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## A stochastic weighted particle method for the Boltzmann equation

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**Abstract.** A class of algorithms for the numerical treatment of the Boltzmann equation is introduced. The basic idea is a more general procedure of modelling collisions between particles. This procedure is based on a random weight transfer from the particles with the pre-collision velocities to the particles with the post-collision velocities.

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# 1. Introduction

This paper is concerned with the numerical solution of the **Boltzmann equation** for dilute monatomic gases ([7])

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

$$\int_{\mathcal{R}^3} dw \int_{S^2} de B(v, w, e) [f(t, x, v^*) f(t, x, w^*) - f(t, x, v) f(t, x, w)],$$

$$f(0, x, v) = f_0(x, v), \quad (1.2)$$

where  $t \geq 0$ ,  $x \in D \subset \mathcal{R}^3$ , and  $v \in \mathcal{R}^3$ . The symbol  $\nabla_x$  denotes the vector of the partial derivatives with respect to  $x$ ,  $D$  is a bounded domain in three-dimensional Euclidean space  $\mathcal{R}^3$ , and  $(\cdot, \cdot)$  is the scalar product. The function  $B$  is called the collision kernel. The symbols  $de$  and  $dw$  denote the uniform surface measure on the unit sphere  $S^2$  and the Lebesgue measure on  $\mathcal{R}^3$ , respectively. The objects  $v^*$  and  $w^*$  are defined as

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

where  $v, w \in \mathcal{R}^3$ ,  $e \in S^2$ . They are interpreted as the post-collision velocities of two particles with the pre-collision velocities  $v$  and  $w$ .

The basic idea of particle methods for the numerical solution of the Boltzmann equation (cf. [16], [8], [13], [17]) is to approximate the measures

$$\lambda(t, dx, dv) = f(t, x, v) dx dv, \quad (1.4)$$

where  $f$  is the solution of Eq. (1.1), by a system of point measures defined by a particle system. The classical particle method introduced by G. A. Bird in 1963 (called "direct simulation Monte Carlo" or DSMC method) was derived on the basis of physical intuition (cf. [3], [6]). In recent years some progress has been achieved in the mathematical foundation of particle methods for the Boltzmann equation. We refer to [1], [2], [19], and [20] concerning convergence results (as the number of particles in the system tends to infinity).

Basing on these results, an even more challenging problem arises – the mathematically rigorous study and the improvement of the efficiency of the simulation schemes in the sense of rates of convergence or even error estimates (see, e.g., the discussion in [5]). In the case of stochastic methods,

an improvement of the convergence behaviour is related to the problem of variance reduction, i.e. the reduction of the random fluctuations around the deterministic limit. We refer to [17] concerning the introduction of low discrepancy sequences instead of sequences of random numbers in some parts of the algorithm called finite pointset method. Weighted particles in connection with this method were considered in [18].

Another approach to the problem of variance reduction is to develop models with certain degrees of freedom, i.e. with such parameters that do not change the deterministic limit but can be chosen in order to reduce the fluctuations.

The purpose of this paper is to introduce a class of particle methods depending on certain parameters (degrees of freedom). For a special choice of these parameters, the standard DSMC method is obtained. Under rather general assumptions concerning the parameters, the deterministic limit (as the number of particles tends to infinity) is the same as for the standard DSMC method. The basic idea is a more general procedure of modelling collisions between particles. They are simulated by a random weight transfer, which is connected with an increase of the number of particles in the system. This idea originates from [11], where random discrete velocity models were introduced (cf. also [9], [12], [10], [21]).

The paper is organized as follows. A general description of the method is given in Section 2. The main part of the method, the modelling of collisions via a random weight transfer, is introduced in Section 3. Results of numerical experiments are presented in Section 4. Section 5 contains some conclusions and remarks.

## 2. General description of the method

In this section we introduce the general framework of particle simulation schemes and explain the main ideas of what we call a stochastic weighted particle method.

A time discretization

$$t_k = k \Delta t, \quad k = 0, 1, \dots, \quad \Delta t > 0, \quad (2.1)$$

is used to split the simulation of the free flow of the particles and the simulation of their collisions. This means that on a small time interval of length  $\Delta t$ ,

at a first step, the free flow is simulated disregarding the possible collisions. Then, at a second step, the collisions are simulated neglecting the free flow.

To describe this procedure rigorously, we introduce two families of particle systems

$$\left(x_i^{(1,k,n)}(t), v_i^{(1,k,n)}(t), g_i^{(1,k,n)}(t)\right), \quad i = 1, \dots, m^{(1,k,n)}(t), \quad (2.2)$$

and

$$\left(x_i^{(2,k,n)}(t), v_i^{(2,k,n)}(t), g_i^{(2,k,n)}(t)\right), \quad i = 1, \dots, m^{(2,k,n)}(t), \quad (2.3)$$

where  $t \in [t_k, t_{k+1}]$ . The indices 1 and 2 indicate the free flow simulation step and the collision simulation step, respectively. The index  $k$  indicates the number of the time interval. The index  $n$  is a parameter governing the approximation of the initial measure

$$\lambda_0(dx, dv) = f_0(x, v) dx dv, \quad (2.4)$$

which corresponds to the function  $f_0$  appearing in the initial condition (1.2) of the Boltzmann equation. Usually, the parameter  $n$  is the number of particles in the system at time zero.

**Remark.** *For simplicity, we will omit the lengthy list of superscripts appearing in (2.2)–(2.3) (or at least a part of it), whenever this (as we hope) does not lead to misunderstanding.*

The symbols  $x_i(t)$  and  $v_i(t)$  denote the position and the velocity of the  $i$ -th particle,  $g_i(t)$  is considered as a weight of the particle. Finally,  $m(t)$  is the number of particles in the system.

The time evolution of the system (2.2) (the **free flow simulation step**) is defined as follows. The initial state of the system is, if  $k = 0$ , an appropriate approximation of the initial measure  $\lambda_0$  given in (2.4), or, otherwise, the final state of the system (2.3) on the time interval  $[t_{k-1}, t_k]$ , i.e.

$$\begin{aligned} x_i^{(1,k,n)}(t_k) &= x_i^{(2,k-1,n)}(t_k), \\ v_i^{(1,k,n)}(t_k) &= v_i^{(2,k-1,n)}(t_k), \\ g_i^{(1,k,n)}(t_k) &= g_i^{(2,k-1,n)}(t_k). \end{aligned}$$

Then, the particles move according to their velocities, i.e.

$$x_i^{(1,k,n)}(t) = x_i^{(1,k,n)}(t_k) + (t - t_k) v_i^{(1,k,n)}(t_k).$$

The velocities do not change unless a particle hits the boundary. In this case, the corresponding velocity changes according to the boundary condition. The weights of the particles remain the same during the free flow simulation.

