A Convergence Proof for Bird's Direct Simulation Monte Carlo Method for the Boltzmann Equation

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Bird's direct simulation Monte Carlo method for the Boltzmann equation is considered. The limit (as the number of particles tends to infinity) of the random empirical measures associated with the Bird algorithm is shown to be a deterministic measure-valued function satisfying an equation close (in a certain sense) to the Boltzmann equation. A Markov jump process is introduced, which is related to Bird's collision simulation procedure via a random time transformation. Convergence is established for the Markov process and the random time transformation. These results, together with some general properties concerning the convergence of random measures, make it possible to characterize the limiting behavior of the Bird algorithm.

KEY WORDS: Boltzmann equation; Bird's direct simulation Monte Carlo method; stochastic numerical algorithm; convergence of random measures; Markov jump processes.

1. INTRODUCTION

Stochastic simulation schemes play an important role in the numerical treatment of the Boltzmann equation.^(10,14,16,20,21) Therefore theoretical results concerning the convergence of these simulation procedures are of considerable interest. Recently a convergence proof for Nanbu's simulation method has been published^(2,3) and the convergence of a procedure based on stochastic differential equations has been established.^(19,23)

The first and best-known simulation procedure for the Boltzmann equation is Bird's^(5,6) "direct simulation Monte Carlo method." This scheme is the main one used in engineering problems. However, the question of its

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convergence remains open. The purpose of the present paper is to fill this gap.

We are concerned with the initial boundary value problem

$$\frac{\partial}{\partial t}f(t, x, v) + (v, \nabla_x)f(t, x, v) = J(f)(t, x, v)$$
(1.1)

 $t \ge t_0, x \in G, v \in \mathbb{R}^3$, with the right-hand side

$$J(f)(t, x, v) = \int_{\mathbb{R}^3} dw \int_{\mathbb{S}^2} de \ q(v, w, e) [f(t, x, v^*) \ f(t, x, w^*) - f(t, x, v) \ f(t, x, w)]$$
(1.2)

where G is a bounded domain in the three-dimensional Euclidean space \mathbb{R}^3 , ∇_x denotes the vector of the partial derivatives with respect to x, de denotes the uniform surface measure on the unit sphere \mathbb{S}^2 , and dw denotes the Lebesgue measure. The function q is called the collision kernel.

Furthermore, v^* and w^* are the postcollision velocities related to the precollision velocities v and w and the collision parameter e via the formulas

$$v^* = v + e(e, w - v)$$

 $w^* = w + e(e, v - w)$
(1.3)

which are consequences of the conservation of momentum and energy.

An initial condition

$$f(t_0, x, v) = f_0(x, v), \qquad (x, v) \in G \otimes \mathbb{R}^3$$
 (1.4)

and deterministic and energy-conserving boundary conditions on $\partial G \otimes \mathbb{R}^3$ are assumed (e.g., specular reflection as considered in Babovsky and Illner⁽³⁾). The initial value f_0 is supposed to be normalized in such a way that

$$\int_{G} \int_{\mathbb{R}^{3}} f_{0}(x, v) \, dv \, dx = 1 \tag{1.5}$$

We refer to $Cercignani^{(7,8)}$ or Lebowitz and $Montroll^{(18)}$ for more details concerning the Boltzmann equation.

The paper is organized as follows. In Section 2, we describe the Bird algorithm. In Section 3, we prove some results concerning the convergence of random measures, which are necessary for the investigation of the Bird algorithm.

Section 4 contains the main result. The limit (as the number of particles tends to infinity) of the random empirical measures associated with the Bird algorithm is shown to be a deterministic measure-valued function satisfying an equation close (in a certain sense) to the Boltzmann equation.

Some comments on the results and related problems are given in Section 5.

In this paper, the following notations are used. The symbols (,) and || denote the scalar product and the norm, respectively, in the Euclidean space. The basic probability measure and the corresponding mathematical expectation are denoted by Prob() and *E*, respectively. The symbol \P_A denotes the indicator function of some set *A*. Finally, the sign \rightarrow is used to denote convergence as the index n=1, 2,... tends to infinity, if no other indication is given. Further notations will be introduced at the beginning of the sections where they are mainly used.

2. THE BIRD ALGORITHM

The Bird algorithm $^{(16,21)}$ defines the time evolution of a random particle system

$$(x_i(t), v_i(t)) \in G \otimes \mathbb{R}^3, \qquad i = 1, \dots, n$$

$$(2.1)$$

 $t \ge t_0$, where *n* is the number of particles. The evolution of the system depends on a time discretization

$$(t_k), \quad k = 0, 1, \dots$$

where $t_{k+1} = t_k + \Delta t$ for some $\Delta t > 0$.

At the time t_0 , the system

$$(x_i(t_0), v_i(t_0)), \quad i = 1, ..., n$$

is sampled in accordance with the initial condition (1.4) of the Boltzmann equation.

Given the state of the system at some time t_k ,

$$(x_i(t_k), v_i(t_k)), \quad i = 1, ..., n$$

k = 0, 1,..., the simulation of the free flow of the particles and the simulation of their collisions on the time interval

$$(t_k, t_{k+1}]$$

are separated. First, the free flow is simulated disregarding the possible collisions. Then, the collisions are simulated neglecting the free flow.

The free flow simulation is done by means of the transformation

$$\Phi_s(x, v) = (X_s(x, v), V_s(x, v)), \qquad s \ge 0$$
(2.2)

which describes the behavior of a particle starting at the time $s_0 = 0$ in the point (x, v). This transformation depends on the domain G and the corresponding boundary conditions used in the formulation of the Boltzmann equation. Let (s_m) , m = 1, 2, ..., be the moments at which the particle interacts with the boundary ∂G . Then, the function $X_s(x, v)$ is piecewise linear in s,

$$X_{s}(x, v) = x + \int_{0}^{s} V_{u}(x, v) \, du$$
(2.3)

and the function $V_s(x, v)$ is piecewise constant in s,

$$V_{s_{m+1}}(x, v) = \Psi(X_{s_{m+1}}(x, v), V_{s_m}(x, v))$$
(2.4)

m = 0, 1,... The transformation Ψ describes the interaction of the particle with the boundary, e.g., specular reflection.⁽³⁾ We suppose that energy is conserved, i.e.,

$$|V_s(x,v)| = |v|, \qquad s \ge 0 \tag{2.5}$$

The system resulting from the free flow simulation on the time interval $(t_k, t_{k+1}]$ is

$$(x_i^{(k)}, v_i^{(k)}) = \Phi_{\Delta t}(x_i(t_k), v_i(t_k)), \qquad i = 1, ..., n$$
(2.6)

The system (2.6) is the starting point for the *collision simulation* on the time interval $(t_k, t_{k+1}]$. This procedure depends on a division of the position space G into a finite number of disjunct cells

$$G_l, \qquad l=1,...,l_c$$

It is assumed that

$$g_l > 0, \qquad l = 1, ..., l_c$$

where g_i denotes the Lebesgue measure of the cell G_i . In each cell, collisions of the particles are simulated neglecting their exact positions. Moreover, the positions of the particles do not change, and there is no interaction between different cells.

We consider a fixed cell G_i and describe Bird's collision simulation procedure by means of a continuous-time process

$$z(t), \quad t \ge t_k$$

with the state space $(G \otimes \mathbb{R}^3)^n$, which we call *Bird's collision process*. In fact, this process depends on *n*, *l*, and *k*. We omit these indices whenever it (as we hope) does not lead to misunderstanding.

The initial value of the process is defined in accordance with (2.6),

$$z(t_k) = ((x_i^{(k)}, v_i^{(k)}), i = 1, ..., n)$$
(2.7)

Let n_i denote the number of particles of the system (2.7) which are in the cell G_i .

In the case $n_i < 2$, the evolution in the cell G_i is trivial in the sense that no collisions take place. Thus, we define

$$z(t) = z(t_k), \qquad t \ge t_k \tag{2.8}$$

In the case $n_l \ge 2$, we introduce a *Markov chain*

$$\kappa(m), \qquad m=0, 1,...$$

with the state space $(G \otimes \mathbb{R}^3)^n$, the initial state

$$\kappa(0) = z(t_k) \tag{2.9}$$

and the following transition rule.

Given the state $\kappa(m) = ((x_i, v_i), i = 1,..., n)$, first, the indices *i* and *j* of the particles due to take part in a collision are generated according to the probabilities

const
$$\P_{G_l}(x_i) \P_{G_l}(x_j) Q(v_i, v_j)$$
 (2.10)

where

$$Q(v, w) = \int_{S^2} q(v, w, e) de$$
 (2.11)

and const is an appropriate normalization factor.

Then, an element $e \in \mathbb{S}^2$ is generated in correspondence with the probability density

$$q(v_i, v_j, e)/Q(v_i, v_j)$$
 (2.12)

Finally, the postcollision velocities v_i^* and v_j^* are calculated according to (1.3).

The state $\kappa(m+1)$ is obtained from $\kappa(m)$ by replacing v_i and v_j by v_i^* and v_i^* , respectively.

Furthermore, a time counter is used, advancing the time by

$$\Delta \tau(m) = [n^{-1}(n_l - 1)(n_l/2) g_l^{-1} Q(v_i, v_j)]^{-1}$$
(2.13)

when the *m*th collision took place. Here, *i* and *j* are the indices of the particles taking part in the *m*th collision, and v_i and v_j are the precollision velocities.

