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A Stochastic Weighted Particle Method for the Boltzmann Equation

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A class of algorithms for the numerical treatment of the Boltzmann equation is introduced. This class generalizes the standard direct simulation Monte Carlo method, which is contained as a particular case. The new algorithms use a more general procedure of modelling collisions between particles. This procedure is based on a random weight transfer from the particles with the precollision velocities to the particles with the postcollision velocities. © 1996 Academic Press, Inc.

1. INTRODUCTION

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

$$\frac{\partial}{\partial t} f(t,x,v) + (v, \nabla_x) f(t,x,v) = \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de\, B(v,w,e)[f(t,x,v^*) f(t,x,w^*) - f(t,x,v) f(t,x,w)], \tag{1.1}$$

$$f(0,x,v) = f_0(x,v), \tag{1.2}$$

where $t \geq 0$, $x \in D \subset \mathscr{R}^3$, and $v \in \mathscr{R}^3$. The symbol ∇_x denotes the vector of the partial derivatives with respect to x, D is a bounded domain in three-dimensional Euclidean space $\mathscr{R}^3$, 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 $\mathscr{S}^2$ and the Lebesgue measure on $\mathscr{R}^3$, respectively. The objects v^* and w^* are defined as

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

where v, $w \in \mathscr{R}^3$, $e \in \mathscr{S}^2$. They are interpreted as the postcollision velocities of two particles with the precollision 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

$$\lambda(t, dx, dv) = f(t,x,v)\, dx\, dv, \tag{1.4}$$

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, 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 mainly related to the problem of variance reduction, i.e., the reduction of the random fluctuations around the deterministic limit.

For example, the problem of calculating a gas flow around an obstacle by particle methods becomes difficult, if there are large differences in the gas density. The gas density behind the obstacle may be some orders of magnitude lower than the gas density in front of the obstacle. Macroscopic quantities of the gas in the low density region cannot be calculated efficiently, since only very few test particles enter this region, or, in statistical terms, the fluctuations of the corresponding estimators are very large.

In order to handle such a situation, it is necessary to have some mechanism for adapting the particle scheme to the concrete problem. For instance, it would be helpful to have the opportunity to blow up or reduce the system of test particles in a certain region, or to enforce test particles to enter the desired region. To this end, it is of interest to develop models with certain parameters that can be used to control the behaviour of the system.

The purpose of this paper is to propose a step into this direction. We generalize the standard DSMC method in such a way that the new class of particle methods contains

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certain 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, 10, 12, 21]). Thus, one obtains some combination of particle schemes (particles with changing velocities and fixed weights) and discrete velocity models (particles with fixed velocities and changing weights).

We refer to [17] concerning another approach to the problem of variance reduction. Low discrepancy sequences were introduced 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].

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

$$t_k = k\,\Delta t, \quad k = 0, 1, ..., \quad \Delta t > 0, \tag{2.1}$$

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 Δt, 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

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

and

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

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

$$\lambda_0(dx, dv) = f_0(x, v)\,dx\,dv, \tag{2.4}$$

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 ith 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 λ_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.,

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

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

$$D = \bigcup_{l=1}^{l_c} D_l \tag{2.5}$$

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 $\mathscr{S}^2$ are chosen randomly. Two new velocities

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

are calculated (cf. (1.3)). Instead of replacing the precollision velocities v_i, v_j of the two particles by the postcollision 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

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

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 a particle with the postcollision 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

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

where δ 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

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

where φ is an appropriate test function, are approximated by the term

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

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 $n \to \infty$, 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

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

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

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

with the initial conditions

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

and

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

and

$$\begin{aligned} \frac{\partial}{\partial t} f^{(2,k)}(t, x, v) = \int_D dy \int_{\mathscr{R}^3} dw \int_{\mathscr{S}^2} de\, h(x, y) B(v, w, e) \\ \times [f^{(2,k)}(t, x, v^*) f^{(2,k)}(t, y, w^*) \\ - f^{(2,k)}(t, x, v) f^{(2,k)}(t, y, w)], \end{aligned} \tag{2.13}$$

with the initial condition

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

The function

$$h(x, y) = \sum_{l=1}^{l_c} \frac{1}{|D_l|} \P_{D_l}(x) \P_{D_l}(y), \tag{2.15}$$

is a mollifying kernel depending on the partition (2.5), where $|D_l|$ denotes the Lebesgue measure of the cell D_l, and $\P$ 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 Section 3.1 we introduce a Markov jump process, which provides the background for the definition of the collision simulation. In Section 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 Section 3.3 in connection with the introduction of fictitious collisions. Some examples are given in Section 3.4. Finally, in Section 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

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

with the infinitesimal generator

$$\begin{aligned}\mathscr{A}^{(n)}(\Phi)(\bar{z}) = \sum_{1\leq i\neq j\leq m} \int_{\mathscr{S}^2} \frac{1}{2} q(\bar{z}, i, j, e) \\ \times [\Phi(J(\bar{z}, i, j, e)) - \Phi(\bar{z})]\, de,\end{aligned} \tag{3.2}$$

where

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

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

and Φ 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

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

and

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

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

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

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

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

so that the weight components of the process remain nonnegative. The *intensity function* q is assumed to be bounded and measurable.