The time evolution of the system (2.3) (the **collision simulation step**) is defined as follows. The initial state of the system is the final state of the system (2.2) on the time interval  $[t_k, t_{k+1}]$ , i.e.

$$\begin{aligned}x_i^{(2,k,n)}(t_k) &= x_i^{(1,k,n)}(t_{k+1}), \\v_i^{(2,k,n)}(t_k) &= v_i^{(1,k,n)}(t_{k+1}), \\g_i^{(2,k,n)}(t_k) &= g_i^{(1,k,n)}(t_{k+1}).\end{aligned}$$

The positions of the particles remain the same during the collision simulation. A partition

$$D = \cup_{l=1}^{l_c} D_l \quad (2.5)$$

of the spatial domain  $D$  into a finite number  $l_c$  of disjoint cells is used. There is no interaction between different cells. In each cell, collisions of the particles are simulated. Here various approaches differ. A detailed description of the approach based on random weight transfer will be given in Section 3. Here we mention only the main idea, on which the elementary interaction (collision between two particles) is based.

Two indices  $i$  and  $j$  as well as an element  $e$  of the unit sphere  $S^2$  are chosen randomly. Two new velocities

$$v_i^* = v_i + e(e, v_j - v_i), \quad v_j^* = v_j + e(e, v_i - v_j) \quad (2.6)$$

are calculated (cf. (1.3)). Instead of replacing the pre-collision velocities  $v_i, v_j$  of the two particles by the post-collision velocities  $v_i^*, v_j^*$ , we replace the pair of particles  $(x_i, v_i, g_i), (x_j, v_j, g_j)$  by a group of four particles

$$(x_i, v_i, g_i - G), \quad (x_j, v_j, g_j - G), \quad (x_i, v_i^*, G), \quad (x_j, v_j^*, G),$$

where  $G$  is a function depending on the state of the system and on the parameters  $i, j, e$ . Thus, each of the particles taking part in the collision gives a part of its weight to an particle with the post-collision velocity.

The numerical method consists in the simulation of the particle systems (2.2)–(2.3), and in the approximation of the measures (1.4) by the corresponding empirical measures

$$\mu^{(n)}(t, dx, dv) = \sum_{i=1}^{m(t)} g_i(t) \delta_{(x_i(t), v_i(t))}(dx, dv), \quad (2.7)$$

where  $\delta$  denotes the Dirac measure. This means that functionals of the solution of Eq. (1.1) (e.g., density, momentum, energy), that are of the form

$$\int_D dx \int_{\mathcal{R}^3} dv \varphi(x, v) f(t, x, v), \quad (2.8)$$

where  $\varphi$  is an appropriate test function, are approximated by the term

$$\sum_{i=1}^{m(t)} g_i(t) \varphi(x_i(t), v_i(t)). \quad (2.9)$$

We use the notion "stochastic weighted particle method" in order to emphasize that the third components in the systems (2.2)–(2.3) are, in general, not constant, and that the time evolution of the systems is stochastic.

As  $n \rightarrow \infty$ , the empirical measures converge to the solution of an approximate Boltzmann equation. We describe the limiting equation, which has been obtained for Bird's DSMC method in [20] and which holds also for the stochastic weighted particle method presented in this paper.

Let the functions

$$f^{(1,k)}(t, x, v), \quad f^{(2,k)}(t, x, v), \quad t \in [t_k, t_{k+1}], \quad x \in D, \quad v \in \mathcal{R}^3,$$

where  $k = 0, 1, \dots$ , be defined as the solutions to the following system of equations,

$$\frac{\partial}{\partial t} f^{(1,k)}(t, x, v) + (v, \nabla_x) f^{(1,k)}(t, x, v) = 0, \quad (2.10)$$

with the initial conditions

$$f^{(1,k)}(t_k, x, v) = f^{(2,k-1)}(t_k, x, v), \quad \text{for } k = 1, 2, \dots, \quad (2.11)$$

and

$$f^{(1,k)}(t_k, x, v) = f_0(x, v), \quad \text{for } k = 0, \quad (2.12)$$



and

$$\frac{\partial}{\partial t} f^{(2,k)}(t, x, v) = \int_D dy \int_{\mathcal{R}^3} dw \int_{S^2} de h(x, y) B(v, w, e) \times \quad (2.13)$$

$$\left[ f^{(2,k)}(t, x, v^*) f^{(2,k)}(t, y, w^*) - f^{(2,k)}(t, x, v) f^{(2,k)}(t, y, w) \right],$$

with the initial condition

$$f^{(2,k)}(t_k, x, v) = f^{(1,k)}(t_{k+1}, x, v). \quad (2.14)$$

The function

$$h(x, y) = \sum_{i=1}^{l_c} \frac{1}{|D_i|} \mathbb{1}_{D_i}(x) \mathbb{1}_{D_i}(y), \quad (2.15)$$

is a mollifying kernel depending on the partition (2.5), where  $|D_i|$  denotes the Lebesgue measure of the cell  $D_i$ , and  $\mathbb{1}$  denotes the indicator function.

The various approximations involved in the algorithm are clearly displayed in the limiting equations. The splitting of the free flow simulation and the collision simulation leads to a corresponding splitting of the Boltzmann equation based on the time discretization (2.1). The introduction of the cell structure during the collision simulation step is represented by the mollifier  $h$  in the limiting equation. The transition from an approximate equation of the type (2.10)–(2.14) to the Boltzmann equation (1.1) has been studied in [2] in connection with Nanbu's simulation scheme.

### 3. Modelling of collisions

In this section we describe the collision simulation on a time interval  $[t_k, t_{k+1}]$ , i.e. the system (2.3). For simplicity, we omit the index  $k$  as well as the index 2 indicating the collision simulation step.

In § 3.1 we introduce a Markov jump process, which provides the background for the definition of the collision simulation. In § 3.2 we study the relationship between the Markov process and the approximate Boltzmann equation (2.13). The pathwise behaviour of the Markov process is described in § 3.3 in connection with the introduction of fictitious collisions. Some examples are given in § 3.4. Finally, in § 3.5 we introduce a reduction method for the number of particles in the system.

