically allocate and deallocate its memory requirements at each collision stage, and the size of the allocation is dependent to the most populated cell. For each cell, this transient layer of subcells is fabricated by a special number of divisions along x (D_x) and y (D_y):

$$D_x = \sqrt{\frac{N^{(l)}}{AR \times Envelop \times PPSC}} \tag{10}$$

$$D_{y} = D_{x} \times AR \; ; \; AR = \frac{\Delta y_{cell}}{\Delta x_{cell}}; \; Envelop = \frac{V^{(l)}}{\Delta y_{cell} \times \Delta x_{cell}} \tag{11}$$

, where AR is the aspect ratio, PPSC is the desired number of particles per subcell and Envelop is used to increase the number of subcells, in case the cell is not fully rectangular.

3.2 SBT-TAS

TAS grid divides the collision cell into equally spaced rectangular divisions, and the SBT procedure can independently operate within their space. Although these divisions are physically rectangular and particle indexing is also made with this consideration, their effect on the probability function is not necessarily based on fully rectangular divisions. By fabricating subcell divisions over a collision cell, we would have three types of subcell (Fig.1-a): (1) The first group is the ones, which are out of the borders of the collision cell and they are not considered in the flow in relative to the current collision cell. (2) The second group is the ones, which are in flow, but they are vacant, and consequently they're assumed inactive in collision occurrence. (3) The third group of subcells is the ones that are totally or partially in the flow and at the same time contain at least one particle. These subcells are called as "inflow active" subcells. SBT scheme can rely on in-flow active subcells as the probable areas for registering a collision. The \forall_m in the probability function of the SBT-TAS scheme (equation (11)) is the available volume that is assigned to the stack of indexed particles. Because the collision cell is considered a homogeneous space, it is possible to assume that cell volume is equally distributed among in-flow active subcells (type 3). Fig.1-b demonstrates how the cell volume is heterogeneously divided among the type3 subcells. In the regards of the new borders, we can modify the probability function in the form of the Equation (11). For each subcell, i.e. for the subcell mth it will be:

$$W_{ij}^{m} = F_n \left(N_m - i \right) \left(\sigma g \right)_{ij} \frac{\Delta t}{\forall_m}; \ \forall_m = \frac{V^{(l)}}{NS_{type\,3}}$$
(11)

, where W_{ij}^m is the probability of the pair (i, j) in the m^{th} subcell, N_m is the number of indexed particles for this subcell, NS_{type 3} is the number of type 3 subcells, and \forall_m is calculated in a way that all the collision cell volume $(V^{(l)})$ is equally distributed among type 3 subcells.





Figure 1: Different subcell types; (a) subcell divisions for indexing particles, (b) subcell divisions based on the assigned volume in the estimation of probability function (divisions are tried to represent an equivalent volume of \forall_m).

Having the modified SBT-TAS collision scheme, now it is possible to simulate the flowfields that are highly dependent on the adaptation of the computational grid.

Using the Bird's DS2V code [17], we implemented the SBT-TAS collision algorithm [11-12] and compared the computational resources and costs of SBT-TAS with respect to the most recent DSMC collision-pair selection algorithm, i.e., No Time Counter-Nearest Neighbor (NTC-NN, or as is called: NN) [18-19]. The hypersonic rarefied gas flow past a cylinder [19] is selected here to show the performance behavior of SBT-TAS. It is a 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 T_s =500 K and a nominal free-stream Knudsen number of 0.01. Tab.1 represents the comparison between the SBT-TAS and NN in the hypersonic cylinder test case.

Scheme	Division	Particle	CPU-time	Sample-Size	Normalized CPU-time	Normalized Sample
	grid	per cell				size
NTC-TAS	100×95	10	61 min	4.0308 E9	1	1
SBT-TAS	100×95	10	33 min	2.2402E9	0.5409	0.5557

 Table 1: Comparison of CPU-time and Sample-size between the collision schemes of NN and SBT-TAS in the simulation of the hypersonic cylinder.

In order to evaluate the performance of SBT-TAS at higher Knudsen numbers, we consider this test for the hypesonic flow over the cylinder geometry in Knudsen numbers of 0.05, 0.5 and 1. Tab.2 presents the comparative performance data between SBT-TAS and NN for this test. This table states that SBT-TAS can employ a smaller number of particles at high Knudsen numbers. This issue could be attributed to the SBT property that for a definite number of particles checks for more number of collisions. Consider that the number of collision checking in the SBT scheme is equal to $N^{(l)}$ -1, where $N^{(l)}$ is the number of particles in the cell/subcell, while in the NTC scheme the number of collision acceptance/rejection checking is a function of collision rate. The positive point for the SBT collision scheme is that in the DSMC method as the Knudsen number increases, the required number of particles within the flow field would start to decline. Consequently, this reduction would help SBT collision scheme to employ smaller amount of particles, and increase the collision scheme efficiency.