Let $\tau(m)$, m = 0, 1,..., be the sequence of random moments generated by (2.13),

$$\tau(0) = t_k$$

 $\tau(m) = \tau(m-1) + \Delta \tau(m), \qquad m = 1, 2,...$
(2.14)

Then, the process z(t) is defined as

$$z(t) = z(\tau(m)),$$
 $t \in [\tau(m), \tau(m+1))$
 $z(\tau(m)) = \kappa(m),$ $m = 0, 1,...$ (2.15)

The collision simulation is performed by generating the processes $z^{(l)}$ in all cells G_l while the corresponding time counters remain less than t_{k+1} . The resulting particle system is

$$(x_i(t), v_i(t)) = \sum_{l=1}^{l_c} \P_{G_l}(x_i^{(k)}) \, z_i^{(l)}(t)$$
(2.16)

 $i=1,...,n, t \in [t_k, t_{k+1}]$, where $z_i^{(l)}$ denotes the *i*th component of the process $z^{(l)}$.

The system

$$(x_i(t_{k+1}), v_i(t_{k+1})), \quad i=1,..., n$$

is the starting point for the algorithm on the next time interval.

It should be mentioned that the time step Δt as well as the partition into cells (G_i) may depend on the time index k. However, we decided not to introduce further indices.

The factor n^{-1} enters formula (2.13) as compared with the corresponding expression in Illner and Neunzert⁽¹⁶⁾ and Ploss,⁽²¹⁾ since we assume the normalization condition (1.5). The factor $(n_l-1)n_l$ instead of n_l^2 is not essential for the limiting behavior, but it is technically more convenient for the proof.

The processes $z^{(l)}(t)$ have been introduced without restricting the positions of the particles to the cells G_l in order to avoid a random dimension of the state space.

3. AUXILIARY RESULTS

In this section, we prove some results concerning the convergence of random measures. We refer to Hennequin and Tortra,⁽¹⁵⁾ Chapter 25, for

basic facts related to the convergence of random variables with values in metric spaces, and to Billingsley⁽⁴⁾ for the theory of weak convergence of measures. In the proofs, we use several ideas from Skorokhod⁽²²⁾ and Smirnov.⁽²³⁾

Let $\mathcal{M} = \mathcal{M}(Z)$ be the space of finite measures on the space $Z = G \otimes \mathbb{R}^3$ equipped with the Borel σ -algebra. Some of the results are valid also for more general metric spaces Z. For any measurable bounded function φ and any $\mu \in \mathcal{M}$, we denote

$$\langle \varphi, \mu \rangle = \int_{Z} \varphi(z) \, \mu(dz)$$

Let $C_b = C_b(Z)$ be the space of bounded continuous functions on Z with the norm

$$\|\varphi\|_{\infty} = \sup_{z \in Z} |\varphi(z)|, \qquad \varphi \in C_b$$

Definition 3.1. A sequence of measures (μ_n) is said to converge weakly to a measure μ if

$$\langle \varphi, \mu_n \rangle \rightarrow \langle \varphi, \mu \rangle$$

for any $\varphi \in C_b$.

Let $C_L = C_L(Z)$ be the space of bounded and Lipschitz-continuous functions on Z with the norm

$$\|\varphi\| = \sup_{z, z' \in \mathbb{Z}} \left(|\varphi(z)| + \frac{|\varphi(z) - \varphi(z')|}{|z - z'|} \right)$$

Then, a metric on \mathcal{M} is defined as

$$\rho_{L}(\mu, \lambda) = \sup_{\|\varphi\| \leq 1} |\langle \varphi, \mu \rangle - \langle \varphi, \lambda \rangle|$$
(3.1)

 μ , $\lambda \in \mathcal{M}$. The metric (3.1) is equivalent to the weak convergence.⁽¹¹⁾

Let, subsequently, μ_n and μ denote random variables with values in \mathcal{M} . Let P_n and P be the corresponding probability measures on \mathcal{M} .

Definition 3.2. The sequence (μ_n) is said to converge to μ in distribution if

$$P_n \rightarrow P$$
 weakly

Definition 3.3. The sequence (μ_n) is said to converge to μ in probability if

$$\rho_L(\mu_n, \mu) \rightarrow 0$$
 in probability

As in the finite-dimensional case, the convergence in probability implies the convergence in distribution. Furthermore, since ρ_L is bounded, the convergence in probability is equivalent to the convergence in the mean,

$$E\rho_L(\mu_n,\mu) \to 0$$

For any measurable transformation T of the space Z into a metric space Z', let D(T) denote the set of discontinuity points of T. In particular, T may be a measurable real-valued function on Z. Furthermore, for any $\lambda \in \mathcal{M}$, let λ^*T^{-1} denote the measure on Z' defined as

$$(\lambda^* T^{-1})(A) = \lambda(T^{-1}(A))$$
(3.2)

for any measurable set $A \subset Z'$.

First we generalize the following result to the case of random measures.

Theorem 3.1 (Billingsley,⁽⁴⁾ Theorem 5.2(iii)). Suppose μ_n , μ to be deterministic and $\mu_n \rightarrow \mu$. Let φ be a measurable bounded function on Z such that

 $\mu(D(\varphi)) = 0$

Then,

$$\langle \varphi, \mu_n \rangle \rightarrow \langle \varphi, \mu \rangle$$

Theorem 3.2. Suppose $\mu_n \rightarrow \mu$ in distribution. Let φ be a measurable bounded function on Z such that

$$E\mu(D(\varphi)) = 0 \tag{3.3}$$

Then

 $\langle \varphi, \mu_n \rangle \rightarrow \langle \varphi, \mu \rangle$ in distribution

Proof. We consider the function

$$F(\lambda) = \exp(it \langle \varphi, \lambda \rangle)$$

on
$$\mathcal{M}$$
, where *i* is the imaginary unit number, and $t \in \mathbb{R}$.
It follows from Theorem 3.1 that

$$D(F) \subset \{\lambda \colon \lambda(D(\varphi)) > 0\}$$

Actually, if $\lambda(D(\varphi)) = 0$ and $\lambda_n \to \lambda$, then

 $\langle \varphi, \lambda_n \rangle \rightarrow \langle \varphi, \lambda \rangle$ and $F(\lambda_n) \rightarrow F(\lambda)$

Consequently,

$$P(D(F)) \leq P(\{\lambda: \lambda(D(\varphi)) > 0\}) = \operatorname{Prob}(\mu(D(\varphi)) > 0) = 0$$

because of (3.3). Applying again Theorem 3.1, we obtain

$$\langle F, P_n \rangle \rightarrow \langle F, P \rangle$$

Thus, the characteristic functions of the random variables $\langle \varphi, \mu_n \rangle$ converge to the characteristic function of $\langle \varphi, \mu \rangle$, and the assertion of the theorem follows.

Now we find a sufficient condition for the convergence in probability of random measures.

Lemma 3.3. Suppose $\langle \varphi, \mu_n \rangle \rightarrow \langle \varphi, \mu \rangle$ in distribution, $\forall \varphi \in C_b$. Then

$$\sup_{n} E\mu_n(|z| > R) \xrightarrow[R \to \infty]{} 0$$

Proof. Since the random variables $\langle \varphi, \mu_n \rangle$ are bounded, it follows that the measures m_n defined as

 $m_n(A) = E\mu_n(A)$ for any measurable set $A \subset Z$

converge weakly to the measure $m = E\mu$. Consequently, the sequence (m_n) is relatively compact, and the assertion is a consequence of the Prokhorov theorem.⁽⁴⁾

Theorem 3.4. Suppose $\langle \varphi, \mu_n \rangle \rightarrow \langle \varphi, \mu \rangle$ in probability, $\forall \varphi \in C_b$. Then

 $\mu_n \rightarrow \mu$ in probability

Proof. Consider the function

$$\chi_{R}(z) = \begin{cases} 1, & |z| \leq R \\ 1+R-|z|, & |z| \in (R, R+1) \\ 0, & |z| \geq R+1 \end{cases}$$
(3.4)

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where R > 0, and a function $\varphi \in C_L$ such that $\|\varphi\| \leq 1$. Then,

$$|\langle \varphi, \mu_n - \mu \rangle| \leq |\langle \varphi \chi_R, \mu_n - \mu \rangle| + \mu_n(|z| > R) + \mu(|z| > R)$$

and

$$\rho_L(\mu_n, \mu) \leq \sup_{\varphi \in D_R} |\langle \varphi, \mu_n - \mu \rangle| + \mu_n(|z| > R) + \mu(|z| > R)$$
(3.5)

where $D_R = \{ \varphi \chi_R : \varphi \in C_L, \|\varphi\| \leq 1 \}.$

Since D_R is compact, there exists a finite ε -set $\{\varphi_i \in C_b\}$ for any $\varepsilon > 0$. Consequently, for $\varphi \in D_R$, we obtain

$$|\langle \varphi, \mu_n - \mu \rangle| \leq \inf_i |\langle \varphi - \varphi_i, \mu_n - \mu \rangle| + \sum_i |\langle \varphi_i, \mu_n - \mu \rangle|$$

and

$$\sup_{\varphi \in D_R} |\langle \varphi, \mu_n - \mu \rangle| \leq 2\varepsilon + \sum_i |\langle \varphi_i, \mu_n - \mu \rangle|$$
(3.6)

From (3.5) and (3.6), it follows that

$$E\rho_L(\mu_n,\mu) \leq 2\varepsilon + \sum_i E |\langle \varphi_i, \mu_n - \mu \rangle| + E\mu_n(|z| > R) + E\mu(|z| > R)$$

and

$$\limsup_{n \to \infty} E\rho_L(\mu_n, \mu) \leq 2\varepsilon + \sup_n E\mu_n(|z| > R) + E\mu(|z| > R)$$

for arbitrary $\varepsilon > 0$. Consequently, the assertion follows from Lemma 3.3.