### 3.1. A Markov jump process

We consider a Markov process

$$Z^{(n)}(t) = \left\{ \left( x_i^{(n)}(t), v_i^{(n)}(t), g_i^{(n)}(t) \right), \quad i = 1, \dots, m^{(n)}(t) \right\}, \quad t \geq t_k, \quad (3.1)$$

with the infinitesimal generator

$$\mathcal{A}^{(n)}(\Phi)(\bar{z}) = \sum_{1 \leq i \neq j \leq m} \int_{S^2} \frac{1}{2} q(\bar{z}, i, j, e) \left[ \Phi(J(\bar{z}, i, j, e)) - \Phi(\bar{z}) \right] de, \quad (3.2)$$

where

$$\bar{z} = ((x_1, v_1, g_1), \dots, (x_m, v_m, g_m)) \in \mathcal{Z}^{(n)},$$

$$\mathcal{Z}^{(n)} = \bigcup_{m=N_{min}^{(n)}}^{N_{max}^{(n)}} \left( D \times \mathcal{R}^3 \times [0, \gamma_{max}^{(n)}] \right)^m,$$

and  $\Phi$  is a measurable bounded test function. The symbols  $N_{min}^{(n)}$  and  $N_{max}^{(n)}$  denote a lower and an upper bound for the number of particles in the system. The symbol  $\gamma_{max}^{(n)}$  denotes an upper bound for the weights of the particles in the system. We assume

$$\gamma_{max}^{(n)} = \frac{C_g}{n}$$

and

$$N_{min}^{(n)} = C_{N,min} n, \quad N_{max}^{(n)} = C_{N,max} n.$$

The collision transformation  $J(\bar{z}, i, j, e) : \mathcal{Z}^{(n)} \rightarrow \mathcal{Z}^{(n)}$  is defined as

$$[J(\bar{z}, i, j, e)]_k = \begin{cases} (x_k, v_k, g_k) & , \text{ if } k \leq m, k \neq i, j, \\ (x_i, v_i, g_i - G(\bar{z}, i, j, e)) & , \text{ if } k = i, \\ (x_j, v_j, g_j - G(\bar{z}, i, j, e)) & , \text{ if } k = j, \\ (x_i, v_i^*, G(\bar{z}, i, j, e)) & , \text{ if } k = m + 1, \\ (x_j, v_j^*, G(\bar{z}, i, j, e)) & , \text{ if } k = m + 2, \end{cases} \quad (3.3)$$

with  $v_i^*, v_j^*$  given in (2.6). Concerning the weight transfer function  $G$  we assume

$$G(\bar{z}, i, j, e) \leq \min(g_i, g_j) \quad (3.4)$$

so that the weight components of the process remain non-negative. The intensity function  $q$  is assumed to be bounded and measurable.

### 3.2. Relation to the Boltzmann equation

Consider a function

$$\Phi(\bar{z}) = \sum_{i=1}^m g_i \varphi(x_i, v_i), \quad \bar{z} = ((x_1, v_1, g_1), \dots, (x_m, v_m, g_m)),$$

where  $\varphi$  is an appropriate function on  $D \times \mathcal{R}^3$ . Notice that

$$\Phi(Z^{(n)}(t)) = \langle \varphi, \mu^{(n)}(t) \rangle, \quad (3.5)$$

where  $Z^{(n)}$  is the Markov process (3.1), and  $\mu^{(n)}$  is the corresponding empirical measure (2.7). Using (3.3), we find

$$\begin{aligned} \Phi(J(\bar{z}, i, j, e)) &= \Phi(\bar{z}) + \\ &G(\bar{z}, i, j, e) [\varphi(x_i, v_i^*) + \varphi(x_j, v_j^*) - \varphi(x_i, v_i) - \varphi(x_j, v_j)], \end{aligned}$$

and, according to (3.2),

$$\begin{aligned} \mathcal{A}^{(n)}(\Phi)(\bar{z}) &= \sum_{1 \leq i \neq j \leq m} \int_{S^2} \frac{1}{2} q(\bar{z}, i, j, e) \times \\ &G(\bar{z}, i, j, e) [\varphi(x_i, v_i^*) + \varphi(x_j, v_j^*) - \varphi(x_i, v_i) - \varphi(x_j, v_j)] de. \end{aligned} \quad (3.6)$$

The following representation holds for any measurable bounded function  $\Phi$ ,

$$\Phi(Z^{(n)}(t)) = \Phi(Z^{(n)}(0)) + \int_0^t \mathcal{A}^{(n)}(\Phi)(Z^{(n)}(s)) ds + M^{(n)}(t), \quad (3.7)$$

where  $M^{(n)}(t)$  is a martingale term.

Assume that the intensity function  $q$  and the weight transfer function  $G$  satisfy the equality

$$q(\bar{z}, i, j, e) G(\bar{z}, i, j, e) = h(x_i, x_j) B(v_i, v_j, e) g_i g_j, \quad (3.8)$$

where  $B$  is the collision kernel of the Boltzmann equation and  $h$  is the mollifying kernel defined in (2.15). Then, using (3.7), (3.5), and (3.6), one obtains the representation

$$\begin{aligned} \langle \varphi, \mu^{(n)}(t) \rangle &= \langle \varphi, \mu^{(n)}(0) \rangle + \int_0^t \int_{D \times \mathcal{R}^3} \int_{D \times \mathcal{R}^3} \int_{S^2} \frac{1}{2} h(x, y) B(v, w, e) \times \\ &[\varphi(x, v^*) + \varphi(y, w^*) - \varphi(x, v) - \varphi(y, w)] \\ &de \mu^{(n)}(s, dy, dw) \mu^{(n)}(s, dx, dv) ds + R^{(n)}, \end{aligned}$$

where  $R^{(n)}$  is a remainder disappearing when  $n \rightarrow \infty$ . Therefore, the limit  $\lambda(t)$  of the empirical measures is expected to satisfy the equation

$$\langle \varphi, \lambda(t) \rangle = \langle \varphi, \lambda(0) \rangle + \int_0^t \int_{D \times \mathcal{R}^3} \int_{D \times \mathcal{R}^3} \int_{S^2} \frac{1}{2} h(x, y) B(v, w, e) \times \quad (3.9)$$

$$[\varphi(x, v^*) + \varphi(y, w^*) - \varphi(x, v) - \varphi(y, w)] de \lambda(s, dy, dw) \lambda(s, dx, dv) ds.$$

Assume the measures  $\lambda(t)$  are absolutely continuous with respect to the Lebesgue measure. Then, after the substitution of the integration variables  $(v, w)$  by  $(v^*, w^*)$  and removing the test function  $\varphi$ , Eq. (3.9) reduces to Eq. (2.13) provided that the kernel  $B$  has the properties

$$B(v, w, e) = B(w, v, e) = B(v^*, w^*, e).$$

Thus, condition (3.8) describes the **basic relationship** between the parameters  $q$  and  $G$  of the stochastic process (3.1) and the parameters  $B$  and  $h$  of the approximate Boltzmann equation (2.13).