3.2. *Relation to the Boltzmann Equation*

Consider a function

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

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

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

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),

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

The following representation holds for any measurable bounded function Φ,

$$\begin{aligned}\Phi(Z^{(n)}(t)) = \Phi(Z^{(n)}(0)) + \int_0^t \mathscr{A}^{(n)}(\Phi)(Z^{(n)}(s))\, ds \\ + M^{(n)}(t),\end{aligned} \tag{3.7}$$

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

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

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

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

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

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

$$\begin{aligned}\langle \varphi, \lambda(t)\rangle = \langle \varphi, \lambda(0)\rangle \\ + \int_0^t \int_{D\times\mathbb{R}^3} \int_{D\times\mathbb{R}^3} \int_{\mathcal{S}^2} \frac{1}{2} h(x, y)B(v, w, e) \qquad (3.9) \\ \times [\varphi(x, v^*) + \varphi(y, w^*) - \varphi(x, v) - \varphi(y, w)] \\ \times de\, \lambda(s, dy, dw)\lambda(s, dx, dv)\, ds.\end{aligned}$$

We refer to [21] concerning a convergence proof.

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 φ, 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.,

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

and

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

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

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

and

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

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

$$\begin{aligned}\mathcal{A}^{(n,l)}(\Phi)(\bar{z}) = \sum_{1\le i\ne j\le m} \int_{\mathcal{S}^2} \frac{1}{2} \P_{D_l}(x_i)\P_{D_l}(x_j)q^{(l)}(\bar{z}, i, j, e) \\ \times[\Phi(J^{(l)}(\bar{z}, i, j, e)) - \Phi(\bar{z})]\, de,\end{aligned} \qquad (3.14)$$

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

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

the generator (3.14) can be transformed as

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

where

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

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

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

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

$$\tilde{\pi}^{(l)}(\bar{z}) = \sum_{1\le i\ne j\le m} \int_{\mathcal{S}^2} \frac{1}{2}\, \P_{D_l}(x_i)\P_{D_l}(x_j)\tilde{q}^{(l)}(\bar{z}, i, j, e)\, de. \tag{3.18}$$

Then, the process jumps from the state $\bar{z}$ into the state $\tilde{J}^{(l)}(\bar{z}, i, j, e, \eta)$. This means that first the condition on η 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, η are distributed according to the density

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

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

$$p_1^{(l)}(i) = \frac{\sum_{j:i\ne j}\int_{\mathcal{S}^2}(1/2)\P_{D_l}(x_i)\P_{D_l}(x_j)\tilde{q}^{(l)}(\bar{z}, i, j, e)\, de}{\tilde{\pi}^{(l)}(\bar{z})}. \tag{3.19}$$

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

$$p_2^{(l)}(j \mid i) = \frac{\int_{\mathcal{S}^2}\P_{D_l}(x_i)\P_{D_l}(x_j)\tilde{q}^{(l)}(\bar{z}, i, j, e)\, de}{\sum_{j:i\ne j}\int_{\mathcal{S}^2}\P_{D_l}(x_i)\P_{D_l}(x_j)\tilde{q}^{(l)}(\bar{z}, i, j, e)\, de}. \tag{3.20}$$

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

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

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 Δt, 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 examples there is a random weight transfer during the collisions. We assume the collision kernel to be bounded (or truncated), i.e.,

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

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 Lebesque 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 η at the right-hand side of (3.17) takes the form

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

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.,

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

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

$$p_3^{(l)}(e \mid i, j) = 1/4\pi. \tag{3.27}$$

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

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

EXAMPLE 2. Next we consider the functions

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

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 η takes the form

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

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

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

EXAMPLE 3. Finally, we consider the functions

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

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 η takes the form

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

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 η 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

$$(x_1, v_1, g_1), ..., (x_m, v_m, g_m). \tag{3.33}$$

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

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

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

$$c_i = \sum_{j=1}^{k_i} g_{i,j}, \tag{3.35}$$

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

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

and

$$\varepsilon_i^2 = \beta_i - \|\alpha_i\|^2, \tag{3.38}$$

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

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

where

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

and

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

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

$$X_i = \{x_{i,j} : j = 1, ..., k_i\}. \tag{3.42}$$

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

Note the conservation properties in each group,

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

where

$$\mu_i = \sum_{j=1}^{k_i} g_{i,j} \delta_{(x_{i,j}, v_{i,j})},$$

$$\tilde{\mu}_i = \tilde{g}_{i,1} \delta_{(\tilde{x}_{i,1}, \tilde{v}_{i,1})} + \tilde{g}_{i,2} \delta_{(\tilde{x}_{i,2}, \tilde{v}_{i,2})},$$

$$i = 1, ..., \hat{m}.$$

In order to estimate the error caused by the reduction procedure, we consider the bounded Lipschitz metric