Knudsen	Scheme	Division Grid	Total collision	Total	Elapsed time	Sample-size
number			cells	particles	(seconds)	
0.05	SBT-TAS	55×45	9553	7.5E4	229	4.57E8
	NTC-TAS	70×35	9455	7.E4	180	4.87E8
0.5	SBT-TAS	45×45	8034	4.E4	143	2.96E8
	NTC-TAS	55×55	12000	10.E4	220	9.79E8
1	SBT-TAS	20×15	1194	3.E4	182	2.84E8
	NTC-TAS	45×25	4480	8.E4	244	12.3E8

Table 2: Comparison of CPU-time and Sample-size between the collision schemes of NN and SBT-TAS in the simulation of the hypersonic cylinder at high Knudsen numbers.

4. THE SIMPLIFIED BERNOULLI TRIALS COLLISION SCHEME WITH INTELLIGENCE OVER PARTICLE DISTANCES

Here we review a modification of the Simplified Bernoulli Trials (SBT) scheme, called the Intelligent Simplified Bernoulli Trials (ISBT) scheme [20], which is capable to create pseudo-circular subcells that reduce approximately 25-32% of the mean collision separation distance (MCS).

ISBT scheme arranges the particle indexing and the collision acceptance-rejection of the SBT scheme in a way that leads to the formation of virtual clusters. These inner-cell clusters then will cause the selection of the 'near-neighbor' pair, which leads to the smaller mean collision separation distances for ISBT compared with SBT. The following procedure will describe the evolution of SBT into ISBT scheme:

The aim of the first step is to define a method for a locally indexing of particles based on the estimated inter-particle distances. The particle indexing should be modified in a way that a semi-perception of distance emerges in the hierarchical order of indexed numbers, i.e. in a collision cell with N⁽¹⁾ particles, we need to have an indexing method that satisfies the condition of $(\delta_i < \delta_j, 0 < i < j \le N^{(l)})$, where δ_i is the distance of the *i*th particle to a reference point \mathbb{R} (see Fig.2-a).

One can easily observe that the indexed points, relative to their hierarchical order, would be closer to each other if points are located in the list with respect to the distance to the corners of a rectangle that surrounds the particles (compare Figs. 2 (b-c) for example). Therefore, we suggest the random selection of cell/subcell corners to efficiently index particles. However, because the δ distance does not consider the angular distances, some particles continue to be indexed successively while they are far from one another. Specifically, this is seen for those particles on opposite sides of the diagonal (e.g., particles 4 and 5 in the Fig. 2-c). Statistically, these particles are not the majority, yet any other means of particle indexing would inevitably create situations where indexed particles would be far from each other.

It is essential to note that while along the indexing direction (diagonal RB in Fig.2-a) particles are prevented to collide in opposite corners (because they are indexed at the bottom and the top of the hierarchical order), along the other one (diagonal AC in Fig.2-a) particles might be indexed as neighbors, and their collision reverse the angular momentum. Since these kinds of collisions might be inevitably supported in the ISBT scheme, as a solution, we suggest using elongated cell/subcells.

In a quadrangular cell/subcell ('RABC' in Fig.2-d) the maximum distance (MD) that two far-indexed particles could have is $\sqrt{2}$ times greater than the side length. It can be shown that the corresponding values in the elongated rectangular cell/subcell ('RDEF' in Fig.2-d) will be smaller than those of equal-area quadrangle (compare the MD_Q value of 'RABC' quadrangle and maximum corresponding value MD_{R1} of 'RDEF' elongated-rectangle).





Figure 2: Distribution of some particles in a cell/subcell; (a) a system of particle indexing based on the distance of particles to a definite center point (e), (b) the indexing results for a group of nine particles when the (e) is located on the center of the cell, (c) when this point is on the left-down corner of the cell, and (d) the geometrical comparison between one quadrangle cell/subcell ("RABC") and its equal-area elongated cell/subcell ("RDEF"), while the calculated values for the maximum distance (*MD*) between two far-indexed particles are shown; they denote that elongated cell/subcell has smaller *MD* value.

In the second step, the objective is to alter the acceptance-rejection method of the SBT scheme in favor of the selection of closer pairs. To perform this as simple as possible, the ISBT scheme just follows the SBT procedure, i.e. the first particle, say *i*, is sequentially selected from 1 to $N^{(l)}$, while its pair, say *j*, at each sequent is randomly selected among the further available particles, identical to the SBT procedure in equation (8).