Theorems 3.2 and 3.4 imply the following result.

Corollary 3.5. Let μ be deterministic. Then, the following conditions are equivalent:

- (i) $\mu_n \rightarrow \mu$ in probability.
- (ii) $\mu_n \rightarrow \mu$ in distribution.
- (iii) $\langle \varphi, \mu_n \rangle \rightarrow \langle \varphi, \mu \rangle$ in probability for any measurable bounded function φ such that $\mu(D(\varphi)) = 0$.
- (iv) $\langle \varphi, \mu_n \rangle \rightarrow \langle \varphi, \mu \rangle$ in distribution, $\forall \varphi \in C_b$.

The next theorem deals with the convergence of restrictions of random measures. Consider a subset $Z_1 \subset Z$. Let λ_1 denote the restriction of a measure $\lambda \in \mathcal{M}$ to Z_1 .

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Theorem 3.6. Let μ be deterministic and such that

$$\mu(\partial Z_1) = 0 \tag{3.7}$$

where ∂Z_1 is the boundary of the set Z_1 .

If $\mu_n \to \mu$ in probability, then $\mu_{n,1} \to \mu_1$ in probability.

Proof. Consider $\varphi_1 \in C_b(Z_1)$, and define a function $\varphi^{(1)}$ on Z, which equals φ_1 on Z_1 and zero on $Z \setminus Z_1$. Since $D(\varphi^{(1)}) \subset \partial Z_1$ and $\langle \varphi_1, \mu_{n,1} \rangle = \langle \varphi^{(1)}, \mu_n \rangle$, the assertion is an immediate consequence of Corollary 3.5 and (3.7).

The following theorem establishes the convergence of transformations of random measures (cf. Billingsley,⁽⁴⁾ Theorem 5.1, concerning the deterministic case). Consider a transformation T of the space Z into a space Z'.

Theorem 3.7. Let μ be deterministic and such that

$$\mu(D(T)) = 0 \tag{3.8}$$

If $\mu_n \to \mu$ in probability, then $\mu_n^* T^{-1} \to \mu^* T^{-1}$ in probability.

Proof. Consider a bounded continuous function ψ on Z', and define a function ψ_T on Z such that

$$\psi_T(z) = \psi(T(z)), z \in \mathbb{Z}$$

Since $D(\psi_T) \subset D(T)$ and $\langle \psi, \mu_n^* T^{-1} \rangle = \langle \psi_T, \mu_n \rangle$, the assertion follows immediately from Corollary 3.5 and (3.8).

We finish this section with some technical lemmas.

Lemma 3.8. Let T be a transformation of the space Z into itself such that

$$|T(z)| \leq C |z|$$

for any $z \in Z$ and some constant C.

Suppose

$$\sup_{n} E\langle |z|^{p}, \mu_{n} \rangle < \infty \qquad \text{for some} \quad p > 0$$

Then,

$$\sup_{n} E\langle |z|^{p}, \mu_{n}^{*}T^{-1}\rangle < \infty$$

Proof. Substitution of the variables in the integral ensures that

$$\langle |z|^p, \mu_n^* T^{-1} \rangle = \langle |T(z)|^p, \mu_n \rangle \leq C^p \langle |z|^p, \mu_n \rangle$$

and the assertion follows.

Lemma 3.9. Suppose $\mu_n \rightarrow \mu$ in probability, and

$$\sup_{n} E\langle |z|^{p}, \mu_{n} \rangle = C < \infty \qquad \text{for some } p > 0$$

Then,

$$E\langle |z|^p, \mu \rangle \leq C$$

Proof. Consider the function χ_R defined in (3.4). The function $|z|^p \chi_R(z)$ is bounded and Lipschitz-continuous; consequently,

$$E |\langle |z|^p \chi_R(z), \mu_n - \mu \rangle| \rightarrow 0$$

Furthermore,

$$E\langle |z|^p \chi_R(z), \mu_n \rangle \leq E\langle |z|^p, \mu_n \rangle \leq C$$

and, therefore,

$$E \langle |z|^p \chi_R(z), \mu \rangle \leq C$$
 for any $R > 0$

The assertion follows immediately.

Lemma 3.10. Consider random measures $\mu_n(t)$, $\mu(t)$, depending on a time index $t \in [t_a, \infty)$. Suppose that

$$E \sup_{t \in [t_a, t_b]} \rho_L(\mu_n(t), \mu(t)) \to 0, \qquad \forall t_b \ge t_a$$
(3.9)

and

$$E \sup_{s \in [t-\delta, t+\delta]} \rho_L(\mu(s), \mu(t)) \xrightarrow[\delta \to 0]{} 0, \quad \forall t > t_a$$
(3.10)

Consider a sequence of random transformations σ_n of the time interval $[t_a, \infty)$ such that

$$\sigma_n(t) \to t$$
 in probability, $\forall t \ge t_a$ (3.11)

Define random measures

$$v_n(t) = \mu_n(\sigma_n(t))$$

Then,

$$E\rho_L(v_n(t), \mu(t)) \to 0, \quad \forall t \ge t_a$$

Proof. Consider the set

$$A_{\varepsilon} = \{ \rho_L(v_n(t), \mu(t)) > \varepsilon \} \text{ for some } t \ge t_a \text{ and } \varepsilon > 0$$

Then, for any $\delta > 0$,

$$\operatorname{Prob}(A_{\varepsilon}) = \operatorname{Prob}(A_{\varepsilon} \cap \{ |\sigma_n(t) - t| > \delta \}) + \operatorname{Prob}(A_{\varepsilon} \cap \{ |\sigma_n(t) - t| \le \delta \})$$
$$\leq \operatorname{Prob}(|\sigma_n(t) - t| > \delta) + \operatorname{Prob}(\sup_{s \in [t - \delta, t + \delta]} \rho_L(\mu_n(s), \mu(t)) > \varepsilon)$$
$$= S_1 + S_2$$

The term S_1 tends to zero as $n \to \infty$ for any fixed δ , because of (3.11). The term S_2 remains to be estimated. Consider the set

$$B_{\varepsilon} = \{ \sup_{s \in [t-\delta, t+\delta]} \rho_L(\mu_n(s), \mu(s)) + \sup_{s \in [t-\delta, t+\delta]} \rho_L(\mu(s), \mu(t)) > \varepsilon \}$$

Then,

$$S_{2} \leq \operatorname{Prob}(B_{\varepsilon})$$

$$\leq \operatorname{Prob}(\sup_{s \in [t-\delta, t+\delta]} \rho_{L}(\mu(s), \mu(t)) > \varepsilon/2)$$

$$+ \operatorname{Prob}(\sup_{s \in [t-\delta, t+\delta]} \rho_{L}(\mu_{n}(s), \mu(s)) > \varepsilon/2)$$

The first term on the right-hand side of the above inequality can be made arbitrarily small by an appropriate choice of δ , because of (3.10). For a fixed δ , the second term tends to zero because of (3.9). Consequently, the assertion of the lemma follows.

4. THE CONVERGENCE RESULT

Let $v^{(n)}(t)$, $t \ge t_0$, denote the empirical measures associated with Bird's particle system (2.1), i.e.,

$$\langle \varphi, v^{(n)}(t) \rangle = n^{-1} \sum_{i=1}^{n} \varphi(x_i(t), v_i(t))$$
 (4.1)

for any measurable bounded function φ on the space $Z = G \otimes \mathbb{R}^3$.

In order to construct the measure-valued function P(t), $t \ge t_0$, that will turn out to be the limit (as the number of particles *n* tends to infinity) of the empirical measures (4.1), we introduce some notations.

Let $\lambda_k(t), t \ge t_k, k = 0, 1,...$, be measure-valued functions such that

$$\lambda_k(t_k) = \lambda_{k-1}(t_k)^* \Phi_{\Delta t}^{-1}, \qquad k = 1, 2, \dots$$
(4.2)

and

$$\lambda_0(t_0) = P_0^* \Phi_{\Delta t}^{-1} \qquad \text{for some} \quad P_0 \in \mathcal{M}$$
(4.3)

where the transformation Φ is defined in (2.2)–(2.5), and the asterisk denotes the operation defined in (3.2).

Let $\lambda_{k,l}(t)$, $l=1,...,l_c$, denote the restrictions of the measures $\lambda_k(t)$ to the spaces $Z_l = G_l \otimes \mathbb{R}^3$. Suppose that the functions $\lambda_{k,l}(t)$ satisfy the equations

$$\frac{d}{dt} \langle \varphi, \lambda_{k,l}(t) \rangle$$

$$= \int_{G_l} \int_{\mathbb{R}^3} \int_{G_l} \int_{\mathbb{R}^3} \left[\int_{\mathbb{S}^2} de \ g_l^{-1} q(v, w, e) \times \left[\varphi(x, v + e(e, w - v)) - \varphi(x, v) \right] \right] \lambda_{k,l}(t, dx, dv) \lambda_{k,l}(t, dy, dw)$$
(4.4)

where the function φ is an arbitrary element of the space $C_L(G_l \otimes \mathbb{R}^3)$.