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

where

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

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

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

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

We obtain

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

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

$$\begin{aligned}
|\varphi(x, v) - \varphi(\hat{x}, v)| &\le \|x - \hat{x}\| \\
&\le \operatorname{diam}(X_i) \quad \forall x \in X_i, \forall v \in \mathscr{R}^3
\end{aligned}$$

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

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

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

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

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

$$\rho(\mu, \tilde{\mu}) \le 2\sum_{i=1}^{\hat{m}} c_i\varepsilon_i + 2\sum_{i=1}^{\hat{m}} \operatorname{diam}(X_i)c_i. \tag{3.46}$$

Note that

$$\begin{aligned}
c_i^2\varepsilon_i^2 &= \left(\sum_{j=1}^{k_i} g_{i,j}\right)\left(\sum_{j=1}^{k_i} g_{i,j}\|v_{i,j}\|^2\right) - \left\|\sum_{j=1}^{k_i} g_{i,j}v_{i,j}\right\|^2 \\
&= \sum_{j=1}^{k_i} g_{i,j}^2\|v_{i,j}\|^2 + \sum_{1\le j_1<j_2\le k_i} g_{i,j_1}g_{i,j_2}(\|v_{i,j_1}\|^2 + \|v_{i,j_2}\|^2) \\
&\quad - \sum_{j=1}^{k_i} g_{i,j}^2\|v_{i,j}\|^2 - 2\sum_{1\le j_1<j_2\le k_i} g_{i,j_1}g_{i,j_2}(v_{i,j_1}, v_{i,j_2}) \\
&= \sum_{1\le j_1<j_2\le k_i} g_{i,j_1}g_{i,j_2}\|v_{i,j_1} - v_{i,j_2}\|^2.
\end{aligned} \tag{3.47}$$

The right-hand side of (3.46) gives an estimate of the error caused by the reduction step. This error is the sum of the errors made in each group (3.34), which are weighted by the masses c_i of the groups. The errors in each group are determined by two components—the maximum difference of the positions and the weighted differences of the velocities (cf. (3.47)).

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

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

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 κ 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.,

$$f_0(x, v) = \frac{1}{(2\pi RT_0)^{3/2}}\exp\left(-\frac{1}{2RT_0}\|v\|^2\right),$$

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

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

and

$$\begin{aligned}
T(t, x) = \frac{1}{3Rd(t, x)}&\left[\int_{\mathscr{R}^3}\|v\|^2 f(t, x, v)\,dv\right. \\
&\left. - \left\|\frac{1}{d(t, x)}\int_{\mathscr{R}^3} vf(t, x, v)\,dv\right\|^2\right].
\end{aligned} \tag{4.2}$$

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), with test functions

$$\varphi_{\alpha,l}(x, v) = \frac{1}{|D_l|}\P_{D_l}(x)\|v\|^\alpha,$$
$$\alpha = 0, 1, 2, \quad l = 1, ..., l_c \quad \text{(cf. (2.15))}.$$

These functionals are approximated by terms of the form (2.9), which are random variables,

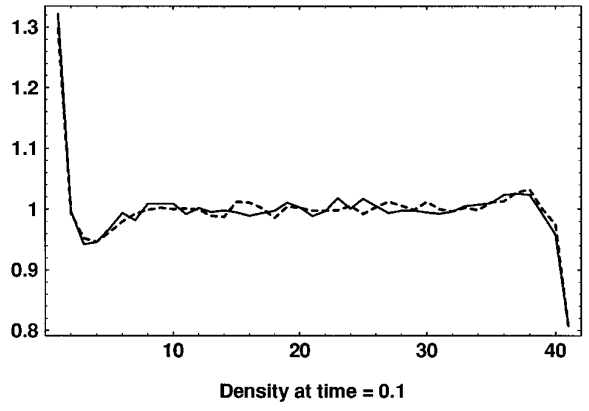

FIGURE 1

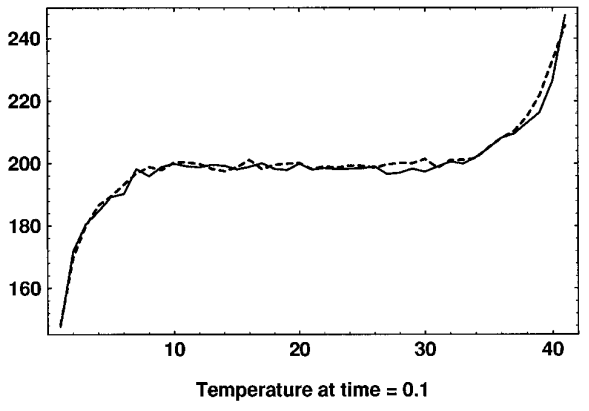

FIGURE 3

$$\xi_{\alpha,l}(t) = \sum_{i=1}^{m(t)} g_i(t)\varphi_{\alpha,l}(x_i(t), v_i(t)). \tag{4.3}$$

