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Stochastic models and Monte Carlo algorithms for Boltzmann type equations

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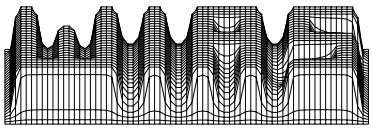

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Abstract

In this paper we are concerned with three typical aspects of the Monte Carlo approach. First there is a certain field of application, namely physical systems described by the Boltzmann equation. Then some class of stochastic models is introduced and its relation to the equation is studied using probability theory. Finally Monte Carlo algorithms based on those models are constructed. Here numerical issues like efficiency and error estimates are taken into account. In Section 1 we recall some basic facts from the kinetic theory of gases, introduce the Boltzmann equation and discuss some applications. Section 2 is devoted to the study of stochastic particle systems related to the Boltzmann equation. The main interest is in the convergence of the system (when the number of particles increases) to the solution of the equation in an appropriate sense. In Section 3 we introduce a modification of the standard "direct simulation Monte Carlo" method, which allows us to tackle the problem of variance reduction. Results of some numerical experiments are presented.

Contents

1. Kinetic theory and Boltzmann equation **1**

2. Stochastic models and convergence **3**

3. Numerical algorithms **10**

References **20**

1. Kinetic theory and Boltzmann equation

Kinetic theory describes a gas as a system of many particles (molecules) performing a chaotic motion. Particles interact through binary collisions, during which the two involved particles change their velocities. It is assumed that momentum and energy are conserved so that the pre-collisional velocities v, w and the post-collisional velocities v^*, w^* are coupled via the relations

$$v^* + w^* = v + w\,, \qquad \|v^*\|^2 + \|w^*\|^2 = \|v\|^2 + \|w\|^2\,. \tag{1}$$

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Since the number of gas molecules is huge (10^{19} per cm^3 at standard conditions), it would be impossible to study the behaviour of each individual molecule. Instead a statistical description is used – some function $f(t,x,v)$ representing the relative amount of gas particles at time t having a position close to x and a velocity close to v. The basis for this statistical theory was provided in the second half of the 19th century. James Clerk Maxwell (1831-1879) found the distribution function of the gas molecule velocities in thermal equilibrium,

$$f_{eq}(v) = \frac{1}{[2\pi\, T]^{3/2}} \exp\left(-\frac{\|v\|^2}{2\,T}\right), \qquad v \in \mathcal{R}^3\,. \tag{2}$$

The number T corresponds to the temperature of the gas. Ludwig Boltzmann (1844-1906) studied the problem if a gas starting from any initial state reaches the Maxwellian distribution (2). In [Bol72] he established the equation

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

governing the time evolution of the distribution function

$$f(t,x,v)\,, \qquad t \geq 0\,, \quad x \in D \subset \mathcal{R}^3\,, \quad v \in \mathcal{R}^3\,.$$

Here ∇ denotes the vector of partial derivatives, $(\,.\,,\,.\,)$ is the scalar product and $\mathcal{S}^2$ is the unit sphere in $\mathcal{R}^3$. The collision transformation

$$\begin{aligned} v^* &= v^*(v,w,e) = v + e\,(e, w-v)\,, \\ w^* &= w^*(v,w,e) = w + e\,(e, v-w) \end{aligned} \tag{4}$$

satisfies (1). The collision kernel B is determined by the interaction potential between molecules. For the hard sphere model (billiard collisions) it takes the form

$$B(v,w,e) = c\,|(v-w,e)|\,, \qquad \text{for some} \quad c > 0\,.$$

The classical Boltzmann equation (3) is used in such applications, where the mean free path (the average distance between subsequent collisions of molecules) is not negligible compared to the characteristic length scale of the problem. This means that either the mean free path is large, or the characteristic length is tiny.

A typical example with large mean free path is the reentry of a space shuttle into the atmosphere. Above an altitude of about $120\,km$, the mean free path is larger than $1\,m$ and collisions between gas molecules can be neglected (free molecular flow). Below an altitude of about $70\,km$, the mean free path is smaller than $1\,mm$ and local equilibria are reached due to the huge number of collisions. The distribution function takes the form

$$f(t,x,v) = \frac{\varrho(t,x)}{[2\pi\, T(t,x)]^{3/2}} \exp\left(-\frac{\|v - U(t,x)\|^2}{2\,T(t,x)}\right),$$

where

$$\begin{aligned} \varrho(t,x) &= \int_{\mathcal{R}^3} f(t,x,v)\,dv\,, \\ U(t,x) &= \frac{1}{\varrho(t,x)} \int_{\mathcal{R}^3} v\, f(t,x,v)\,dv\,, \\ T(t,x) &= \frac{1}{3\,\varrho(t,x)} \int_{\mathcal{R}^3} \|v - U(t,x)\|^2\, f(t,x,v)\,dv \end{aligned}$$

are the local density, bulk velocity and temperature. The time evolution of these macroscopic quantities is determined by the fluid dynamics equations. Instead of finding one function of seven variables one has to find five functions of four variables each, which is much easier. Between the free molecular regime and the fluid dynamics regime the Boltzmann equation is relevant. Its solution delivers the necessary input information for the fluid dynamics equations. Another field of application, where the mean free path is large, is vacuum technology (e.g., material processing via vapour deposition).

However, there are also applications in our common environment. At standard atmospheric pressure and temperature $25^0\,C$, the mean free path of an oxygen molecule is about $50\,nm$. The molecule travels at an average velocity of about $500\,m/s$ suffering about 10^{10} collisions per second. Its diameter is about $0.3\,nm$ so that it travels a distance of 150 times its diameter between collisions. Applications with a tiny characteristic length scale are engineering of micro-electro-mechanical systems (MEMS) or calculating the flows in a disc drive (read/write head floats less than $50\,nm$ above the surface of the spinning platter).

The physical values mentioned above are only rough estimates, but they illustrate the qualitative picture. We refer to [Cer88], [CIP94] concerning the theory of the Boltzmann equation, and to [Cer98] concerning the history of kinetic theory.

2. Stochastic models and convergence

In this section some sketch of the history of the subject is given. Stochastic models for the Boltzmann equation are based on systems of particles imitating the behaviour of the gas molecules in a probabilistic way. The main interest is in proving rigorously the convergence of the system (when the number of particles increases) to the solution of the equation in an appropriate sense.