Theorem 4.1 (Convergence of the Bird algorithm). Let the following assumptions be fulfilled.

A1. Suppose that there exist solutions $\lambda_k(t)$, $\lambda_{k,l}(t)$, $t \ge t_k$, $k = 0, 1, ..., l = 1, ..., l_c$, of the system of equations (4.2)–(4.4) such that

$$\sup_{\epsilon \ [t_k, \ T]} \int |z|^2 \lambda_k(t, dz) < \infty, \qquad \forall T > t_k$$
(4.5)

A2. Suppose that the functions λ_k , k = 0, 1,..., and the domains G_l , $l = 1,..., l_c$, are such that

$$\lambda_k(t_k)(G_l \otimes \mathbb{R}^3) > 0 \tag{4.6}$$

and

t

$$\lambda_k(t_k)(\partial G_l \otimes \mathbb{R}^3) = 0 \tag{4.7}$$

A3. Suppose that the collision kernel q satisfies the conditions

$$q(v, w, e) = q(w, v, e), \qquad \forall v, w \in \mathbb{R}^3, \quad e \in \mathbb{S}^2$$
(4.8)

$$\int_{\mathbb{S}^2} q(v, w, e) \, de \leq Q_{\max} < \infty, \qquad \forall v, w \in \mathbb{R}^3 \tag{4.9}$$

$$\int_{\mathbb{S}^2} |q(v, w, e) - q(v', w, e)| \ de \leq C \ |v - v'|, \qquad \forall v, v', w \in \mathbb{R}^3 \quad (4.10)$$

$$\int_{\mathbb{S}^2} q(v, w, e) \, de \ge Q_{\min} > 0, \qquad \forall v, w \in \mathbb{R}^3 \tag{4.11}$$

for some constants Q_{max} , C, and Q_{min} .

A4. Suppose that the initial value $v^{(n)}(t_0)$ of the Bird algorithm satisfies the conditions

$$E\rho_L(v^{(n)}(t_0), P_0) \to 0$$
 (4.12)

and

$$\sup_{n} E\langle |z|^2, v^{(n)}(t_0) \rangle < \infty$$
(4.13)

where the measure P_0 is the same as in (4.3).

Then,

$$E\rho_L(v^{(n)}(t), P(t)) \to 0$$
 (4.14)

and

$$\sup_{n} E\langle |z|^2, v^{(n)}(t) \rangle < \infty$$
(4.15)

for any $t \ge t_0$, where the measure-valued function P(t), $t \ge t_0$, is defined via the relations

$$P(t) = \lambda_k(t), \quad t \in (t_k, t_{k+1}], \quad k = 0, 1, \dots$$

and

$$P(t_0) = P_0$$

Theorem 4.1 is a consequence of the following convergence results concerning the two parts of the Bird algorithm.

Theorem 4.2 (Convergence of the free flow simulation). Let $v_k^{(n)}$ denote the empirical measure associated with the particle system (2.6).

Let the assumption A1 of Theorem 4.1 be fulfilled.

Suppose that the functions λ_k , k = 0, 1,..., are such that

$$\lambda_k(t_k)(\partial G \otimes \mathbb{R}^3) = 0 \tag{4.16}$$

Suppose that

$$E\rho_L(\mathbf{v}^{(n)}(t_k), P(t_k)) \to 0 \tag{4.17}$$

and

$$\sup_{n} E\langle |z|^2, v^{(n)}(t_k) \rangle < \infty$$
(4.18)

for some $k = 0, 1, \dots$

Then,

$$E\rho_L(\nu_k^{(n)}, \lambda_k(t_k)) \to 0 \tag{4.19}$$

and

$$\sup_{n} E\langle |z|^2, v_k^{(n)} \rangle < \infty \tag{4.20}$$

Theorem 4.3. (Convergence of the collision simulation). Let $\mu^{(n)}(t), t \ge t_k$, denote the empirical measures associated with Bird's collision process z(t) defined in (2.7)–(2.15). Let $\mu_l^{(n)}(t)$ denote the restriction of the measure $\mu^{(n)}(t)$ to the space $G_l \otimes \mathbb{R}^3$.

Let the assumptions A1–A3 of Theorem 4.1 be fulfilled. Suppose that

$$E\rho_L(\mu_l^{(n)}(t_k), \lambda_{k,l}(t_k)) \to 0 \tag{4.21}$$

and

$$\sup_{n} E\langle |z|^2, \, \mu_l^{(n)}(t_k) \rangle < \infty \tag{4.22}$$

for some k = 0, 1, ...

Then

 $E\rho_L(\mu_l^{(n)}(t), \lambda_{k,l}(t)) \rightarrow 0$

and

$$\sup_{n} E\langle |z|^2, \, \mu_l^{(n)}(t) \rangle < \infty, \qquad \forall t \ge t_k$$

Proof of Theorem 4.1. It follows from (4.12), (4.13), and the definition of the function P that the assertions (4.14) and (4.15) are fulfilled for $t = t_0$.

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Let (4.14) and (4.15) hold for $t = t_k$ and some $k = 0, 1, \dots$. We show that then (4.14) and (4.15) are fulfilled for any $t \in (t_k, t_{k+1}]$.

It follows from (2.16) that

$$v_l^{(n)}(t) = \mu_l^{(n)}(t), \quad \forall t \in (t_k, t_{k+1}], \quad l = 1, ..., l_c$$
 (4.23)

Furthermore, (2.7) implies that

$$\mu^{(n)}(t_k) = \nu_k^{(n)} \tag{4.24}$$

Assumption (4.16) follows from (4.7), and Theorem 4.2 together with (4.24) ensure that

$$E\rho_L(\mu^{(n)}(t_k), \lambda_k(t_k)) \to 0 \tag{4.25}$$

and

$$\sup_{n} E\langle |z|^2, \, \mu^{(n)}(t_k) \rangle < \infty \tag{4.26}$$

Assumption (4.21) follows from (4.25), (4.7), and Theorem 3.6. Assumption (4.22) follows immediately from (4.26). Thus, by virtue of Theorem 4.3 and (4.23), we obtain

$$E\rho_L(v_l^{(n)}(t), \lambda_{k,l}(t)) \to 0 \tag{4.27}$$

and

$$\sup_{n} E\langle |z|^2, v_i^{(n)}(t) \rangle < \infty$$
(4.28)

for any $t \in (t_k, t_{k+1}]$ and $l = 1, ..., l_c$.

It can be shown easily that

$$\rho_L(\boldsymbol{v}^{(n)}(t), \lambda_k(t)) \leq \sum_{l=1}^{l_c} \rho_L(\boldsymbol{v}_l^{(n)}(t), \lambda_{k,l}(t))$$

Thus, assertion (4.14) follows from (4.27) and the definition of *P*. Furthermore, assertion (4.15) follows immediately from (4.28).

Proof of Theorem 4.2. It follows from (2.6) and (3.2) that

$$v_k^{(n)} = v^{(n)}(t_k)^* \Phi_{\Delta t}^{-1}$$

Furthermore,

$$\lambda_k(t_k) = P(t_k)^* \Phi_{At}^{-1}$$

according to (4.2) and the definition of *P*. The transformation $\Phi_{\Delta t}$ defined in (2.2)–(2.5) is discontinuous in (x, v) iff $\Phi_{\Delta t}(x, v) \in \partial G \otimes \mathbb{R}^3$. Hence, (4.19) follows from (4.17) and Theorem 3.7, if

$$P(t_k)(\Phi_{\mathcal{A}t}^{-1}(\partial G \otimes \mathbb{R}^3)) = 0$$

This is ensured by assumption (4.16).

The transformation Φ_{At} satisfies the inequality

$$|\Phi_{\Delta t}(x,v)| \le (1 + \Delta t)(|x| + |v|)$$
(4.29)

Consequently, (4.18) and (4.29) imply (4.20), according to Lemma 3.8.

In order to prove Theorem 4.3, we introduce a Markov jump process related to Bird's collision process, and establish convergence for this process. Then, we show that the Bird process converges to the same limit. For this purpose, we use a random time transformation that connects the Bird process and the Markov process.

We consider a continuous-time Markov jump process (cf., e.g., Feller,⁽¹²⁾ Chapter 10)

$$z^M(t), \qquad t \ge t_k$$

with the state space Z^n . Let the infinitesimal generator of the process be of the form

$$\mathscr{A}F(z^{(n)}) = n^{-1} \sum_{i < j} \int_{\mathbb{S}^2} de \left[F(z^{(n)} + \zeta^{(i, j)}(z^{(n)}, e)) - F(z^{(n)}) \right] \\ \times g_l^{-1} \P_{G_l}(x_i) \P_{G_l}(x_j) q(v_i, v_j, e)$$
(4.30)

where $z^{(n)} \in \mathbb{Z}^n$, with the components $z_i^{(n)} = (x_i, v_i)$, i = 1, ..., n, F is an arbitrary bounded measurable function on \mathbb{Z}^n , and $\zeta^{(i,j)}(z^{(n)}, e) \in \mathbb{Z}^n$, with the components

$$[\zeta^{(i, j)}(z^{(n)}, e)]_m = \begin{cases} (0, 0), & m \neq i, j \\ (0, e(e, v_j - v_i)), & m = i \\ (0, e(e, v_i - v_j)), & m = j \end{cases}$$

m = 1, ..., n. The initial value of the process is

$$z^M(t_k) = z(t_k) \tag{4.31}$$

where $z(t_k)$ is defined in (2.7).