In order to estimate the fluctuations of the random variables (4.3), a number N of independent ensembles of particles is generated. The corresponding values of the random variables are denoted by $\xi_{\alpha,l}^{(1)}(t), \ldots, \xi_{\alpha,l}^{(N)}(t)$. Then the empirical mean

$$\frac{1}{N}\sum_{j=1}^{N} \xi_{\alpha,l}^{(j)}(t) \tag{4.4}$$

converges as $N \to \infty$ to the expectation of the random variable (4.3). The statistical fluctuations around this deterministic limit are characterized by the quantity $\sqrt{\mathscr{D}_{\alpha,l}(t)/N}$, where $\mathscr{D}_{\alpha,l}(t)$ denotes the mean square deviation of the random variable (4.3) from its expectation. The order of convergence of the fluctuations is $1/\sqrt{N}$. However, the actual values depend strongly on the factor $\mathscr{D}_{\alpha,l}(t)$.

The spatial domain [0, 1] is divided into $l_c = 41$ cells D_l 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 $T_{\text{left}} = 100$ at the left plate and $T_{\text{right}} = 300$ 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., $1/\sqrt{2RT_0}$.

An averaging over $N = 100$ independent runs of the algorithm was performed (cf. (4.4)). The bounds for the fluctuations are at a level of about 5% of the expected values for both algorithms; i.e., the confidence intervals (corresponding to the confidence level 0.99) have a length of 0.05 in our figures. We decided not to display the confidence intervals in order not to overload the figures.

The results of the calculations are shown in Figs. 1–4. The dashed lines represent the results for the stochastic weighted particle method (cf. Example 2), while the solid

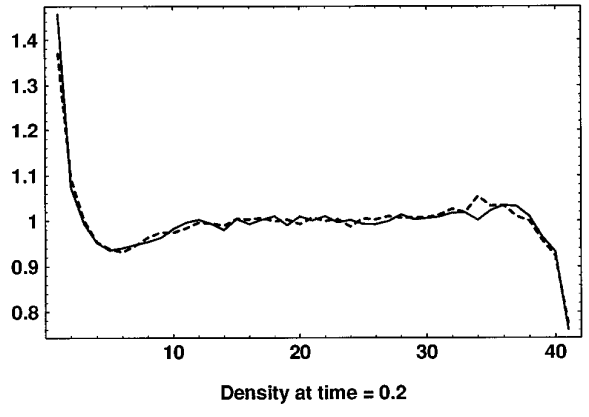

FIGURE 2

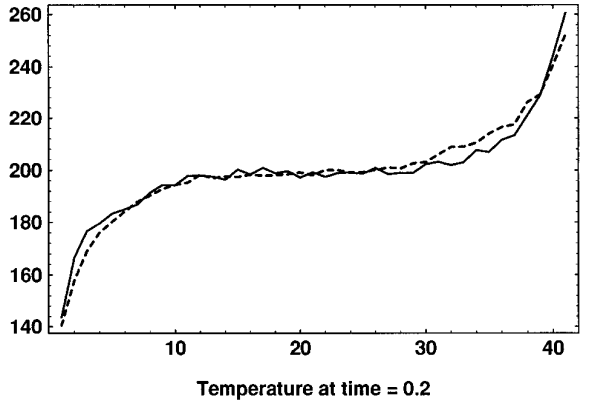

FIGURE 4

lines represent the results obtained with the standard DSMC method (cf. Example 1).

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 blowup of the system. This idea can be interpreted in the following sense. Particles in a numerical procedure should be considered as test particles rather than physical particles. They represent quite big ensembles of real particles. From this point of view, it is natural that a collision causes a change of velocities only for a part of the big ensemble. This part is determined by an appropriate weighting factor.

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 algorithm 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 check the method in such applications, where the additional degrees of freedom turn out to be useful. The weighting factor G is a very general function (cf. the conditions (3.4) and (3.8)). In particular, the collision simulation procedure may depend on the spatial coordinates, on the velocities of the colliding particles, and even on the direction parameter e that determines the postcollision velocities (cf. (3.13)). Thus, it becomes 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. The investigation of such test cases will be the main subject of future work.

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