We consider a stochastic particle system

$$Z^{(n)}(t) = \Big(x_1(t), v_1(t); \ldots; x_n(t), v_n(t)\Big), \qquad t \geq 0\,, \tag{5}$$

determined by an infinitesimal generator of the form

$$\begin{aligned} \mathcal{A}^{(n)}(\Phi)(z) = \sum_{i=1}^{n} (v_i, \nabla_{x_i})(\Phi)(z) + \\ \frac{1}{2\,n} \sum_{1 \leq i \neq j \leq n} \int_{\mathcal{S}^2} \Big[\Phi(J(z,i,j,e)) - \Phi(z)\Big]\, q^{(n)}(x_i, v_i, x_j, v_j, e)\,de\,, \end{aligned} \tag{6}$$

where Φ is an appropriate test function,

$$z = (x_1, v_1; \ldots; x_n, v_n)\,, \qquad x_i, v_i \in \mathcal{R}^3\,, \quad i = 1, \ldots, n\,,$$

$q^{(n)}$ is an intensity function and

$$[J(z,i,j,e)]_k = \begin{cases} (x_k, v_k) & , \quad \text{if} \quad k \neq i,j\,, \\ (x_i, v_i + e\big(e, v_j - v_i\big)) & , \quad \text{if} \quad k = i\,, \\ (x_j, v_j + e\big(e, v_i - v_j\big)) & , \quad \text{if} \quad k = j\,, \end{cases} \tag{7}$$

is the jump transformation. Here we assume $D = \mathcal{R}^3$ so that no boundary conditions are involved. We recall the pathwise behaviour of the system (5), which is a piecewise-deterministic process in the sense of [Dav93, Section 2]. Starting at z the process moves according to the free flow, i.e.

$$Z^{(n)}(t) = \Big(x_1 + t\,v_1, v_1; \ldots; x_n + t\,v_n, v_n\Big),$$

until a random jump time τ_1 is reached. The probability distribution of this time is determined by

$$\text{Prob}(\tau_1 > t) = \exp\left(-\int_0^t \lambda^{(n)}(Z^{(n)}(s))\,ds\right), \qquad t \geq 0\,,$$

where

$$\lambda^{(n)}(z) = \frac{1}{2\,n} \sum_{1 \leq i \neq j \leq n} \int_{S^2} q^{(n)}(x_i, v_i, x_j, v_j, e)\,de\,. \tag{8}$$

At the random time τ_1 the process jumps into a state z_1, which is obtained from the state $z' = (x_1', v_1'; \ldots; x_n', v_n')$ of the process just before the jump by a two-particle interaction. Namely, two indices i, j and a direction vector e are chosen according to the probability density

$$\frac{q^{(n)}(x_i', v_i', x_j', v_j', e)}{2\,n\,\lambda^{(n)}(z')} \tag{9}$$

and the velocities v_i', v_j' are replaced using the collision transformation (4).

The study of the relationship between the process (5) and the Boltzmann equation (3) was started by M. A. Leontovich (1903-1981) in the paper [Leo35] in 1935. Note that a version of Kolmogorov's forward equation for a Markov process with density p and generator $\mathcal{A}$ reads

$$\frac{\partial}{\partial t}\,p(t,z) = \mathcal{A}^*\,p(t,z)\,. \tag{10}$$

Let $p^{(n)}(t,z)$ denote the n–particle distribution function of the process (5). Applying properties of the collision transformation (4) and some symmetry assumption on

$q^{(n)}$, one obtains from (10) the equation

$$\frac{\partial}{\partial t}\, p^{(n)}(t,z) + \sum_{i=1}^{n} \left(v_i, \nabla_{x_i}\right) p^{(n)}(t,z) = \tag{11}$$
$$\frac{1}{2\,n} \sum_{1\le i\ne j\le n} \int_{S^2} \Big[p^{(n)}(t, J(z,i,j,e)) - p^{(n)}(t,z)\Big] q^{(n)}(x_i, v_i, x_j, v_j, e)\, de\,.$$

Using the method of generating functions, Leontovich first studied the cases of "monomolecular processes" (independent particles) and of "bimolecular processes" with discrete states (e.g., a finite number of velocities). Under some assumptions on the initial state, he showed that the expectations of the relative numbers of particles in the bimolecular scheme asymptotically (as $n \to \infty$) solve the corresponding deterministic equation. In the case of the full Boltzmann equation the stochastic process was described via (11) (even including a boundary condition of specular reflection). Concerning the asymptotic behaviour of the process, Leontovich pointed out the following. Let $p_k^{(n)}$ denote the marginal distributions corresponding to the density $p^{(n)}$. If

$$\lim_{n\to\infty}\, p_2^{(n)}(t, x_1, v_1, x_2, v_2) = \lim_{n\to\infty}\, p_1^{(n)}(t, x_1, v_1) \lim_{n\to\infty}\, p_1^{(n)}(t, x_2, v_2)$$

and

$$\lim_{n\to\infty}\, q^{(n)}(x, v, y, w, e) = \delta(x-y)\, B(v, w, e)\,, \tag{12}$$

where δ denotes Dirac's delta–function, then the function

$$f(t,x,v) = \lim_{n\to\infty}\, p_1^{(n)}(t,x,v) \tag{13}$$

solves the Boltzmann equation. Leontovich noted that he was not able to prove a limit theorem in analogy with the discrete case, though he strongly believes that such theorem holds.

For example, (12) is satisfied for the choice

$$q^{(n)}(x, v, y, w, e) = h^{(n)}(x, y)\, B(v, w, e) \tag{14}$$

and

$$h^{(n)}(x,y) = \begin{cases} c_n^{-1}\,, & \text{if} \quad \|x-y\| \le \varepsilon^{(n)}\,, \\ 0 \quad , & \text{otherwise}\,, \end{cases}$$

where c_n is the volume of the ball of radius $\varepsilon^{(n)} \to 0$. In this case, according to (9), only those particles can collide which are closer to each other than the interaction distance $\varepsilon^{(n)}$.