Theorem 4.4. Let $\mu^{M}(t)$, $t \ge t_k$, denote the empirical measures associated with the process $z^{M}(t)$. Let $\mu_l^{M}(t)$ denote the restriction of the measure $\mu^{M}(t)$ to the space $G_l \otimes \mathbb{R}^3$.

Let the assumptions A1 and A2 of Theorem 4.1 be fulfilled. Suppose that the collision kernel q satisfies (4.8)–(4.10). Suppose that

$$E\rho_L(\mu_l^M(t_k), \lambda_{k,l}(t_k)) \to 0 \tag{4.32}$$

and

$$\sup_{n} E\langle |z|^2, \, \mu_I^M(t_k) \rangle < \infty \tag{4.33}$$

for some k = 0, 1, ...

Then,

$$E \sup_{t \in [t_k, T]} \rho_L(\mu_l^M(t), \lambda_{k,l}(t)) \to 0, \qquad \forall T \ge t_k$$

The process $z^{\mathcal{M}}(t)$ is closely related to Bird's collision process defined in (2.7)–(2.15). Their initial values as well as their behavior in the case $n_l < 2$ are identical. In the case $n_l \ge 2$, the process $z^{\mathcal{M}}(t)$ can be described on the basis of the Markov chain $\kappa(m)$ defined in (2.9)–(2.12).

Let $\tau^{M}(m)$, m = 0, 1, ..., be a sequence of random moments

$$\tau^{M}(0) = t_{k}$$

$$\tau^{M}(m) = \tau^{M}(m-1) + \Delta \tau^{M}(m), \qquad m = 1, 2,...$$
(4.34)

where the random variables $\Delta \tau^{M}(m)$, m = 1, 2,..., are independent and exponentially distributed with the parameters

$$n^{-1} \sum_{i < j} \P_{G_i}(x_i) \P_{G_i}(x_j) g_i^{-1} Q(v_i, v_j)$$
(4.35)

which depend on the state $\kappa(m-1) = ((x_i, v_i), i = 1,..., n)$ of the Markov chain. Then, the process $z^M(t)$ can be represented in the form

$$z^{M}(t) = z^{M}(\tau^{M}(m)), \qquad t \in [\tau^{M}(m), \tau^{M}(m+1))$$

$$z^{M}(\tau^{M}(m)) = \kappa(m), \qquad m = 0, 1, ...$$
(4.36)

Consequently, one can introduce a random transformation σ of the time interval $[t_k, \infty)$ such that

$$z(t) = z^{M}(\sigma(t)), \qquad t \ge t_{k} \tag{4.37}$$

In the case $n_1 < 2$, we define

$$\sigma(t) = t, \qquad t \ge t_k$$

In the case $n_l \ge 2$, relation (4.37) is fulfilled if

$$\sigma(t) \in [\tau^M(m), \tau^M(m+1)) \tag{4.38}$$

for $t \in [\tau(m), \tau(m+1))$, $m = 0, 1, \dots$ This follows from (2.15) and (4.36). Let σ be the continuous and piecewise linear function satisfying (4.38) and

$$\sigma(t_k) = t_k \tag{4.39}$$

Theorem 4.5. Let the assumptions A1 and A2 of Theorem 4.1 be fulfilled. Suppose that the collision kernel q satisfies (4.8), (4.9), and (4.11). Suppose that μ^M satisfies (4.32).

Then,

$$\sigma(t) \to t$$
 in probability, $\forall t \ge t_k$

Now we are in the position to prove Theorem 4.3.

Proof of Theorem 4.3. Since

$$\mu(t_k) = \mu^M(t_k)$$

according to (4.31), the assumptions (4.21) and (4.22) imply (4.32) and (4.33), and the conclusions of Theorems 4.4 and 4.5 are valid.

It follows from (4.37) that

$$\mu(t) = \mu^{M}(\sigma(t)), \qquad \forall t \ge t_{k}$$

Theorems 4.4 and 4.5 ensure (3.9) and (3.11), respectively. In order to apply Lemma 3.10, we check the property (3.10) of the function $\lambda_{k,l}(t)$. Notice that Eq. (4.4) is equivalent to the equation

$$\langle \varphi, \lambda_{k,l}(t) \rangle = \langle \varphi, \lambda_{k,l}(t_k) \rangle$$

+ $\int_{t_k}^t \int_{G_l} \int_{\mathbb{R}^3} \int_{G_l} \int_{\mathbb{R}^3} B(\varphi)(z_1, z_2)$
 $\times \lambda_{k,l}(s, dz_1) \lambda_{k,l}(s, dz_2) ds$ (4.40)

The function $B(\varphi)$ is defined as

$$B(\varphi)(z_1, z_2) = \int_{\mathbb{S}^2} de \ g_l^{-1} q(v_1, v_2, e)(1/2) \\ \times \left[\varphi(x_1, v_1^*) - \varphi(x_1, v_1) + \varphi(x_2, v_2^*) - \varphi(x_2, v_2) \right]$$
(4.41)

where we use the notation (1.3), and $z_i = (x_i, v_i)$, i = 1, 2.

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The function $B(\varphi)$ defined in (4.41) is symmetric in their arguments. As a function of each of the arguments, it belongs to $C_L(Z_l)$ if φ does. Using the assumption (4.9), one easily checks that

$$\|B(\varphi)(\cdot, z_2)\| \leq 2g_l^{-1}Q_{\max} \|\varphi\|, \qquad \forall z_2 \in Z_l$$

$$(4.42)$$

and the property (3.10) follows. Hence, Lemma 3.10 implies the first assertion of Theorem 4.3.

The second assertion of Theorem 4.3 follows from the equation

$$\langle |z|^2, \mu_l(t) \rangle = \langle |z|^2, \mu_l(t_k) \rangle, \quad \forall t \ge t_k$$
(4.43)

and the assumption (4.22). The property (4.43) is a consequence of the energy conservation during the collision simulation.

Thus, the proof is completed.

It remains to prove Theorems 4.4 and 4.5.

To prepare the proof of Theorem 4.4, we consider a function F of the form

$$F(z^{(n)}) = n^{-1} \sum_{i=1}^{n} \varphi(z_i), \qquad z^{(n)} \in \mathbb{Z}^n$$
(4.44)

where φ is an arbitrary bounded measurable function on Z. Notice that

$$F(z^{M}(t)) = \langle \varphi, \mu^{M}(t) \rangle$$
(4.45)

It follows from general properties of Markov processes (cf. Skorokhod,⁽²²⁾ p. 3, or Davis,⁽⁹⁾ p. 26) that the process

$$M(\varphi, t) = F(z^{M}(t)) - F(z^{M}(t_{k})) - \int_{t_{k}}^{t} \mathscr{A}(F)(z^{M}(s)) \, ds \qquad (4.46)$$

is a martingale, and

$$EM(\varphi, t)^2 = E \int_{t_k}^t \left[\mathscr{A}(F^2) - 2F\mathscr{A}(F) \right] (z^M(s)) \, ds \tag{4.47}$$

It follows directly from (4.30) that

$$\mathscr{A}F(z^{(n)}) = n^{-2} \sum_{i < j} \int_{\mathbb{S}^2} de \left[\varphi(x_i, v_i^*) - \varphi(x_i, v_i) + \varphi(x_j, v_j^*) - \varphi(x_j, v_j) \right] \\ \times g_l^{-1} \P_{G_l}(x_i) \, \P_{G_l}(x_j) \, q(v_i, v_j, e)$$
(4.48)

From (4.44), (4.46), and (4.48), we obtain the estimate

$$|M(\varphi, t)| \le 2 \|\varphi\|_{\infty} \left[1 + g_l^{-1} Q_{\max}(t - t_k)\right]$$
(4.49)

Elementary but lengthy calculations show that

$$[\mathscr{A}(F^{2}) - 2F\mathscr{A}(F)](z^{(n)})$$

= $n^{-3} \sum_{i < j} \int_{\mathbb{S}^{2}} de [\varphi(x_{i}, v_{i}^{*}) - \varphi(x_{i}, v_{i}) + \varphi(x_{j}, v_{j}^{*}) - \varphi(x_{j}, v_{j})]^{2}$
 $\times g_{l}^{-1} \P_{G_{l}}(x_{i}) \P_{G_{l}}(x_{j}) q(v_{i}, v_{j}, e)$ (4.50)

From (4.47) and (4.50), we obtain the estimate

$$E[M(\varphi, t)]^{2} \leq 8 \|\varphi\|_{\infty}^{2} g_{l}^{-1} Q_{\max}(t - t_{k}) n^{-1}$$
(4.51)

It follows from (4.45), (4.46), and (4.48), that

$$\langle \varphi, \mu^{M}(t) \rangle = \langle \varphi, \mu^{M}(t_{k}) \rangle$$
$$+ \int_{t_{k}}^{t} \int_{G_{l}} \int_{\mathbb{R}^{3}} \int_{G_{l}} \int_{\mathbb{R}^{3}} B(\varphi)(z_{1}, z_{2})$$
$$\times \mu^{M}(s, dz_{1}) \mu^{M}(s, dz_{2}) ds + M(\varphi, t)$$
(4.52)

for any bounded measurable function φ on Z, where we used the notation (4.41).

Now we are ready to prove Theorem 4.4. The main ideas of the proof are due to Smirnov,⁽²³⁾ where a numerical procedure based on stochastic differential equations with respect to Poisson measures was shown to converge to the solution of the spatially homogeneous Boltzmann equation.