### 3.3. Pathwise behaviour and fictitious collisions

Taking into account the special form (2.15) of the mollifying kernel  $h$  and the condition (3.8), we assume that the functions  $q$  and  $G$  are of the same structure, i.e.

$$q(\bar{z}, i, j, e) = \sum_{l=1}^{l_c} \mathbb{1}_{D_l}(x_i) \mathbb{1}_{D_l}(x_j) q^{(l)}(\bar{z}, i, j, e) \quad (3.10)$$

and

$$G(\bar{z}, i, j, e) = \sum_{l=1}^{l_c} \mathbb{1}_{D_l}(x_i) \mathbb{1}_{D_l}(x_j) G^{(l)}(\bar{z}, i, j, e). \quad (3.11)$$

Then, the particle system (3.1) can be divided into independent subsystems corresponding to the spatial cells, provided that the functions  $q^{(l)}$  and  $G^{(l)}$  depend only on particles belonging to the cell  $D_l$ . For example, this is fulfilled, if

$$q^{(l)}(\bar{z}, i, j, e) = q^{(l)}(x_i, x_j, v_i, v_j, e) \quad (3.12)$$

and

$$G^{(l)}(\bar{z}, i, j, e) = G^{(l)}(x_i, x_j, v_i, v_j, e). \quad (3.13)$$

For a fixed cell  $D_l$ , we consider the generator of the corresponding process,

$$\begin{aligned} \mathcal{A}^{(n,l)}(\Phi)(\bar{z}) = & \quad (3.14) \\ & \sum_{1 \leq i \neq j \leq m} \int_{S^2} \frac{1}{2} \mathbb{1}_{D_l}(x_i) \mathbb{1}_{D_l}(x_j) q^{(l)}(\bar{z}, i, j, e) [\Phi(J^{(l)}(\bar{z}, i, j, e)) - \Phi(\bar{z})] de, \end{aligned}$$

where  $J^{(l)}$  denotes the transformation (3.3) with  $G$  replaced by  $G^{(l)}$ .

The generation of a trajectory of the Markov process can be simplified significantly by means of the following procedure, which is called the introduction of fictitious jumps. Under the assumption

$$q^{(l)}(\bar{z}, i, j, e) \leq \tilde{q}^{(l)}(\bar{z}, i, j, e), \quad (3.15)$$

the generator (3.14) can be transformed as follows,

$$\begin{aligned} \mathcal{A}^{(n,l)}(\Phi)(\bar{z}) = & \quad (3.16) \\ & \sum_{1 \leq i \neq j \leq m} \int_{S^2} \int_0^1 \frac{1}{2} \mathbb{1}_{D_l}(x_i) \mathbb{1}_{D_l}(x_j) \times \\ & \tilde{q}^{(l)}(\bar{z}, i, j, e) [\Phi(\tilde{J}^{(l)}(\bar{z}, i, j, e, \eta)) - \Phi(\bar{z})] d\eta de, \end{aligned}$$

where

$$\tilde{J}^{(l)}(\bar{z}, i, j, e, \eta) = \begin{cases} J^{(l)}(\bar{z}, i, j, e), & \text{if } \eta \leq \frac{q^{(l)}(\bar{z}, i, j, e)}{\tilde{q}^{(l)}(\bar{z}, i, j, e)}, \\ \bar{z}, & \text{otherwise.} \end{cases} \quad (3.17)$$

The behaviour of the Markov process with the generator (3.16) is as follows. Given a state

$$\bar{z} = ((x_1, v_1, g_1), \dots, (x_m, v_m, g_m)),$$

the process waits a random time having an exponential distribution with the parameter

$$\tilde{\pi}^{(l)}(\bar{z}) = \sum_{1 \leq i \neq j \leq m} \int_{S^2} \frac{1}{2} \mathbb{1}_{D_l}(x_i) \mathbb{1}_{D_l}(x_j) \tilde{q}^{(l)}(\bar{z}, i, j, e) de. \quad (3.18)$$

Then, the process jumps from the state  $\bar{z}$  into the state  $\bar{J}^{(l)}(\bar{z}, i, j, e, \eta)$ . This means that first the condition on  $\eta$  at the right-hand side of (3.17) is checked. If the condition is not satisfied, then nothing happens and the jump (or the collision) is called fictitious. Otherwise, a jump is performed according to the jump transformation defined in (3.3). The jump (collision) parameters  $i, j, e, \eta$  are distributed according to the density

$$p^{(l)}(i, j, e, \eta) = \frac{\frac{1}{2} \mathbb{1}_{D_i}(x_i) \mathbb{1}_{D_i}(x_j) \tilde{q}^{(l)}(\bar{z}, i, j, e)}{\tilde{\pi}^{(l)}(\bar{z})}.$$

Thus, the parameter  $\eta$  is uniformly distributed on the unit time interval  $[0, 1]$ . The distribution of the parameter  $i$  is

$$p_1^{(l)}(i) = \frac{\sum_{j: i \neq j} \int_{S^2} \frac{1}{2} \mathbb{1}_{D_i}(x_i) \mathbb{1}_{D_i}(x_j) \tilde{q}^{(l)}(\bar{z}, i, j, e) de}{\tilde{\pi}^{(l)}(\bar{z})}. \quad (3.19)$$

The distribution of the parameter  $j$  given the value of  $i$  is

$$p_2^{(l)}(j | i) = \frac{\int_{S^2} \mathbb{1}_{D_i}(x_i) \mathbb{1}_{D_i}(x_j) \tilde{q}^{(l)}(\bar{z}, i, j, e) de}{\sum_{j: i \neq j} \int_{S^2} \mathbb{1}_{D_i}(x_i) \mathbb{1}_{D_i}(x_j) \tilde{q}^{(l)}(\bar{z}, i, j, e) de}. \quad (3.20)$$

Finally, the distribution of the parameter  $e$  given the values of  $i$  and  $j$  is

$$p_3^{(l)}(e | i, j) = \frac{\tilde{q}^{(l)}(\bar{z}, i, j, e)}{\int_{S^2} \tilde{q}^{(l)}(\bar{z}, i, j, e) de}. \quad (3.21)$$

In the case  $q^{(l)} = \tilde{q}^{(l)}$ , the behaviour of the original process (without fictitious jumps) is obtained from the above procedure. An appropriate choice of the function  $\tilde{q}^{(l)}$  may lead to a substantial simplification of the modelling of the process (note that the distribution of the process remains the same).

In particular, if the parameter of the waiting time distribution is easy to calculate, then the time step between two collisions is approximated by the value  $\tilde{\pi}^{(l)}(\bar{z})^{-1}$ . These approximate time steps are added to a variable called the **time counter**. If the value of this variable reaches  $\Delta t$ , then the collision simulation step is finished. Note that both fictitious and real collisions are counted.

The general idea of the introduction of fictitious collisions is to generate more collisions by a much simplified stochastic mechanism and to play an

additional game of chance to reduce the number of collisions to the right one. This idea is present in many of the algorithms used in practical calculations, as the null-collision technique [14], the majorant-frequency scheme [13], the no-time-counter scheme [4], or the scheme based on stochastic differential equations with respect to Poisson measures [15].