Independently, the problem was tackled by M. Kac (1914-1984) in the paper [Kac56a] in 1956. Considering the spatially homogeneous Boltzmann equation

$$\frac{\partial}{\partial t}\, f(t,v) = \int_{R^3} \int_{S^2} B(v,w,e) \times \tag{15}$$
$$\Big[f(t, v^*(v,w,e))\, f(t, w^*(v,w,e)) - f(t,v)\, f(t,w)\Big]\, de\, dw$$

Kac introduced a process

$$Z^{(n)}(t) = \Big(v_1(t), \dots, v_n(t)\Big), \qquad t \geq 0\,, \tag{16}$$

governed by the Kolmogorov equation

$$\frac{\partial}{\partial t}\, p^{(n)}(t,z) = \tag{17}$$
$$\frac{1}{2\,n} \sum_{1 \leq i \neq j \leq n} \int_{S^2} \Big[p^{(n)}(t, J(z,i,j,e)) - p^{(n)}(t,z)\Big]\, B(v_i, v_j, e)\, de\,,$$

where $z = (v_1, \dots, v_n)$ and J is appropriately adapted, compared to (7). He studied its asymptotic behaviour and proved (in a simplified situation) that $\lim_{n\to\infty} p_1^{(n)}$ satisfies the Boltzmann equation. We cite from p.175 (using our notations): "To get (15) one must only assume that

$$p_2^{(n)}(t, v, w) \sim p_1^{(n)}(t, v)\, p_1^{(n)}(t, w)$$

for all v, w in the allowable range. One is immediately faced with the difficulty that since $p^{(n)}(t,z)$ is uniquely determined by $p^{(n)}(0,z)$ no additional assumptions on $p^{(n)}(t,z)$ can be made unless they can be deduced from some postulated properties of $p^{(n)}(0,z)$. A moment's reflection will convince us that in order to derive (15) the following theorem must first be proved.

BASIC THEOREM Let $p^{(n)}(t,z)$ be a sequence of probability density functions ... having the "Boltzmann property"

$$\lim_{n\to\infty} p_k^{(n)}(0, v_1, \dots, v_k) = \prod_{i=1}^{k} \lim_{n\to\infty} p_1^{(n)}(0, v_i)\,. \tag{18}$$

Then $p^{(n)}(t,z)$ [that is, solutions of (17)] also have the "Boltzmann property":

$$\lim_{n\to\infty} p_k^{(n)}(t, v_1, \dots, v_k) = \prod_{i=1}^{k} \lim_{n\to\infty} p_1^{(n)}(t, v_i)\,. \tag{19}$$

In other words, the Boltzmann property propagates in time!" Kac calls equation (17) **master equation** referring to the paper [NLU40].

The two books [Kac56b] and [Kac59] contain more material related to the stochastic approach to the Boltzmann equation. In [Kac56b] the factorization property (19) is called "chaos property" (indicating asymptotic independence), and the statement of the basic theorem is called **propagation of chaos**. The following remark is made in [Kac59, p.131]: "The primary disadvantage of the master equation approach ... lies in the difficulty (if not impossibility!) of extending it to the nonspatially uniform case." Research in the field of stochastic particle systems related to the Boltzmann equation was restricted to the **spatially homogeneous** case during a long period after the paper [Kac56a]. We refer to [McK66], [McK75], [Grü71], [Pic72], [Tan73],

[Tan78], [Tan83], [Mur77], [Szn82], [Szn84], [Szn91], [Smi89], [HK90]. It turns out (cf., e.g., [Tan83], [Szn84], [Uch87]) that the chaos property (18) (i.e., the asymptotic factorization) is equivalent to the convergence in distribution of the **empirical measures** (cf. (16))

$$\mu^{(n)}(t, dv) = \frac{1}{n} \sum_{i=1}^{n} \delta_{v_i(t)}(dv) \tag{20}$$

to a deterministic limit. The objects (20) are considered as random variables with values in the space of measures on the state space of a single particle. Thus, the basic theorem can be reformulated as the propagation of convergence of empirical measures. In this setup, it is natural to study convergence not only for fixed t, but also in the space of measure–valued functions of t (functional law of large numbers).

The **spatially inhomogeneous** case was treated by C. Cercignani in the paper [Cer83] in 1983. He considered a system of "soft spheres", where "molecules collide at distances randomly given by a probability distribution", and proved propagation of chaos (modulo a uniqueness theorem). The limiting equation is the so-called mollified Boltzmann equation (cf. [Cer88, Section VIII.3])

$$\begin{aligned} &\frac{\partial}{\partial t} f(t,x,v) + (v, \nabla_x) f(t,x,v) = \\ &\quad \int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} h(x,y)\, B(v,w,e) \times \\ &\quad \Big[f(t,x,v^*(v,w,e))\, f(t,y,w^*(v,w,e)) - f(t,x,v)\, f(t,y,w) \Big] de\, dw\, dy\,. \end{aligned} \tag{21}$$

This equation was introduced in [Mor55] and reduces formally to the Boltzmann equation (3) if the "mollifier" h is a delta-function.

A more general approach was developed by A.V. Skorokhod in the book [Sko83] published in 1983. In Chapter 2 he considered a Markov process

$$Z^{(n)}(t) = \Big(Z_1(t), \ldots, Z_n(t) \Big), \qquad t \geq 0\,,$$

(describing it via stochastic differential equations with respect to Poisson measures) with the generator

$$\begin{aligned} \mathcal{A}^{(n)}(\Phi)(z) \;\; = \;\; & \sum_{i=1}^{n} (b(z_i), \nabla_{z_i})(\Phi)(z) + \\ & \frac{1}{2n} \sum_{1 \leq i \neq j \leq n} \int_{\Theta} \Big[\Phi(J(z,i,j,\vartheta)) - \Phi(z) \Big]\, \pi(d\vartheta)\,, \end{aligned}$$

where Φ is an appropriate test function, $z = (z_1, \ldots, z_n) \in \mathcal{Z}^n$, and

$$[J(z,i,j,e)]_k = \begin{cases} z_k & \text{, if} \quad k \neq i,j\,, \\ z_i + a(z_i, z_j, \vartheta)\,, & \text{if} \quad k = i\,, \\ z_j + a(z_j, z_i, \vartheta)\,, & \text{if} \quad k = j\,. \end{cases}$$

The symbol $\mathcal{Z}$ denotes the state space of a single particle, π is a measure on a parameter set Θ, and a is a function on $\mathcal{Z} \times \mathcal{Z} \times \Theta$. This model is more general than the Leontovich model (6), (7), as far as the gradient terms and the jump transformation J are concerned. However, the distribution π of the jump parameter ϑ does not depend on the state z. It was proved that the corresponding empirical measures (cf. (20)) converge (for any t) to a deterministic limit $F(t)$ which satisfies the equation

$$\frac{d}{dt}\int_{\mathcal{Z}} \varphi(z)\, F(t,dz) = \int_{\mathcal{Z}} (b(z),\nabla_z)(\varphi)(z)\, F(t,dz) + \int_{\mathcal{Z}}\int_{\mathcal{Z}} \left\{ \int_{\Theta} \Big[\varphi(z_1 + a(z_1,z_2,\vartheta)) - \varphi(z_1)\Big]\, \pi(d\vartheta) \right\} F(t,dz_1)\, F(t,dz_2)\,,$$

for appropriate test functions φ.