Proof of Theorem 4.4. In the following calculations we will write $\mu(t)$ and $\lambda(t)$ instead of $\mu_i^M(t)$ and $\lambda_{k,l}(t)$, respectively. We also use simply the sign sup for the supremum over all $t \in [t_k, T]$. We consider a function $\varphi \in C_L(Z_l)$ and denote $\varphi_R = \varphi \chi_R$, where R is a positive real number and the function χ_R is defined in (3.4). Furthermore, the functions on Z_l are continued by zero to functions on Z, when Eq. (4.52) is used. Using (4.52) and (4.40), we obtain the following inequality:

$$\begin{split} |\langle \varphi, \mu(t) - \lambda(t) \rangle| \\ &\leq |\langle \varphi_R, \mu(t) - \lambda(t) \rangle| + |\langle \varphi - \varphi_R, \mu(t) - \lambda(t) \rangle| \\ &\leq \|\varphi\| \left(\mu(t)(|z| \ge R) + \lambda(t)(|z| \ge R) \right) + \left| \langle \varphi_R, \mu(t_k) \rangle + M(\varphi_R, t) \right. \\ &+ \int_{t_k}^t \int_{G_l} \int_{\mathbb{R}^3} \int_{G_l} \int_{\mathbb{R}^3} B(\varphi_R)(z_1, z_2) \, \mu(s, dz_1) \, \mu(s, dz_2) \, ds \\ &- \langle \varphi_R, \lambda(t_k) \rangle \\ &- \int_{t_k}^t \int_{G_l} \int_{\mathbb{R}^3} \int_{G_l} \int_{\mathbb{R}^3} B(\varphi_R)(z_1, z_2) \, \lambda(s, dz_1) \, \lambda(s, dz_2) \, ds \Big| \end{split}$$

$$\leq \|\varphi\| (\sup \mu(t)(|z| \geq R) + \sup \lambda(t)(|z| \geq R)) + \sup |M(\varphi_R, t)|$$

+ $|\langle \varphi_R, \mu(t_k) - \lambda(t_k) \rangle| + \left| \int_{t_k}^t \int_{G_l} \int_{\mathbb{R}^3} \int_{G_l} \int_{\mathbb{R}^3} B(\varphi_R)(z_1, z_2) \right|$
 $\times [\mu(s, dz_1) \mu(s, dz_2) - \lambda(s, dz_1) \lambda(s, dz_2)] ds$ (4.53)

Notice that $\|\varphi_R\| \leq 2 \|\varphi\|$. Thus, we obtain, from (4.53) and (4.42), that

$$\rho_L(\mu(t), \lambda(t)) \leq \sup \mu(t)(|z| \geq R) + \sup \lambda(t)(|z| \geq R) + S_1$$
$$+ 2\rho_L(\mu(t_k), \lambda(t_k)) + 4g_l^{-1}Q_{\max} \int_{t_k}^t \rho_L(\mu(s), \lambda(s)) \, ds$$

where

$$S_1 = \sup_{\|\varphi\| \le 1} \sup_{t} |M(\varphi_R, t)|$$
(4.54)

Now the Gronwall lemma allows to conclude that

$$\sup \rho_{L}(\mu(t), \lambda(t))$$

$$\leq \exp[4g_{l}^{-1}Q_{\max}(T-t_{k})]$$

$$\times \{\sup \mu(t)(|z| \ge R) + \sup \lambda(t)(|z| \ge R) + S_{1}$$

$$+ 2\rho_{L}(\mu(t_{k}), \lambda(t_{k}))\}$$
(4.55)

First we estimate the expectation of the term S_1 defined in (4.54).

The set $D_R = \{\varphi_R : \varphi \in C_L(Z_l), \|\varphi\| \le 1\}$ is compact in the space of continuous functions on $\{z \in Z_l : |z| \le R+1\}$. Consequently, for any $\varepsilon > 0$, there exists a finite set of functions $\{\varphi_i \in C_b\}$ such that

$$\min_{i} \|\varphi - \varphi_{i}\|_{\infty} \leq \varepsilon, \qquad \forall \varphi \in D_{R}$$

Thus, we obtain the estimate

$$|M(\varphi_R, t)| \leq \min_i |M(\varphi_R - \varphi_i, t)| + \max_i |M(\varphi_i, t)|$$
$$\leq \sup_{\|\psi\|_{\infty} \leq \varepsilon} |M(\psi, t)| + \sum_i |M(\varphi_i, t)|$$

Consequently, it follows that

$$ES_1 \leq E \sup_{t} \sup_{\|\psi\|_{\infty} \leq \varepsilon} |M(\psi, t)| + \sum_{i} E \sup_{t} |M(\varphi_i, t)|$$
(4.56)

Applying (4.49) to the first term, and the martingale inequality and (4.51) to the second term on the right-hand side of (4.56), we obtain

$$ES_1 \leq \varepsilon \cdot \text{const} + C(\varepsilon) n^{-1/2}$$

and

$$\limsup_{n \to \infty} ES_1 \leq \varepsilon \cdot \text{const}, \qquad \forall \varepsilon > 0$$

Hence,

$$\lim ES_1 = 0, \quad \forall R > 0 \tag{4.57}$$

We conclude from Chebychev's inequality and the energy conservation law governing the transformation (1.3) that

$$\mu(t)(|z| \ge R) \le R^{-2} \langle |z|^2, \, \mu(t) \rangle = R^{-2} \langle |z|^2, \, \mu(t_k) \rangle$$

Consequently, we obtain

$$\limsup_{n \to \infty} E \sup_{t} \mu(t)(|z| \ge R) \le R^{-2} \sup_{n} E\langle |z|^2, \mu(t_k) \rangle$$
(4.58)

Thus, using (4.32), (4.57), and (4.58), we conclude from (4.55) that

$$\limsup_{n \to \infty} E \sup_{t} \rho_L(\mu(t), \lambda(t))$$

$$\leq \operatorname{const} \{ R^{-2} \sup_{n} E \langle |z|^2, \mu(t_k) \rangle + \sup_{t} \lambda(t)(|z| \ge R) \}, \quad \forall R > 0$$

The right-hand side of the last inequality tends to zero as $R \to \infty$ because of the assumptions (4.33) and (4.5). Thus, the proof is completed.

To prepare the proof of Theorem 4.5, we introduce two auxiliary random time transformations.

Let σ^M be the inverse transformation of σ . Thus, σ^M is piecewise linear. Moreover,

$$\sigma^M(t) = t, \qquad t \ge t_k \tag{4.59}$$

in the case $n_l < 2$, and

$$\sigma^{M}(\tau^{M}(m)) = \tau(m), \qquad m = 0, 1, \dots$$
(4.60)

in the case $n_l \ge 2$, according to (4.38), (4.39).

Furthermore, let σ_0^M be the function defined as

$$\sigma_0^M(t) = t, \qquad t \ge t_k \tag{4.61}$$

in the case $n_l < 2$, and

$$\sigma_0^M(t) = \tau(m) \tag{4.62}$$

for $t \in [\tau^{M}(m), \tau^{M}(m+1)), m = 0, 1, ..., in the case <math>n_{l} \ge 2$.

Now we prove two assertions concerning the random time transformations σ_0^M and σ^M .

Lemma 4.6. Suppose the assumptions of Theorem 4.5 to be fulfilled. Then,

$$\sup_{t \in [t_k, T]} |\sigma_0^M(t) - t| \to 0 \quad \text{in probability,} \qquad \forall T \ge t_k$$

Proof. We consider the Markov process

$$(z^{M}(t), u^{M}(t)), \qquad t \ge t_{k} \tag{4.63}$$

with the state space $Z^n \otimes \mathbb{R}$. Let the infinitesimal generator of the extended process (4.63) have the following form, which is a slight modification of (4.30):

$$\mathscr{A}F(z^{(n)}, u) = n^{-1} \sum_{i < j} \int_{\mathbb{S}^2} de [F(z^{(n)} + \zeta^{(i, j)}(z^{(n)}, e), u + n^{-1}Q(v_i, v_j)^{-1}) - F(z^{(n)}, u)] g_l^{-1} \P_{G_l}(x_i) \P_{G_l}(x_j) q(v_i, v_j, e)$$
(4.64)

where F is an arbitrary bounded measurable function on $Z^n \otimes \mathbb{R}$. The initial value of the additional component is

$$u^{M}(t_{k}) = 0 \tag{4.65}$$

Thus, the component $u^{M}(t)$ jumps at the random moments $\tau^{M}(m)$, m = 1, 2,..., defined in (4.34). Because of the assumption (4.11), the maximum value of the jumps is $n^{-1}Q_{\min}^{-1}$. The mean number of jumps on a time interval $[t_k, T]$ increases when the parameter (4.35) of the waiting time distribution is replaced by the value $ng_l^{-1}Q_{\max}$, which does not depend on the current state. The number of jumps related to this waiting times has a Poisson distribution with the parameter $ng_l^{-1}Q_{\max}(T-t_k)$. Consequently, the expectation of the component $u^{M}(T)$ can be estimated uniformly in n,

$$Eu^{M}(T) \leq Q_{\min}^{-1} g_{l}^{-1} Q_{\max}(T - t_{k})$$
(4.66)