Here we restate equation (8) in the following form with a new name for the generated random number as $Ranf_I \in [0, 1)$:

$$j = (i+1) + int \left(Ranf_I \times \left(N^{(l)} - i \right) \right)$$
(12)

The important point is that the acceptance-rejection sections of the SBT and ISBT collision schemes differ by their random numbers. In fact in the ISBT scheme instead of regenerating the second random number, which happens in the acceptance-rejection section of the SBT scheme (in inequality (9)), here ISBT does not call any new random number for the acceptance-rejection section and implements the first generated one. In other words, the condition for acceptance-rejection of the collision pair (i,j) in the ISBT scheme would be as follows:

$$W_{ij} = kF_n \frac{\sigma_{ij}g_{ij}\tau}{V^{(l)}} > Ranf_I \tag{13}$$

Fig.3 compares the sequences of the ISBT and SBT procedures, in selection of the first and second collision pairs. Note that the main differences lie on the indexing section (the way to arrange particle numbers) and also in the acceptance/rejection section (the decision to generate or not the new random number $Ranf_I$).





Figure 3: The Simplified Bernoulli trials (SBT) and the Intelligent Simplified Bernoulli trials (ISBT) collision schemes, compared by their collision procedures.

As a result of this modification, pseudo-circular subcells (Fig.4) will be created that allow an easier acceptance for closer-pairs and a more superior condition for far from each other particles; it is because that smaller number for j, as the second particle in the hierarchical list of indexed numbers, is only obtained if the $Ranf_I$ is closer to zero, and conversely, greater number for j, as the second particle, is merely obtained if the $Ranf_I$ is further from zero.



• The 4th -10th indexed particles that are randomly chosen as the second collision pair $\langle i \rangle$

Figure 4: Pseudo-circular subcells in the ISBT scheme that causes a biased selection for closer collision pairs.

4.1.1 ISBT analysis in micro cavity

Having described the ISBT scheme, let's consider a square lid-driven cavity, shown in Fig.5-a, as a study tool to investigate the validation of primary properties of the ISBT collision scheme. Fig.5-b, represents the accuracy of the ISBT collision scheme relative to its other counterparts, the SBT and Nearest Neighbor (NN) schemes, in prediction of the velocity components along the cavity center lines.





Figure 5: (a) the lid-driven cavity used to investigate the validation of the ISBT scheme, (b) comparison of velocity components of the lid-driven cavity along the center lines, between NN, ISBT, and SBT schemes, in two different division grids of 100×100 and 200×200 with 10 particles per collision cell.

The dimensionless number, SOF, which is the mean collision separation distance (MCS) divided by the local mean free path (λ), is selected as a parameter for measuring the quality of collisions. Tab.3 averts that the ISBT, compared with the SBT collision scheme, reduced the *SOF* value about one-third.

Collision scheme	Division size	SOF value	SOF normalized by the resembling NN value	SOF normalized by the resembling SBT value
NN	100-100	0.0477	1	0.182
ISBT	100-100	0.1740	3.66	0.666
SBT	100-100	0.2621	5.49	1

Table 3: Comparison of the *SOF* $\left(\frac{MCS}{\lambda}\right)$ value in the lid-driven cavity flow between NN, ISBT and SBT collision schemes.

5. CONCLUSIONS

In general, the collision schemes used in the DSMC method can be categorized in two groups. The popular ones, e.g. NTC, are constructed on the estimation of maximum collision rate per time step. We paid our attention on the second group which are based on the Kac collision model. We demonstrated that their algorithm construction allows these collision schemes to avoid repeat collisions and therefore employ smaller number of particles per cell. Furthermore, the performance and accuracy analyses of the Bernoulli-trials family of collision schemes presented. It was shown that the simplification done in the Bernoulli Trials (BT) collision scheme lets the SBT collision algorithm to improve its efficiency. We reviewed how it is possible to implement the combination of the SBT collision scheme with the Transient Adaptive Subcell (TAS) over the curved boundary geometries. The performance-test data of SBT-TAS and NN schemes at the Hypersonic flow over the cylinder referred to the SBT-TAS method as a reliable collision scheme - the intelligent simplified Bernoulli-trial (ISBT) scheme, which is supplied with a rule for estimation of inter-particle distances and is able to prioritize the collision acceptance of closer pairs. We noticed that ISBT compared with the SBT scheme, is able to reduce approximately one third of the overall mean collision separation (MCS) distance.



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