Further references concerning the spatially inhomogeneous case are [Fun86], [Ars88], [NT89], [Luk89], [LP90], [BFGR94], [Wag94a], [Wag96], [GM97]. Developing the stochastic approach to the Boltzmann equation, systems with a general binary interaction between particles and a general (Markovian) single particle evolution (including spatial motion) were considered. Results concerning the approximation of the solution to the corresponding nonlinear kinetic equation by the particle system were obtained in the case of bounded intensities, thus being restricted to the mollified Boltzmann equation (21). Partial results concerning the non-mollified case are contained in [CP95] (one-dimensional model), [Rez96a], [Rez96b], [RT97] (discrete velocities), [Mel98] (small initial data).

Finally we mention a result from [CPW98] concerning **convergence in the stationary case**. In many applications studying the equilibrium behaviour of gas flows is of primary interest. To this end, time averaging over trajectories of the corresponding particle system is used,

$$\frac{1}{k}\sum_{j=1}^{k}\left[\frac{1}{n}\sum_{i=1}^{n}\varphi(x_i(t_j),v_i(t_j))\right], \qquad t_j = \bar{t} + j\,\Delta t\,,$$

where φ is some test function and $\bar{t}$ is the starting time for averaging. To justify this procedure (for $k \to \infty$), one has to study the connection between the stationary density of the process and the stationary Boltzmann equation. From the results mentioned above one can obtain information about the limit $\lim_{t\to\infty}\lim_{n\to\infty} p_1^{(n)}(t,x,v)$ while here one is interested in the limit $\lim_{n\to\infty}\lim_{t\to\infty} p_1^{(n)}(t,x,v)$. The identity of both quantities is not at all obvious.

Before formulating the convergence theorem, we recall some facts concerning **boundary conditions** for the Boltzmann equation. A rather general form is

$$f(t,x,v')\,(v',n(x)) = \int_{\{(v,n(x))<0\}} R(x,v,v')\, f(t,x,v)\, |(v,n(x))|\, dv\,,$$

for all $x \in \partial D$ and $v' : (v',n(x)) > 0$, where $n(x)$ denotes the unit inner normal at the point x of the boundary ∂D. The reflection density R, which determines the

behaviour of particles hitting the boundary, is assumed to satisfy

$$\int_{\{(v',n(x))>0\}} R(x,v,v')\,dv' = 1\,, \qquad v\,:\,(v,n(x)) < 0\,.$$

The so-called "Maxwell boundary condition" is obtained for the choice

$$\begin{aligned} R(x,v,v') \;&=\; (1-\alpha)\,\delta(v-v'+2\,n(x)\,(n(x),v')) + \\ &\qquad \alpha\,\frac{1}{2\pi\,[T_b(x)]^2}\exp\left(-\frac{\|v'\|^2}{2\,T_b(x)}\right)(v',n(x))\,, \end{aligned}$$

where $\alpha \in [0,1]$ and $T_b(x)$ is the temperature of the wall. The special case $\alpha = 0$ corresponds to specular reflection,

$$f(t,x,v') = f(t,x,v'-2\,n(x)\,(n(x),v'))\,.$$

The special case $\alpha = 1$ corresponds to diffuse reflection (or complete accommodation),

$$\begin{aligned} &f(t,x,v') = \\ &\quad \frac{1}{2\pi\,[T_b(x)]^2}\exp\left(-\frac{\|v'\|^2}{2\,T_b(x)}\right)\int_{\{(v,n(x))<0\}} f(t,x,v)\,|(v,n(x))|\,dv\,. \end{aligned}$$

Consider the (mollified) stationary Boltzmann equation

$$\begin{aligned} (v,\nabla_x)\,\bar f(x,v) = \varepsilon\int_D\int_{\mathcal{R}^3}\int_{\mathcal{S}^2} h(x,y)\,B(v,w,e)\times \qquad (22)\\ \Big[\bar f(x,v^*(v,w,e))\,\bar f(y,w^*(v,w,e)) - \bar f(x,v)\,\bar f(y,w)\Big]\,de\,dw\,dy\,, \end{aligned}$$

with the boundary condition of "diffuse reflection", and introduce the notation

$$\bar f_k(x_1,v_1,\ldots,x_k,v_k) = \prod_{i=1}^k \bar f(x_i,v_i)\,.$$

Consider the stationary density $\bar p^{(n)}$ of the corresponding n-particle process and the marginals

$$\bar p_k^{(n)}(x_1,v_1,\ldots,x_k,v_k)\,.$$

Then the following result holds.

THEOREM [CPW98, Theorem 2.5] There exists $\varepsilon_0 > 0$ such that

$$\|\bar p_k^{(n)} - \bar f_k\|_{L_1} \;\le\; \frac{c^k}{n}\,, \qquad \forall\; n > k\,,$$

for any $0 < \varepsilon \le \varepsilon_0$ and $k = 1,2,\ldots$, where c does not depend on ε, k, n.

Note that, beside the asymptotic factorization itself, one obtains even an order of convergence. The main restriction, the smallness of the right-hand side of the Boltzmann equation (22), is due to the fact that in the proof a perturbation technique is applied to the collision-less situation. Further assumptions concern the domain D (smooth, convex, bounded), the collision kernel B (bounded) and some cut-off of small velocities.

3. Numerical algorithms

This section is devoted to algorithmic and numerical aspects. Since the dimensionality of the Boltzmann equation is high (time, space, velocity), its numerical treatment is a typical application field of Monte Carlo algorithms. We discuss the "direct simulation Monte Carlo" (or DSMC) algorithm and its recently developed generalization called stochastic weighted particle method (SWPM). The new method contains several degrees of freedom which are used for the purpose of variance reduction. A convergence theorem for SWPM is presented, and some results of numerical experiments are given.

DSMC is presently the most widely used numerical algorithm in kinetic theory. The method goes back to the papers [Bir63] (homogeneous gas relaxation problem) and [Bir65] (shock structure problem) by G.A. Bird. We refer to [Bir76] and [Bir94] (e.g., Sections 9.4, 11.1) concerning remarks on the historical development. The history of the subject is also well reflected in the proceedings of the bi-annual conferences on "Rarefied Gas Dynamics" ranging from 1960 [RGD60] to the present [RGD01]. The method is based on the process (5) but includes several numerically motivated modifications.