According to (4.62), (4.65), (2.13), and (2.14), the transformation $\sigma_0^M(t)$ is connected with the additional component $u^M(t)$ via the relation

$$\sigma_0^M(t) i_l = (t_k + \alpha_n u^M(t)) i_l$$

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where i_l denotes the indicator of the set $\{n_l \ge 2\}$, and

$$\alpha_n = \begin{cases} [n^{-2}(n_l - 1)(n_l/2) g_l^{-1}]^{-1}, & \text{if } n_l \ge 2\\ 0, & \text{if } n_l < 2 \end{cases}$$

We consider the function

$$\varphi_R(u) = u\chi_R(u), \qquad u \in \mathbb{R}$$

where R > 0, and χ_R is defined in (3.4). One easily shows that

$$\|\varphi_R\| \leq (R+1)$$

Let B_1 denote the interval $[0, R - n^{-1}Q_{\min}^{-1}]$ and $B_2 = [0, \infty) \setminus B_1$. Now we start the estimation of the term $(\sigma_0^M(t) - t)$, which equals $(\sigma_0^M(t) - t) i_i$ because of (4.61). We obtain

$$(\sigma_{0}^{M}(t) - t) = [\alpha_{n} \varphi_{R}(u^{M}(t)) - (t - t_{k})] i_{l} \P_{B_{1}}(u^{M}(T)) + [\alpha_{n} \varphi_{R}(u^{M}(t)) - (t - t_{k})] i_{l} \P_{B_{2}}(u^{M}(T)) + \alpha_{n} u^{M}(t) [1 - \chi_{R}(u^{M}(t))] i_{l}$$
(4.67)

Applying the appropriate modification of the formula (4.46) to the process (4.63), the infinitesimal generator (4.64), and the function

$$F(z^{(n)}, u) = \varphi_R(u)$$

we obtain

$$\varphi_R(u^M(t)) = \int_{t_k}^t \mathscr{A}(F)(z^M(s), u^M(s)) \, ds + M(t)$$

where the martingale M(t) has the second moment [cf. (4.47)]

$$EM(t)^{2} = E \int_{t_{k}}^{t} \left[\mathscr{A}(F^{2}) - 2F\mathscr{A}(F) \right] (z^{M}(s), u^{M}(s)) \, ds$$

If $u \in B_1$, then

$$\mathscr{A}F(z^{(n)}, u) = n^{-1} \sum_{i < j} \int_{\mathbb{S}^2} de [\varphi_R(u + n^{-1}Q(v_i, v_j)^{-1}) - \varphi_R(u)]$$

 $\times g_I^{-1} \P_{G_I}(x_i) \P_{G_I}(x_j) q(v_i, v_j, e)$
 $= n^{-2}(n_I - 1)(n_I/2) g_I^{-1}$

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Notice that the function $u^{M}(t)$ is increasing in t. Consequently, the first term on the right-hand side of (4.67) takes the form

$$\begin{aligned} & \left[\alpha_{n}\varphi_{R}(u^{M}(t))-(t-t_{k})\right]i_{l}\P_{B_{1}}(u^{M}(T)) \\ & = \left\{\alpha_{n}\left[\int_{t_{k}}^{t}n^{-2}(n_{l}-1)(n_{l}/2)g_{l}^{-1}ds+M(t)\right]-(t-t_{k})\right\}i_{l}\P_{B_{1}}(u^{M}(T)) \\ & = \alpha_{n}M(t)i_{l}\P_{B_{1}}(u^{M}(T)) \end{aligned}$$

Thus, we conclude from (4.67) that

$$\sup_{t} |\sigma_{0}^{M}(t) - t| \leq \alpha_{n} \sup_{t} |M(t)| + [\alpha_{n}(R+1) + (T-t_{k})] \P_{B_{2}}(u^{M}(T)) + \alpha_{n}u^{M}(T) \P_{(R,\infty)}(u^{M}(T))$$
(4.68)

One finds, in analogy with (4.50),

$$(\mathscr{A}F^{2} - 2F\mathscr{A}F)(z^{(n)}, u)$$

= $n^{-1} \sum_{i < j} \int_{\mathbb{S}^{2}} de [\varphi_{R}(u + n^{-1}Q(v_{i}, v_{j})^{-1}) - \varphi_{R}(u)]^{2}$
 $\times g_{l}^{-1} \P_{G_{l}}(x_{i}) \P_{G_{l}}(x_{j}) q(v_{i}, v_{j}, e) \leq (R+1)^{2} n^{-1}Q_{\min}^{-1}g_{l}^{-1}$

Consequently,

$$EM(T)^{2} \leq (R+1)^{2} n^{-1} Q_{\min}^{-1} g_{l}^{-1} (T-t_{k})$$

and it follows from the martingale inequality that

$$\sup_{t} |M(t)| \xrightarrow[n \to \infty]{} 0 \quad \text{in probability,} \quad \forall R > 0 \tag{4.69}$$

We conclude from the assumptions (4.32) and (4.7) and Corollary 3.5(iii) that

$$n_l/n = \mu_l^M(t_k)(G_l \otimes \mathbb{R}^3) \to \lambda_{k,l}(t_k)(G_l \otimes \mathbb{R}^3)$$
 in probability

Because of assumption (4.6), we obtain that

$$\alpha_n \to (2g_l) [\lambda_k(t_k)(G_l \otimes \mathbb{R}^3)]^{-2} > 0$$
(4.70)

in probability.

$$Prob\{\sup_{t} |\sigma_{0}^{M}(t) - t| > \varepsilon\}$$

$$\leq Prob\{\alpha_{n} \sup_{t} |M(t)| > \varepsilon/3\}$$

$$+ Prob\{[\alpha_{n}(R+1) + (T-t_{k})] \P_{B_{2}}(u^{M}(T)) > \varepsilon/3\}$$

$$+ Prob\{\alpha_{n}u^{M}(T) \P_{(R,\infty)}(u^{M}(T)) > \varepsilon/3\}$$

$$\leq Prob\{\alpha_{n} \sup_{t} |M(t)| > \varepsilon/3\} + Prob\{u^{M}(T) > R - n^{-1}Q_{\min}^{-1}\}$$

$$+ Prob\{u^{M}(T) > R\}$$

Using Chebychev's inequality, (4.66), (4.69), and (4.70), we obtain

$$\limsup_{n \to \infty} \operatorname{Prob} \{ \sup_{t} |\sigma_0^M(t) - t| > \varepsilon \} \leq 2R^{-1}Q_{\min}^{-1}Q_{\max} g_l^{-1}(T - t_k)$$

for any R > 0 and $\varepsilon > 0$. Consequently, the assertion of the lemma follows.

Lemma 4.7. Suppose the assumptions of Theorem 4.5 to be fulfilled. Then

$$\sup_{t \in [t_k, T]} |\sigma^M(t) - t| \to 0 \quad \text{in probability,} \qquad \forall T \ge t_k$$

Proof. If $n_l < 2$, then

$$\sup_{t \in [t_k, T]} |\sigma^M(t) - t| = 0$$

according to (4.59). We suppose in the following that $n_l \ge 2$.

Consider the set

$$A_{\varepsilon} = \{ \sup_{t \in [t_k, T]} |\sigma^M(t) - t| > \varepsilon \}, \qquad \varepsilon > 0$$

and let m_T be such that

$$T \in [\tau^M(m_T), \tau^M(m_T+1))$$

It follows from the piecewise linearity of σ^M that

$$\sup_{t \in [t_k, T]} |\sigma^M(t) - t| \leq \sup_{m \leq m_T + 1} |\sigma^M(\tau^M(m)) - \tau^M(m)|$$

Consequently, we obtain

$$\operatorname{Prob}(A_{\varepsilon}) \leq \operatorname{Prob}(\sup_{m \leq m_T} |\sigma^M(\tau^M(m)) - \tau^M(m)| > \varepsilon) + \operatorname{Prob}(B_{\varepsilon})$$

where

$$B_{\varepsilon} = \left\{ |\sigma^{M}(\tau^{M}(m_{T}+1)) - \tau^{M}(m_{T}+1)| > \varepsilon \right\}$$

Since

$$\sigma^M(\tau^M(m)) = \sigma^M_0(\tau^M(m))$$

according to (4.60), (4.62), it follows that

$$\operatorname{Prob}(A_{\varepsilon}) \leq \operatorname{Prob}(\sup_{t \in [t_k, T]} |\sigma_0^M(t) - t| > \varepsilon) + \operatorname{Prob}(B_{\varepsilon} \cap \{\tau^M(m_T + 1) \leq T + \delta\}) + \operatorname{Prob}(B_{\varepsilon} \cap \{\tau^M(m_T + 1) > T + \delta\})$$

for any $\delta > 0$.

The function σ_0^M is piecewise constant. Thus, if

$$\tau^M(m_T+1) > T+\delta$$

then

$$\sup_{t \in [T, T+\delta]} |\sigma_0^M(t) - t| \ge \delta/2$$

Consequently,

$$\operatorname{Prob}(A_{\varepsilon}) \leq 2 \operatorname{Prob}(\sup_{t \in [t_k, T+\delta]} |\sigma_0^M(t) - t| > \varepsilon) + \operatorname{Prob}(\sup_{t \in [t_k, T+\delta]} |\sigma_0^M(t) - t| \ge \delta/2)$$

The right-hand side of the last inequality tends to zero, for arbitrary ε and δ , because of Lemma 4.6. This completes the proof.

Theorem 4.5 is now an immediate consequence of Lemma 4.7.