### 3.4. Examples

We give three examples of functions  $q$  and  $G$  of the form (3.10)–(3.13) satisfying condition (3.8) and assumption (3.4). The first example reduces to the standard particle simulation scheme (like DSMC) in the case of identical initial weights. In the second and the third example there is a random weight transfer during the collisions. We assume the collision kernel to be bounded (or truncated), i.e.

$$B(v, w, e) \leq B_{\max}, \quad \forall v, w \in \mathcal{R}^3, \quad \forall e \in \mathcal{S}^2.$$

**Example 1** *First we consider the functions*

$$G^{(l)}(\bar{z}, i, j, e) = \min(g_i, g_j) \tag{3.22}$$

and

$$q^{(l)}(\bar{z}, i, j, e) = \frac{1}{|D_l|} B(v_i, v_j, e) \max(g_i, g_j),$$

where  $|D_l|$  is the Lebesgue measure of the cell  $D_l$ . We introduce (cf. (3.15))

$$\tilde{q}^{(l)}(\bar{z}, i, j, e) = \frac{1}{|D_l|} B_{\max} C_{g, \max}(l), \tag{3.23}$$

where  $C_{g, \max}(l)$  denotes the maximum of the weights of the particles in the cell  $D_l$ . The condition on  $\eta$  at the right-hand side of (3.17) takes the form

$$\eta \leq \frac{B(v_i, v_j, e) \max(g_i, g_j)}{B_{\max} C_{g, \max}(l)}. \tag{3.24}$$

From (3.18), we obtain

$$\tilde{\pi}^{(l)}(\bar{z}) = \frac{1}{2} 4\pi \frac{1}{|D_l|} B_{\max} C_{g, \max}(l) m_l (m_l - 1), \tag{3.25}$$

where  $m_l$  denotes the current number of particles in the cell  $D_l$ . Therefore, according to (3.19)–(3.20), the parameters  $i$  and  $j$  are distributed uniformly among the particles belonging to the cell  $D_l$ , i.e.

$$p_1^{(l)}(i) = \frac{1}{m_l}, \quad p_2^{(l)}(j | i) = \frac{1}{m_l - 1}. \quad (3.26)$$

According to (3.21), the parameter  $e$  is distributed uniformly on the unit sphere, i.e.

$$p_3^{(l)}(e | i, j) = \frac{1}{4\pi}. \quad (3.27)$$

According to (3.25), the time step is of the form

$$\left[ 2\pi \frac{1}{|D_l|} B_{\max} C_{g, \max}(l) m_l (m_l - 1) \right]^{-1}. \quad (3.28)$$

**Example 2** Next we consider the functions

$$G^{(l)}(\bar{z}, i, j, e) = \frac{g_i g_j}{g_i + g_j} \quad (3.29)$$

and

$$q^{(l)}(\bar{z}, i, j, e) = \frac{1}{|D_l|} B(v_i, v_j, e) (g_i + g_j).$$

We introduce (cf. (3.15))

$$\tilde{q}^{(l)}(\bar{z}, i, j, e) = \frac{1}{|D_l|} B_{\max} 2 C_{g, \max}(l).$$

The condition on  $\eta$  takes the form

$$\eta \leq \frac{B(v_i, v_j, e)}{B_{\max}} \frac{g_i + g_j}{2 C_{g, \max}(l)}.$$

The distribution of the parameters  $i, j, e$  remains the same as given in (3.26), (3.27). The time step is of the form

$$\left[ 4\pi \frac{1}{|D_l|} B_{\max} C_{g, \max}(l) m_l (m_l - 1) \right]^{-1}. \quad (3.30)$$



**Example 3** Finally, we consider the functions

$$G^{(l)}(\bar{z}, i, j, e) = \frac{B(v_i, v_j, e)}{B_{max}} \min(g_i, g_j) \quad (3.31)$$

and

$$q^{(l)}(\bar{z}, i, j, e) = \frac{1}{|D_l|} B_{max} \max(g_i, g_j).$$

We use the function  $\tilde{q}^{(l)}$  given in (3.23). The condition on  $\eta$  takes the form

$$\eta \leq \frac{\max(g_i, g_j)}{C_{g,max}(l)}. \quad (3.32)$$

The distribution of the parameters  $i, j, e$  and the time step remain the same as given in (3.26)–(3.28).

Consider Example 1 in the case of identical initial weights. The function  $G$  reduces to a constant so that there is a complete weight transfer during each collision. One obtains the standard DSMC method.

Comparing Example 2 and Example 1, we notice that even in the case  $g_i = g_j$  only half of the weight is transferred (cf. (3.29)). On the other hand, the time step is also divided by the factor 2 (compare (3.28) and (3.30)). Thus, the number of collisions (including fictitious) increases twice. This means that there are more collisions but a smaller weight transfer during each collision.

Comparing Example 3 and Example 1, we mention that the time step is the same in both examples. Therefore, the number of collisions (including fictitious) is (roughly) the same. But the portion of fictitious collisions is less in Example 3, since the condition on  $\eta$  is weaker (compare (3.24) and (3.32)). On the other hand, the amount of weight transferred during a collision is also less in Example 3 (compare (3.22) and (3.31)). This means that in many situations, i.e. for many configurations of the parameters  $i, j, e$ , instead of "performing" a fictitious collision, a small part of the weight is transferred.

### 3.5. Reduction of the number of particles

In general, the number of particles in the system increases during each collision. Thus, this number has to be reduced when it becomes too large.

Suppose we are given a system of particles

$$(x_1, v_1, g_1), \dots, (x_m, v_m, g_m). \quad (3.33)$$

The problem is to construct a system with a reduced number of particles but such that the corresponding empirical measures do still approximate the solution of the Boltzmann equation.

We divide the system (3.33) into  $\hat{m}$  groups of particles

$$(x_{i,j}, v_{i,j}, g_{i,j}), \quad i = 1, \dots, \hat{m}, \quad j = 1, \dots, k_i. \quad (3.34)$$

Each group will be replaced by two particles in such a way that mass, momentum and energy are preserved. To this end, we introduce the notations

$$c_i = \sum_{j=1}^{k_i} g_{i,j}, \quad (3.35)$$

$$\alpha_i = \frac{1}{c_i} \sum_{j=1}^{k_i} g_{i,j} v_{i,j}, \quad (3.36)$$

$$\beta_i = \frac{1}{c_i} \sum_{j=1}^{k_i} g_{i,j} \|v_{i,j}\|^2, \quad (3.37)$$

and

$$\varepsilon_i^2 = \beta_i - \|\alpha_i\|^2, \quad (3.38)$$

where  $i = 1, \dots, \hat{m}$ . Now the reduced system is defined as

$$(\tilde{x}_{i,j}, \tilde{v}_{i,j}, \tilde{g}_{i,j}), \quad i = 1, \dots, \hat{m}, \quad j = 1, 2, \quad (3.39)$$

where

$$\tilde{v}_{i,1} = \alpha_i + \varepsilon_i e_i, \quad \tilde{g}_{i,1} = \frac{1}{2} c_i \quad (3.40)$$

and

$$\tilde{v}_{i,2} = \alpha_i - \varepsilon_i e_i, \quad \tilde{g}_{i,2} = \frac{1}{2} c_i. \quad (3.41)$$

The new positions  $\tilde{x}_{i,j}$  are chosen from the set (cf. (3.34))

$$X_i = \{x_{i,j} : j = 1, \dots, k_i\}. \quad (3.42)$$

The vectors  $e_i \in \mathcal{S}^2$  are arbitrary.