Independent motion (free flow) of the particles and their pairwise interactions (collisions) are separated using a splitting procedure with a time increment Δt. During the **free flow step**, particles move according to their velocities,

$$x_i(t+\Delta t) = x_i(t) + \int_t^{t+\Delta t} v_i(s)\, ds\,, \qquad i = 1, \ldots, n\,,$$

and do not collide. At this step boundary conditions are taken into account.

During the **collision step**, particles do not change their positions. At this step some partition

$$D = \cup_{l=1}^{l_c} D_l$$

of the spatial domain into a finite number l_c of disjoint cells is introduced. Using a mollifying function of the form

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

where $|.|$ denotes the volume and χ is the indicator function, leads to a decoupling of collision processes in different cells. The cell process is determined by the generator (cf. (6), (14))

$$\mathcal{A}_l^{(n)}(\Phi)(z) = \qquad (23)$$
$$\frac{1}{2\,n\,|D_l|} \sum_{i\neq j\,:\,x_i,x_j\in D_l} \int_{S^2} \Big[\Phi(J(z,i,j,e)) - \Phi(z)\Big]\, B(v_i,v_j,e)\, de\,.$$

The parameter of the waiting time between jumps takes the form (cf. (8))

$$\lambda_l^{(n)}(z) = \frac{1}{2\,n\,|D_l|} \sum_{i\neq j\,:\,x_i,x_j\in D_l} \int_{\mathcal{S}^2} B(v_i, v_j, e)\, de\,.$$

The jump consists in choosing two indices i, j (of particles with positions in the cell D_l) and a direction vector e (from the unit sphere $\mathcal{S}^2$) according to the probability density (cf. (9))

$$\frac{B(v_i, v_j, e)}{2\,n\,|D_l|\,\lambda_l^{(n)}(z)}$$

and replacing the velocities v_i, v_j by $v^*(v_i, v_j, e), w^*(v_i, v_j, e)$ according to (4).

A third numerically motivated modification (beside splitting and cell structure) is the introduction of **fictitious collisions**. Note that the generator (23) can be written in the form

$$\mathcal{A}_l^{(n)}(\Phi)(z) = \frac{1}{2\,n\,|D_l|} \sum_{i\neq j\,:\,x_i,x_j\in D_l} \left\{ \int_{\mathcal{S}^2} \Big[\Phi(J(z,i,j,e)) - \Phi(z)\Big]\, B(v_i, v_j, e)\, de + \Big[\Phi(z) - \Phi(z)\Big] \left[\hat{B} - \int_{\mathcal{S}^2} B(v_i, v_j, e)\, de\right] \right\},$$

where

$$\int_{\mathcal{S}^2} B(v_i, v_j, e)\, de \le \hat{B}\,, \qquad \text{for some} \quad \hat{B} > 0\,.$$

This suggests an alternative way of generating trajectories of the process. The waiting time parameter is

$$\hat{\lambda}_l^{(n)}(z) = \frac{1}{2\,n\,|D_l|} \sum_{i\neq j\,:\,x_i,x_j\in D_l} \hat{B} = \frac{\hat{B}\,n_l\,(n_l-1)}{2\,n\,|D_l|}\,,$$

where n_l denotes the number of particles in the cell D_l. Indices i, j are chosen uniformly among particles belonging to the cell. With probability

$$1 - \frac{\int_{\mathcal{S}^2} B(v_i, v_j, e)\, de}{\hat{B}}$$

the process does not change, i.e. performs a fictitious jump. With the remaining probability, a random vector e is chosen according to the density

$$\frac{B(v_i, v_j, e)}{\int_{\mathcal{S}^2} B(v_i, v_j, e)\, de}$$

and the two collision partners change their velocities according to (4).

The idea of fictitious collisions is applicable in general situations (cf. [EK86, Section 4.2]). In the context of the Boltzmann equation it has been introduced under different names in [Kou86] (null-collision technique), [IR88] (majorant frequency scheme), [Bir89] (no time counter scheme). The interest in studying the connection between stochastic simulation procedures in rarefied gas dynamics and the Boltzmann equation was stimulated by K. Nanbu's paper [Nan80] (cf. the survey papers [Nan83], [Nan86], [IN87]). Starting from the Boltzmann equation, the author derived a method that, however, suffered from certain deficiencies (quadratic effort in the number of particles, conservation of momentum and energy only on average). Later Nanbu's original method was considerably improved (cf. [Bab86], [Plo87], [Bab89]) so that it did successfully work in applications like the reentry problem (cf. [NGS91], [NS95], [NKS96], [Bab98]). Convergence for the Nanbu scheme and its modifications was studied in [Bab89] (spatially homogeneous case) and [BI89] (spatially inhomogeneous case). Convergence for Bird's scheme (with the original time counter) was proved in [Wag92]. Among the numerous russian sources on stochastic algorithms for the Boltzmann equation we mention papers related to the Leontovich-Kac-process ([BY75a], [BY75b], [Kon86], [Khi86], [IR89], [IR90]), papers using branching processes ([ENS84], [EM87]) and papers following the Skorokhod approach through stochastic differential equations with respect to Poisson measures ([Ars87], [LS89]). Modifications of DSMC related to dense gases were introduced in [AGA95], [AGA97]. The corresponding limiting equation was found in [GW00].

A basic problem in many applications of DSMC (e.g., flows with high density gradients, or low Mach number flows) are large statistical fluctuations so that variance reduction is a challenging task. To this end, a modification of DSMC called **stochastic weighted particle method** (SWPM) was proposed in [RW96]. In SWPM a system of weighted particles is used, which allows one to resolve low density regions with a moderate number of simulation particles (cf. [RW01]). SWPM is based on a partial random weight transfer during collisions, leading to an increase in the number of particles. Therefore appropriate reduction procedures are needed to control that quantity. Various deterministic procedures with different conservation properties were proposed in [RSW98], and some error estimates were found. Further references related to weighted particles are [Sch93] and [Boy96].

Partial convergence results (not including reduction) were obtained in [Wag94b], [RW98]. A convergence proof for SWPM with reduction has recently been proposed in [MW02]. The basic idea was the introduction of new stochastic reduction procedures that, on the one hand, do not possess all conservation properties of the deterministic procedures, but, on the other hand, have the correct expectation for a much larger class of functionals. This idea is quite natural in the context of stochastic particle methods. Here we formulate an improved version of the convergence theorem, which includes the case of deterministic reduction. The proof, which is rather extensive, will be presented elsewhere.