Proof of Theorem 4.5. Since σ^M is increasing and $\sigma^M = \sigma^{-1}$, we obtain

$$\begin{aligned} \operatorname{Prob}(|\sigma(t) - t| > \varepsilon) &= \operatorname{Prob}(\sigma(t) < t - \varepsilon) + \operatorname{Prob}(\sigma(t) > t + \varepsilon) \\ &= \operatorname{Prob}(t < \sigma^{M}(t - \varepsilon)) + \operatorname{Prob}(t > \sigma^{M}(t + \varepsilon)) \end{aligned}$$

for any $\varepsilon > 0$ and $t \ge t_k$. The right-hand side of this inequality tends to zero according to Lemma 4.7.

5. COMMENTS AND OUTLOOK

The considerations of the present paper have been restricted to the limiting behavior of the Bird algorithm when the number of particles tends to infinity. In this final section, we will give some comments concerning the results, and mention some related problems that have not been considered.

First of all, some remarks about the relationship between the limit P(t) of the Bird algorithm and the solution of the Boltzmann equation are necessary. We sketch the derivation (at least on a heuristic level) of the system of equations (4.2)-(4.4) from the Boltzmann equation (1.1)-(1.4).

First, one introduces a mollifying kernel

$$h(x, y) = \sum_{l=1}^{l_c} g_l^{-1} \P_{G_l}(x) \P_{G_l}(y)$$
(5.1)

and replaces the right-hand side of Eq. (1.1) by

$$J_{\text{mol}}(f)(t, x, v) = \int_{G} dy \int_{\mathbb{R}^{3}} dw \int_{\mathbb{S}^{2}} de h(x, y) q(v, w, e)$$
$$\times [f(t, x, v^{*}) f(t, y, w^{*}) - f(t, x, v) f(t, y, w)]$$
(5.2)

Then, one introduces a time discretization

$$(t_k), \quad k = 0, 1, \dots$$

and performs the splitting of the free flow term and the collision term on each time interval

$$[t_k, t_{k+1}], \quad k=0, 1,...$$

After a transformation of the equations with respect to densities into equations with respect to measures, one arrives at the system of equations

$$\frac{d}{dt} \langle \varphi, \lambda_k(t) \rangle = \int_G \int_{\mathbb{R}^3} \int_G \int_{\mathbb{R}^3} \left\{ \int_{\mathbb{S}^2} de \ h(x, \ y) \ q(v, \ w, \ e) \right.$$

$$\times \left[\varphi(x, \ v^*) - \varphi(x, \ v) \right] \left\} \lambda_k(t, \ dx, \ dv) \ \lambda_k(t, \ dy, \ dw) \qquad (5.3)$$

$$t \in [t_k, \ t_{k+1}], \qquad k = 0, \ 1, \dots$$

$$\lambda_k(t_k) = \lambda_{k-1}(t_k)^* \ \Phi_{At}^{-1}, \qquad k = 1, \ 2, \dots \qquad (5.4)$$

$$\lambda_0(t_0) = P_0^* \Phi_{At}^{-1}$$

where the measure P_0 has the density f_0 appearing in (1.4), and h is defined in (5.1). Obviously, the measure-valued functions defined in (4.2)-(4.4) satisfy the system (5.3), (5.4).

The approximation error depends on the time discretization (t_k) and on the division of the space into cells (G_l) , which influences the mollified collision term (5.2). The behavior of the solutions of the system (5.3), (5.4) should be investigated when $\Delta t \rightarrow 0$ and $\Delta x \rightarrow 0$, where Δx denotes the maximum diameter of the cells G_l , $l = 1,..., l_c$. This problem can be tackled similarly to what is done in Babovsky and Illner,⁽³⁾ where the Nanbu algorithm is treated.

Second, we give some comments on the assumptions of Theorem 4.1.

The assumption concerning the existence of the limiting measures λ_k probably could be removed by using the strong properties of q and standard techniques.^(1,13) The essential assumptions concerning λ_k are (4.6) and (4.7), which seem to be rather reasonable. Indeed, the Bird algorithm will not work well if the measure to be approximated has a positive mass on the boundary of some cell. Also, undesirable effects may appear if some cell has the mass zero. Assumption (4.7) is fulfilled if the measures λ_k are absolutely continuous, and the transformation Φ preserves this property.

The assumptions (4.9)-(4.11) concerning the collision kernel q are not fulfilled for realistic q. However, in many cases of practical importance, these assumptions are satisfied for the function

$$q^{(r,R)}(v,w,e) = \begin{cases} R & \text{if } q(v,w,e) \ge R \\ r & \text{if } q(v,w,e) \le r \\ q(v,w,e) & \text{otherwise} \end{cases}$$

 $0 < r < R < \infty$. The behavior of the truncation error resulting from such an approximation should be analyzed when $R \to \infty$ and $r \to 0$ (cf. Arsen'ev⁽¹⁾ for the case $R \to \infty$).

The assumptions concerning the initial value $v^{(n)}(t_0)$ of the Bird algorithm imply that

$$\langle |z|^2, P_0 \rangle < \infty \tag{5.5}$$

according to Lemma 3.9. If one supposes (5.5), then the assumptions (4.12) and (4.13) are fulfilled for the initial measure $v^{(n)}(t_0)$ generated by independent samples of the probability measure P_0 . However, the initial measure $v^{(n)}(t_0)$ can also be deterministic.

It seems to be worth mentioning that no assumption concerning an "initial chaos" is needed. What we have shown is "propagation of the convergence of the empirical measures." The usual chaos property follows from the convergence of the empirical measures under an appropriate symmetry assumption concerning the distribution function of the particle system. This fact has already been mentioned in the literature.⁽²⁴⁾

In finishing this paper, we give an example illustrating further applications of the concept of embedding the discrete Bird algorithm into the framework of Markov processes.

Suppose that the collision kernel q satisfies the condition

$$q(v, w, e) \leq H(e), \qquad \forall v, w \in \mathbb{R}^3, \quad e \in \mathbb{S}^2$$
(5.6)

where $\int_{\mathbb{S}^2} H(e) de < \infty$. Under the assumption (5.6), the infinitesimal generator (4.30) can be transformed into the form

$$\mathscr{A}F(z^{(n)}) = n^{-1} \sum_{i < j} \int_{\mathbb{S}^2} de \int_0^1 d\eta [F(z^{(n)} + \psi^{(i,j)}(z^{(n)}, e, \eta)) - F(z^{(n)})] g_l^{-1} \P_{G_l}(x_i) \P_{G_l}(x_j) H(e)$$
(5.7)

with

$$\psi^{(i,j)}(z^{(n)}, e, \eta) = \begin{cases} \zeta^{(i,j)}(z^{(n)}, e) & \text{if } \eta < q(v_i, v_j, e) / H(e) \\ 0 & \text{otherwise} \end{cases}$$
(5.8)

The form (5.7), (5.8) of the generator suggests the following description of the Markov process, which is different from (4.34)–(4.36).

Given the state $((x_i, v_i), i = 1, ..., n)$, the process waits a random time which is exponentially distributed with the parameter

$$n^{-1} \sum_{i < j} \P_{G_{l}}(x_{i}) \P_{G_{l}}(x_{j}) g_{l}^{-1} \int_{\mathbb{S}^{2}} H(e) de$$

= $n^{-1}(n_{l}-1)(n_{l}/2) g_{l}^{-1} \int_{\mathbb{S}^{2}} H(e) de$ (5.9)

instead of (4.35). After that time, the process jumps in the following way.

First, the indices i and j of the particles due to take part in a collision are generated according to the probabilities

const
$$\cdot \P_{G_l}(x_i) \P_{G_l}(x_j)$$

[instead of (2.10)], i.e., uniformly in the cell G_l .

Then, an element $e \in \mathbb{S}^2$ is generated in correspondence with the probability density

const
$$\cdot H(e)$$

[instead of (2.12)], and a random number η is sampled from the uniform distribution on the interval [0, 1].

Finally, if

$$\eta < q(v_i, v_j, e)/H(e) \tag{5.10}$$

the new state is obtained from the old one by replacing v_i and v_j by v_i^* and v_j^* , respectively, which are calculated according to (1.3). If (5.10) is not fulfilled, then no change takes place in the system, and the collision is called fictitious.

The relationship between the time counter (2.13) and the parameters (4.35) suggests the modified time counter

$$\Delta \tau_f(m) = \left[n^{-1} (n_l - 1) (n_l/2) g_l^{-1} \int_{\mathbb{S}^2} H(e) de \right]^{-1}$$
(5.11)

which is analogously related to the parameters (5.9). We call the algorithm based on the time counter (5.11) the "modified Bird algorithm with fictitious collisions."

The modified time counter (5.11) counts the fictitious collisions, too. Moreover, it is deterministic, so that the number of (possibly fictitious) collisions in a cell can be calculated at the beginning of the collision simulation step. The convergence of the modified Bird algorithm can be proved in a completely analogous way, even without the assumption (4.11).

It should be mentioned that the modified Bird process in a cell is just the same as that obtained by Lukshin and Smirnov⁽¹⁹⁾ in the spatially homogeneous case for the algorithm based on stochastic differential equations, where the Poisson distribution for the number of jumps on a time interval has been replaced by its mathematical expectation. The complete algorithm using the modified Bird process in the cells is very similar to the so-called null-collision technique introduced by Koura.⁽¹⁷⁾

The concept based on Markov processes seems to be very useful for a unification and even a deeper understanding of various stochastic particle simulation procedures for the Boltzmann equation. It can also be employed for developing new algorithms.

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