Note the conservation properties in each group,

$$\begin{aligned} \langle 1, \tilde{\mu}_i \rangle &= c_i = \langle 1, \mu_i \rangle, \\ \langle v, \tilde{\mu}_i \rangle &= \frac{1}{2} c_i 2 \alpha_i = \langle v, \mu_i \rangle, \\ \langle \|v\|^2, \tilde{\mu}_i \rangle &= \frac{1}{2} c_i (\|\alpha_i + \varepsilon_i e_i\|^2 + \|\alpha_i - \varepsilon_i e_i\|^2) \\ &= \frac{1}{2} c_i (2 \|\alpha_i\|^2 + 2 \varepsilon_i^2) \\ &= c_i (\|\alpha_i\|^2 + \beta_i - \|\alpha_i\|^2) = \langle \|v\|^2, \mu_i \rangle, \end{aligned}$$

where

$$\mu_i = \sum_{j=1}^{k_i} g_{i,j} \delta_{(x_{i,j}, v_{i,j})}, \quad \tilde{\mu}_i = \tilde{g}_{i,1} \delta_{(\tilde{x}_{i,1}, \tilde{v}_{i,1})} + \tilde{g}_{i,2} \delta_{(\tilde{x}_{i,2}, \tilde{v}_{i,2})}, \quad i = 1, \dots, \hat{m}.$$

We consider the bounded Lipschitz metric

$$\varrho(\nu_1, \nu_2) = \sup_{\|\varphi\|_L \leq 1} \left| \int_{D \times \mathcal{R}^3} \varphi(x, v) \nu_1(dx, dv) - \int_{D \times \mathcal{R}^3} \varphi(x, v) \nu_2(dx, dv) \right|,$$

where

$$\|\varphi\|_L = \max \left( \sup_{x,v} |\varphi(x, v)|, \sup_{(x,v) \neq (y,w)} \frac{|\varphi(x, v) - \varphi(y, w)|}{\|x - y\| + \|v - w\|} \right).$$

This metric is equivalent to weak convergence of measures. We will estimate the distance  $\varrho(\mu, \tilde{\mu})$ , where

$$\mu = \sum_{i=1}^m g_i \delta_{(x_i, v_i)}, \quad \tilde{\mu} = \sum_{i=1}^{\hat{m}} \left[ \tilde{g}_{i,1} \delta_{(\tilde{x}_{i,1}, \tilde{v}_{i,1})} + \tilde{g}_{i,2} \delta_{(\tilde{x}_{i,2}, \tilde{v}_{i,2})} \right]$$

are the empirical measures associated with the original system (3.33) and the reduced system (3.39), respectively.

We obtain

$$\begin{aligned}
& |\langle \varphi, \mu \rangle - \langle \varphi, \tilde{\mu} \rangle| = \\
& = \left| \sum_{i=1}^{\hat{m}} \sum_{j=1}^{k_i} g_{i,j} \varphi(x_{i,j}, v_{i,j}) - \sum_{i=1}^{\hat{m}} \frac{1}{2} c_i [\varphi(\tilde{x}_{i,1}, \tilde{v}_{i,1}) + \varphi(\tilde{x}_{i,2}, \tilde{v}_{i,2})] \right| \\
& \leq \sum_{i=1}^{\hat{m}} \left| \sum_{j=1}^{k_i} g_{i,j} \varphi(\hat{x}, v_{i,j}) - \frac{1}{2} c_i [\varphi(\hat{x}, \tilde{v}_{i,1}) + \varphi(\hat{x}, \tilde{v}_{i,2})] \right| \\
& \quad + 2 \sum_{i=1}^{\hat{m}} \text{diam}(X_i) c_i, \tag{3.43}
\end{aligned}$$

where  $\hat{x} \in X_i$  is a fixed position (cf. (3.42)), and the obvious inequality

$$|\varphi(x, v) - \varphi(\hat{x}, v)| \leq \|x - \hat{x}\| \leq \text{diam}(X_i), \quad \forall x \in X_i, \quad \forall v \in \mathcal{R}^3,$$

has been used. Using (3.36), (3.40), and (3.41), the term inside the first sum on the right-hand side of (3.43) is estimated as follows,

$$\begin{aligned}
& \left| \sum_{j=1}^{k_i} g_{i,j} \varphi(\hat{x}, v_{i,j}) - \frac{1}{2} c_i [\varphi(\hat{x}, \tilde{v}_{i,1}) + \varphi(\hat{x}, \tilde{v}_{i,2})] \right| \leq \\
& \leq \sum_{j=1}^{k_i} g_{i,j} |\varphi(\hat{x}, v_{i,j}) - \varphi(\hat{x}, \alpha_i)| + |c_i \varphi(\hat{x}, \alpha_i) - \frac{1}{2} c_i [\varphi(\hat{x}, \tilde{v}_{i,1}) + \varphi(\hat{x}, \tilde{v}_{i,2})]| \\
& \leq \sum_{j=1}^{k_i} g_{i,j} \|v_{i,j} - \alpha_i\| + c_i \varepsilon_i. \tag{3.44}
\end{aligned}$$

Finally, using (3.35), (3.37), and (3.38), we estimate

$$\begin{aligned}
& \sum_{j=1}^{k_i} g_{i,j} \|v_{i,j} - \alpha_i\| \leq (c_i)^{1/2} \left( \sum_{j=1}^{k_i} g_{i,j} \|v_{i,j} - \alpha_i\|^2 \right)^{1/2} \\
& = (c_i)^{1/2} \left( c_i \beta_i - 2 c_i \|\alpha_i\|^2 + c_i \|\alpha_i\|^2 \right)^{1/2} = c_i \varepsilon_i. \tag{3.45}
\end{aligned}$$

Thus, we obtain from (3.43), (3.44), and (3.45)

$$\varrho(\mu, \tilde{\mu}) \leq 2 \sum_{i=1}^{\hat{m}} c_i \varepsilon_i + 2 \sum_{i=1}^{\hat{m}} \text{diam}(X_i) c_i.$$