The main modification in SWPM (compared to DSMC) concerns the collision simulation. During this step, the particle system approximates the solution of the spatially homogeneous Boltzmann equation (15). So we restrict our considerations

to that case. We introduce a family of Markov processes

$$Z^{(n)}(t) = \Big((v_i^{(n)}(t), g_i^{(n)}(t)) \,, \quad i = 1, \ldots, m^{(n)}(t) \Big), \qquad t \geq 0 \,, \tag{24}$$

and study its asymptotic behaviour as $n \to \infty$. The process (24) has the **state space**

$$\mathcal{Z}^{(n)} \;=\; \left\{ z \in \mathcal{Z} \,:\; \sum_{i=1}^{m} g_i \leq C_\mu \,, \quad \max_{i=1,\ldots,m} g_i \leq g_{\max}(n) \right\}, \tag{25}$$

where

$$\begin{aligned} \mathcal{Z} \;=\; \Big\{ & \Big(m; (g_1, v_1), \ldots, (g_m, v_m) \Big) : \\ & m = 0, 1, 2, \ldots \,, \qquad g_i > 0 \,,\; v_i \in \mathcal{R}^3 \,, \quad i = 1, \ldots, m \Big\}. \end{aligned}$$

Here $C_\mu > 0$ is some bound for the mass in the system, and $g_{\max}(n) > 0$ is some bound for the individual particle weights.

The **time evolution** of the process is determined by the generator

$$\mathcal{A}^{(n)}(\Phi)(z) = \int_{\mathcal{Z}^{(n)}} [\Phi(\tilde{z}) - \Phi(z)] \, Q^{(n)}(z, d\tilde{z}) \,, \qquad z \in \mathcal{Z}^{(n)} \,,$$

where Φ is an appropriate test function and

$$Q^{(n)}(z, d\tilde{z}) = \begin{cases} Q_{\text{coll}}(z; d\tilde{z}) \,, & \text{if} \quad m \leq m_{\max}(n) \,, \\ Q_{\text{red}}^{(n)}(z; d\tilde{z}) \,, & \text{otherwise.} \end{cases} \tag{26}$$

Here $m_{\max}(n) > 0$ is some particle number bound indicating reduction. The transition measure, corresponding to **collision jumps**, is

$$Q_{\text{coll}}(z; d\tilde{z}) = \frac{1}{2} \sum_{1 \leq i \neq j \leq m} \int_{\mathcal{S}^2} \delta_{J_{\text{coll}}(z;i,j,e)}(d\tilde{z}) \, p_{\text{coll}}(z; i, j, e) \, de \,, \tag{27}$$

with the jump transformation (cf. (4))

$$[J_{\text{coll}}(z; i, j, e)]_k =$$
$$\begin{cases} (v_k, g_k) & , \quad \text{if} \quad k \leq m \,,\; k \neq i, j \,, \\ (v^*(v_i, v_j, e), \gamma_{\text{coll}}(z; i, j, e)) & , \quad \text{if} \quad k = i \,, \\ (w^*(v_i, v_j, e), \gamma_{\text{coll}}(z; i, j, e)) & , \quad \text{if} \quad k = j \,, \\ (v_i, g_i - \gamma_{\text{coll}}(z; i, j, e)) & , \quad \text{if} \quad k = m + 1 \,, \\ (v_j, g_j - \gamma_{\text{coll}}(z; i, j, e)) & , \quad \text{if} \quad k = m + 2 \,. \end{cases}$$

The weight transfer function has the form

$$\gamma_{\text{coll}}(z; i, j, e) = \frac{1}{1 + \kappa(z; i, j, e)} \, \min(g_i, g_j) \,, \tag{28}$$

where the weight transfer parameter satisfies

$$0 \le \kappa(z;i,j,e) \le C_\kappa\,, \qquad \text{for some} \quad C_\kappa > 0\,. \tag{29}$$

Particles with zero weights are removed from the system. The intensity function has the form

$$p_{\rm coll}(z;i,j,e) = (1+\kappa(z;i,j,e))\,\max(g_i,g_j)\,B(v_i,v_j,e)\,.$$

Note that

$$J_{\rm coll}(z;i,j,e) \in \mathcal{Z}^{(n)}\,, \qquad \forall\, z \in \mathcal{Z}^{(n)}\,,\ 1 \le i \ne j \le m\,,\ e \in \mathcal{S}^2\,, \tag{30}$$

since collision jumps are mass-preserving and do not increase the maximum particle weight. The transition measure, corresponding to **reduction jumps**, has the form

$$Q^{(n)}_{\rm red}(z;d\tilde z) = \lambda_{\rm red}(n)\,P^{(n)}_{\rm red}(z;d\tilde z)\,,$$

where $\lambda_{\rm red}(n) > 0$ is some waiting time parameter. The reduction measure is assumed to satisfy

$$P^{(n)}_{\rm red}(z;\mathcal{Z}^{(n)}) = 1\,, \qquad \forall\, z \in \mathcal{Z}^{(n)}\ :\ m > m_{\max}(n)\,, \tag{31}$$

i.e. for all possible starting point of a reduction jump (cf. (26)). It follows from (30), (31) that the process stays in $\mathcal{Z}^{(n)}$, once the initial state belongs to $\mathcal{Z}^{(n)}$. Using (29) and the assumption concerning the collision kernel

$$\int_{\mathcal{S}^2} B(v,w,e)\,de \ \ \le \ \ C_B\,, \tag{32}$$

we obtain (cf. (27), (25))

$$\begin{aligned}
\lambda^{(n)}_{\rm coll}(z) &= Q^{(n)}_{\rm coll}(z,\mathcal{Z}^{(n)}) \\
&= \frac{1}{2}\sum_{1\le i\ne j\le m}\int_{\mathcal{S}^2}[1+\kappa(z;i,j,e)]\,\max(g_i,g_j)\,B(v_i,v_j,e)\,de \\
&\le (1+C_\kappa)\,C_B\,m\sum_{i=1}^m g_i \le (1+C_\kappa)\,C_B\,C_\mu\,m_{\max}(n)\,.
\end{aligned}$$

Thus, the generator $\mathcal{A}^{(n)}$ is bounded, for any fixed n.

We consider the bounded Lipschitz metric as a distance between two measures ν_1 and ν_2 defined as

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

where

$$\|\varphi\|_L = \max\left\{\|\varphi\|_\infty\,;\ \sup_{v\ne w\in\mathcal{R}^3}\frac{|\varphi(v)-\varphi(w)|}{\|v-w\|}\right\}$$

and

$$\|\varphi\|_\infty = \sup_{v\in\mathcal{R}^3} |\varphi(v)| \,.$$

For any $r > 0$, we introduce the function

$$\varphi_r(v) = \varphi(v)\,\beta_r(v)\,, \qquad v \in \mathcal{R}^3\,,$$

where

$$\beta_r(v) = \begin{cases} 1 & , \quad \text{if} \quad \|v\| \le r\,, \\ r+1-\|v\|\,, & \text{if} \quad \|v\| \in [r, r+1]\,, \\ 0 & , \quad \text{if} \quad \|v\| \ge r+1\,, \end{cases}$$

and the set

$$\mathcal{D}_r := \{\varphi_r \;:\; \|\varphi\|_L \le 1\}\,. \tag{33}$$

Let

$$\mu^{(n)}(t, dv) = \sum_{i=1}^{m^{(n)}(t)} g_i^{(n)}(t)\,\delta_{v_i^{(n)}(t)}(dv) \tag{34}$$

denote the empirical measure of the process (24).

We assume that the **initial state** of the process belongs to $\mathcal{Z}^{(n)}$ and satisfies

$$\limsup_{n\to\infty} E\int_{\mathcal{R}^3} \|v\|^2\,\mu^{(n)}(0, dv) < \infty$$

and

$$\lim_{n\to\infty} E\varrho(\mu^{(n)}(0), F_0) = 0\,,$$

for some finite measure F_0 such that

$$\int_{\mathcal{R}^3} \|v\|^2\,F_0(dv) < \infty\,,$$

where the symbol E denotes mathematical expectation. The **collision kernel** is assumed to satisfy (32) and

$$\int_{\mathcal{S}^2} |B(v, w, e) - B(v_1, w_1, e)|\,de \le C_L\Big[\|v - v_1\| + \|w - w_1\|\Big].$$

The first assumption concerning the **reduction procedure** is

$$P_{\text{red}}^{(n)}\left(z; \left\{z \in \mathcal{Z}^{(n)} \;:\; m \le (1-\delta)\,m_{\max}(n)\right\}\right) = 1\,, \tag{35}$$

for some $\delta \in (0,1)$ and all $z \in \mathcal{Z}^{(n)}$ such that $m > m_{\max}(n)$. This assumption assures that the reduction effect is sufficiently strong. The second assumption is that reduction should be sufficiently precise, namely (cf. (33))

$$\lim_{n\to\infty} \sup_{\psi\in\mathcal{D}_r} \sup_{z\in\mathcal{Z}^{(n)}\,:\,m>m_{\max}(n)} \int_{\mathcal{Z}^{(n)}} [\Phi(\tilde{z}) - \Phi(z)]^2 \; P_{\mathrm{red}}^{(n)}(z; d\tilde{z}) = 0\,, \tag{36}$$

for any $r > 0$, where

$$\Phi(z) = \sum_{i=1}^{m} g_i\, \psi(v_i)\,, \qquad z \in \mathcal{Z}\,. \tag{37}$$

Furthermore, we need some bound on the possible energy increase,

$$\int_{\mathcal{Z}^{(n)}} \Phi(\tilde{z})\, P_{\mathrm{red}}^{(n)}(z; d\tilde{z}) \le c\, \Phi(z)\,, \qquad \forall\, z \in \mathcal{Z}^{(n)} \,:\, m > m_{\max}(n)\,, \tag{38}$$

for some $c > 0$, where Φ denotes the function (37) with $\psi(v) = \|v\|^2$. Finally, we assume that the **particle weight bound** satisfies

$$\lim_{n\to\infty} g_{\max}(n) \;=\; 0\,, \tag{39}$$

that the **particle number bound** indicating reduction satisfies

$$\lim_{n\to\infty} m_{\max}(n) \;=\; \infty$$

and that the parameter of the **waiting time before reduction** satisfies

$$\lim_{n\to\infty} \lambda_{\mathrm{red}}(n) \;=\; \infty\,.$$

Theorem 3.1 *Let the above assumptions be fulfilled. Then (cf. (34))*

$$\lim_{n\to\infty} E \sup_{t\in[0,S]} \varrho(\mu^{(n)}(t), F(t)) = 0\,, \qquad \forall\, S > 0\,,$$

where F is a solution of the equation

$$\begin{aligned} \int_{\mathcal{R}^3} \varphi(v)\, F(t, dv) = \int_{\mathcal{R}^3} \varphi(v)\, F_0(dv) + \\ \frac{1}{2} \int_0^t \int_{\mathcal{R}^3} \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} \Big[\varphi(v^*(v,w,e)) + \varphi(w^*(v,w,e)) - \varphi(v) - \varphi(w)\Big] \times \\ B(v,w,e)\, de\, F(s, dv)\, F(s, dw)\, ds\,, \end{aligned} \tag{40}$$

for continuous bounded test functions φ.

Note that equation (40) is a weak form of the Boltzmann equation (15).

The notion of the reduction procedure $P_{\rm red}^{(n)}$ is very general. Here we give one specific example and check the conditions of the convergence theorem. The first step of the reduction procedure consists in arranging the particle system z into groups

$$G_i^{(n)}(z) = \Big((g_{i,j}, v_{i,j}) \,, \quad j = 1, \ldots, m_i \Big), \qquad i = 1, \ldots, \gamma^{(n)}(z) \,. \tag{41}$$

At a second step, each group is replaced by one particle

$$(\tilde{g}_i, \tilde{v}_i) = \left(\sum_{j=1}^{m_i} g_{i,j}, v_{i,k} \right), \tag{42}$$

where the index k is chosen at random according to the probabilities

$$\frac{g_{i,k}}{\sum_{j=1}^{m_i} g_{i,j}} \,, \qquad k = 1, \ldots, m_i \,. \tag{43}$$

Thus, the state after reduction is

$$\tilde{z} = \Big(\tilde{g}_1, \tilde{v}_1, \ldots, \tilde{g}_{\gamma^{(n)}(z)}, \tilde{v}_{\gamma^{(n)}(z)} \Big).$$

The group reduction procedures are assumed to be independent of each other.