Note that

$$\begin{aligned}
c_i^2 \varepsilon_i^2 &= \left( \sum_{j=1}^{k_i} g_{i,j} \right) \left( \sum_{j=1}^{k_i} g_{i,j} \|v_{i,j}\|^2 \right) - \left\| \sum_{j=1}^{k_i} g_{i,j} v_{i,j} \right\|^2 \\
&= \sum_{j=1}^{k_i} g_{i,j}^2 \|v_{i,j}\|^2 + \sum_{1 \leq j_1 < j_2 \leq k_i} g_{i,j_1} g_{i,j_2} \left( \|v_{i,j_1}\|^2 + \|v_{i,j_2}\|^2 \right) \\
&\quad - \sum_{j=1}^{k_i} g_{i,j}^2 \|v_{i,j}\|^2 - 2 \sum_{1 \leq j_1 < j_2 \leq k_i} g_{i,j_1} g_{i,j_2} (v_{i,j_1}, v_{i,j_2}) \\
&= \sum_{1 \leq j_1 < j_2 \leq k_i} g_{i,j_1} g_{i,j_2} \|v_{i,j_1} - v_{i,j_2}\|^2.
\end{aligned}$$

## 4. Numerical experiments

In this section we present results of numerical experiments performed with the stochastic weighted particle method. We consider the problem of heat transfer between parallel plates. In this case, the spatial domain is of the form

$$D = \{x \in \mathcal{R}^3 : x_1 \in [0, 1]\}.$$

We assume homogeneity in  $x_2$  and  $x_3$ , so that the problem reduces to a one-dimensional with respect to the spatial coordinates.

We consider the collision kernel that corresponds to the case of hard sphere molecules, i.e.

$$B(v, w, e) = \frac{1}{2\sqrt{2\pi} \kappa} |(v - w, e)|,$$

with a truncation that is adapted during the calculation. The symbol  $\kappa$  denotes the mean free path between collisions, which is equal to the Knudsen number in our case.

The initial distribution (cf. (1.2)) is supposed to be Maxwellian, i.e.

$$f_0(x, v) = \frac{1}{(2\pi R T_0)^{3/2}} \exp\left(-\frac{1}{2R T_0} \|v\|^2\right),$$

where  $T_0$  is the initial temperature, and  $R$  is the gas constant.

The boundary condition is diffuse reflection with the temperatures  $T_{left}$  and  $T_{right}$  at the left and the right plate, respectively.

We calculate the time evolution of the macroscopic variables  $d$  and  $T$  that describe the density and the temperature of the gas, respectively. These quantities are defined as

$$d(t, x) = \int_{\mathcal{R}^3} f(t, x, v) dv \quad (4.1)$$

and

$$T(t, x) = \frac{1}{3Rd(t, x)} \left[ \int_{\mathcal{R}^3} \|v\|^2 f(t, x, v) dv - \left\| \int_{\mathcal{R}^3} v f(t, x, v) dv \right\|^2 \right]. \quad (4.2)$$

Using some smoothing with respect to the position variable  $x$ , the quantities (4.1) and (4.2) are expressed via functionals of the form (2.8), and are approximated by terms of the form (2.9).

The spatial domain  $[0, 1]$  is divided into 41 cells of equal length. The initial number of particles is 200 per cell. The mean free path is  $\kappa = 0.05$ .

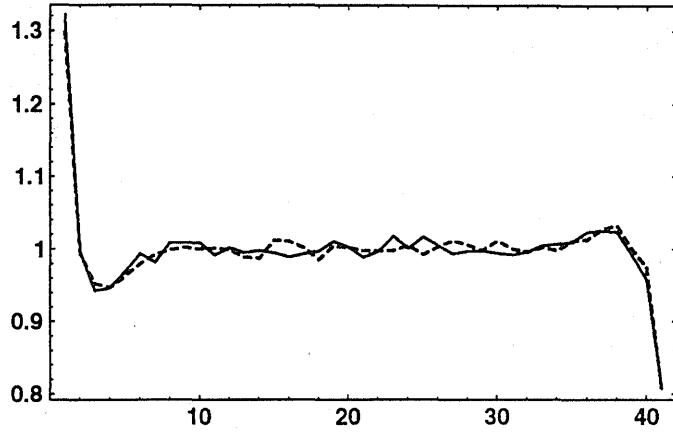
The initial temperature of the gas is  $T_0 = 200$ , the temperature of the boundary is  $T_{left} = 100$  at the left plate, and  $T_{right} = 300$  at the right plate.

The density (4.1) and the temperature (4.2) of the gas have been calculated at the time  $t_1 = 0.1$  and at the time  $t_2 = 0.2$ , where the time unit is the quotient of the distance between the plates and the mean thermic velocity, i.e.  $1/\sqrt{2RT_0}$ .

The results have been averaged over 100 independent runs of the algorithm. The fluctuations are at a level of about 5% of the expected values for both algorithms. We decided not to display the confidence intervals in order not to overload the figures.

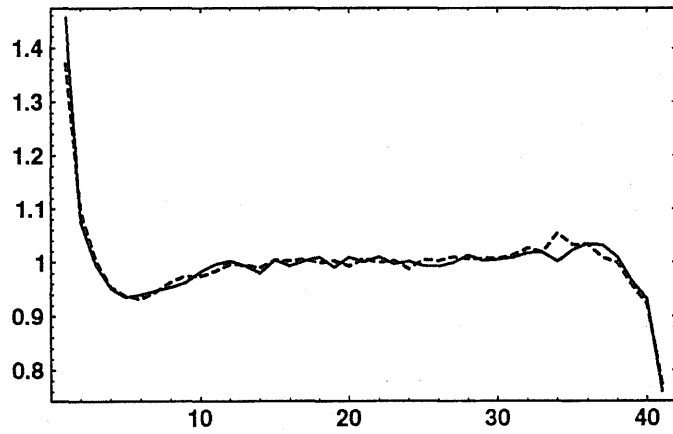
The results are shown in the figures below. The dashed lines represent the results for the stochastic weighted particle method (cf. Example 2), while the other lines represent the results obtained with the standard DSMC method (cf. Example 1).

Density



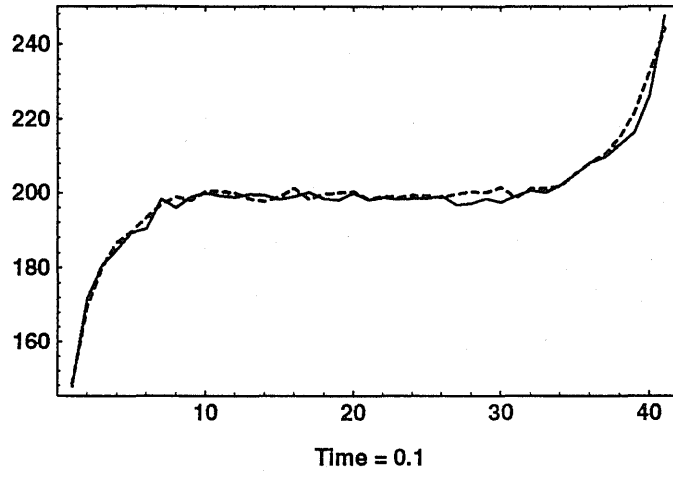
Time = 0.1

Density

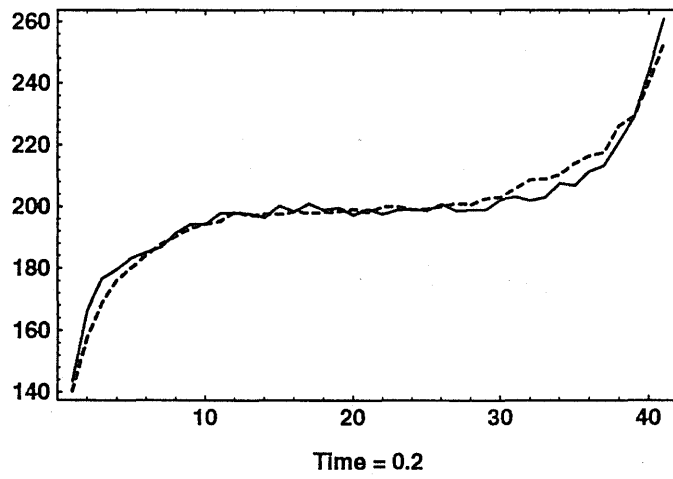


Time = 0.2

Temperature



Temperature





## 5. Concluding remarks

Summarizing the results of this paper, we point out what we consider as the main achievements and the most important open problems.

We have developed a class of algorithms for the numerical treatment of the Boltzmann equation. This class contains the standard DSMC method as a special case. In general, collisions between particles are simulated by means of a random weight transfer, which is connected with a random blow-up of the system.

The algorithms were tested in the case of heat transfer between parallel plates (one-dimensional position space). The time evolution of various macroscopic quantities was studied as well as the random fluctuations. The results of the algorithm with weight transfer and reduction of the system turned out to be comparable with those obtained with the standard DSMC method.

On the one hand, the new class of algorithms contains some degrees of freedom in the collision simulation procedure. On the other hand, additional effort is necessary to use these degrees of freedom. Thus, there are two main directions for further study.

The first direction is to develop more sophisticated techniques for the reduction of the number of particles. This step is very time-consuming at present. The general problem is that of clustering, i.e. of reducing the amount of data while preserving the main information. We will study the reduction procedure in more detail in the relaxation problem (zero-dimensional position space).

The second direction is to look for applications, where the additional degrees of freedom turn out to be useful. The collision simulation procedure may depend on the spatial coordinates and on the velocities of the colliding particles. Thus, it seems to be possible to "direct" particles into spatial regions, where the density is very small. To study this problem, it is necessary to consider at least a two-dimensional position space.

## References

- [1] H. Babovsky. A convergence proof for Nanbu's Boltzmann simulation scheme. *European J. Mech. B Fluids*, 8(1), 41–55, 1989.
- [2] H. Babovsky and R. Illner. A convergence proof for Nanbu's simulation method for the full Boltzmann equation. *SIAM J. Numer. Anal.*, 26(1), 45–65, 1989.
- [3] G. A. Bird. *Molecular Gas Dynamics*. Clarendon Press, Oxford, 1976.
- [4] G. A. Bird. Perception of numerical methods in rarefied gas dynamics. *Progr. Astronaut. Aeronaut.*, 118, 211–226, 1989.
- [5] G. A. Bird. Efficiency and discrepancy in the direct simulation methods. In A. E. Beylich, editor, *Proc. of the 17th International Symposium on Rarefied Gas Dynamics*, 655–662, Aachen, 1990.
- [6] G. A. Bird. *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. Clarendon Press, Oxford, 1994.
- [7] C. Cercignani. *The Boltzmann Equation and its Applications*. Springer, New York, 1988.
- [8] R. Illner and H. Neunzert. On simulation methods for the Boltzmann equation. *Transport Theory Statist. Phys.*, 16(2&3), 141–154, 1987.
- [9] R. Illner and S. Rjasanow. Random discrete velocity models: Possible bridges between the Boltzmann equation, discrete velocity models and particle simulation? In V. C. Boffi, F. Bampi, and G. Toscani, editors, *Nonlinear kinetic theory and mathematical aspects of hyperbolic systems*, 152–158. World Scientific, Singapore, 1992.
- [10] R. Illner and S. Rjasanow. Numerical solution of the Boltzmann equation by random discrete velocity models. *European J. Mech. B Fluids*, 13(2), 197–210, 1994.
- [11] R. Illner and W. Wagner. A random discrete velocity model and approximation of the Boltzmann equation. *J. Statist. Phys.*, 70(3/4), 773–792, 1993.

- [12] R. Illner and W. Wagner. Random discrete velocity models and approximation of the Boltzmann equation. Conservation of momentum and energy. *Transport Theory Statist. Phys.*, 23(1-3), 27-38, 1994.
- [13] M. S. Ivanov and S. V. Rogazinskij. Analysis of numerical techniques of the direct simulation Monte Carlo method in the rarefied gas dynamics. *Soviet J. Numer. Anal. Math. Modelling*, 3(6), 453-465, 1988.
- [14] K. Koura. Null-collision technique in the direct-simulation Monte Carlo method. *Phys. Fluids*, 29(11), 3509-3511, 1986.
- [15] A. V. Lukshin and S. N. Smirnov. An efficient stochastic algorithm for solving the Boltzmann equation. *U.S.S.R. Comput. Math. and Math. Phys.*, 29(1), 83-87, 1989.
- [16] K. Nanbu. Interrelations between various direct simulation methods for solving the Boltzmann equation. *J. Phys. Soc. Jpn.*, 52(10), 3382-3388, 1983.
- [17] H. Neunzert, F. Gropengiesser, and J. Struckmeier. Computational methods for the Boltzmann equation. In R. Spigler, editor, *Applied and Industrial Mathematics*, 111-140. Kluwer Acad. Publ., Dordrecht, 1991.
- [18] M. Schreiner. Weighted particles in the finite pointset method. *Transport Theory Statist. Phys.*, 22(6), 793-817, 1993.
- [19] S. N. Smirnov. On the justification of a stochastic method for solving the Boltzmann equation. *Zh. Vychisl. Mat. i Mat. Fiz.*, 29(2), 270-276, 1989. (in Russian).
- [20] W. Wagner. A convergence proof for Bird's direct simulation Monte Carlo method for the Boltzmann equation. *J. Statist. Phys.*, 66(3/4), 1011-1044, 1992.
- [21] W. Wagner. Stochastic systems of particles with weights and approximation of the Boltzmann equation. The Markov process in the spatially homogeneous case. *Stochastic Anal. Appl.*, 12(5), 1994. to be published.



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118. Herbert Gajewski, Konrad Gröger: Reaction-diffusion processes of electrically charged species.
119. Johannes Elschner, Siegfried Prössdorf, Ian H. Sloan: The qualocation method for Symm's integral equation on a polygon.