Since the reduction procedure is mass-preserving, assumption (31) reduces to

$$\max_{i=1,\ldots,\gamma^{(n)}(z)} \sum_{j=1}^{m_i} g_{i,j} \le g_{\max}(n) \,, \qquad \forall\, z \in \mathcal{Z}^{(n)} \,:\, m > m_{\max}(n) \,. \tag{44}$$

Assumption (35) takes the form

$$\gamma^{(n)}(z) \le (1 - \delta)\, m_{\max}(n) \,, \qquad \forall\, z \in \mathcal{Z}^{(n)} \,:\, m > m_{\max}(n) \,. \tag{45}$$

According to (42), (43) one obtains

$$E\, \tilde{g}_i\, \psi(\tilde{v}_i) = \sum_{k=1}^{m_i} g_{i,k}\, \psi(v_{i,k}) \,, \qquad \forall\, i = 1, \ldots, \gamma^{(n)}(z) \,, \tag{46}$$

and

$$\int_{\mathcal{Z}^{(n)}} \Phi(\tilde{z})\, P_{\rm red}^{(n)}(z; d\tilde{z}) =$$

$$\sum_{i=1}^{\gamma^{(n)}(z)} \int_{\mathcal{Z}^{(n)}} \tilde{g}_i\, \psi(\tilde{v}_i)\, P_{\rm red}^{(n)}(z; d\tilde{z}) = \sum_{i=1}^{\gamma^{(n)}(z)} \sum_{k=1}^{m_i} g_{i,k}\, \psi(v_{i,k}) = \Phi(z) \,,$$

where the function Φ is defined in (37). Thus, assumption (38) is fulfilled. Using (46), (44) and independence, one obtains

$$\int_{\mathcal{Z}^{(n)}} [\Phi(\tilde{z}) - \Phi(z)]^2 P_{\rm red}^{(n)}(z; d\tilde{z}) \le$$

$$\sum_{i=1}^{\gamma^{(n)}(z)} \int_{\mathcal{Z}^{(n)}} [\tilde{g}_i\, \psi(\tilde{v}_i)]^2 P_{\rm red}^{(n)}(z; d\tilde{z}) \le g_{\max}(n)\, \|\psi\|_\infty^2\, C_\mu \,.$$

Consequently, assumption (36) follows from assumption (39). Thus, the remaining restrictions on the reduction procedure concern the group formation (41). Namely, the group weights should satisfy (44) and the number of groups should satisfy (45). Note that a necessary condition for the consistency of these restrictions is (cf. (25))

$$C_\mu \leq (1-\delta) \inf_n m_{\max}(n)\, g_{\max}(n)\,.$$

Finally, we present results of numerical experiments from [MW02]. They illustrate both convergence and considerable variance reduction, for the specific problem of calculating tails of the velocity distribution. Another example (flow with large density gradient) can be found in [RW01]. We consider the relaxation of a mixture of two Maxwellians

$$f_0(v) \;=\; \alpha\, M_1(v) + (1-\alpha)\, M_2(v)\,,$$

where

$$M_i(v) \;=\; \frac{1}{(2\pi\, T_i)^{3/2}} \exp\left(-\frac{\|v-V_i\|}{2\, T_i}\right)$$

and

$$\alpha = 0.1\,, \qquad V_1 = (94.82, 0, 0)\,, \qquad V_2 = (-10.54, 0, 0)\,, \qquad T_1 = T_2 = 1\,,$$

to a Maxwellian $M_\infty(v)$ with

$$V_\infty = (0,0,0)\,, \qquad T_\infty = 334\,.$$

We calculate the tail functional

$$\int_{\{\|v\|>105\}} f(t,v)\, dv\,, \qquad t \in [0,50]\,, \tag{47}$$

i.e. the mass outside some ball with large radius. The relevant parameters are

$$n = 10^5\,, \qquad m_{\max}(n) = 2\,n\,, \qquad g_{\max}(n) = \frac{2}{n}\,, \qquad \kappa = 1\,.$$

Confidence bands for the functional (47), calculated with DSMC and SWPM, are displayed in **Figure 1**. The left graph shows that both algorithms model the same time evolution. The right graph shows how the algorithms approximate the very small value at equilibrium,

$$\int_{\{\|v\|>105\}} M_\infty(v)\, dv \;=\; 3.2 \cdot 10^{-7}\,.$$

Beside convergence, these results illustrate the effect of variance reduction, which was the motivation for introducing SWPM. The number of repetitions is chosen in such a way that DSMC and SWPM need almost the same CPU time. In this particular example, SWPM is about 16 times more time consuming (per trajectory),

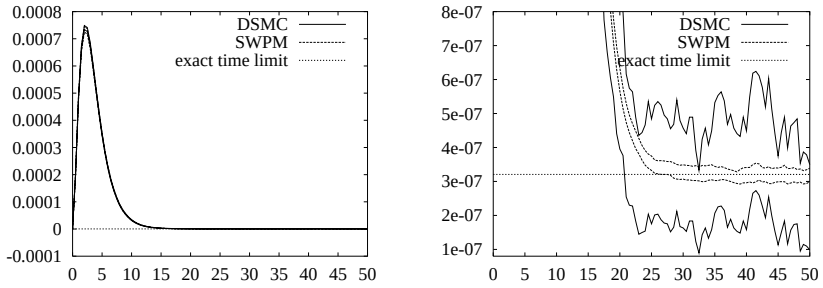

Figure 1: Tail functional (47) and zoom (right).

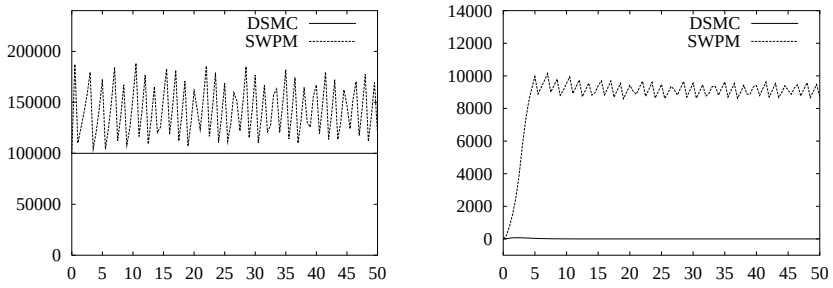

Figure 2: Number of particles in the system (left) and in the tail (right).

so that the gain factor in efficiency of about 50 results from a tremendous variance reduction.

An interesting feature of SWPM is the variable number of simulation particles displayed in **Figure 2**. First we note that SWPM produces a correct result despite the strong fluctuation in the overall number of particles (left graph) and the correspondingly large number of reduction steps. The variance reduction effect is explained best by looking at the curves for the number of simulation particles in the tail (right graph). At the beginning, both algorithms do not have particles inside the tail. Then SWPM produces such particles rather quickly and keeps them. At the end, in SWPM 10% of the particles are in the tail, while in DSMC the relative amount corresponds to the value of the functional. However, the number of particles is just an illustrative quantity, the important point is that they have appropriate weights. This is achieved by dividing the velocity space into a relatively large number of shells and keeping the number of simulation particles in all shells almost equal. Thereby a sufficient "communication" between different parts of the velocity space is guaranteed. Here we use the freedom provided by the reduction procedure.

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