Institut für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Convergence of particle schemes for the Boltzmann equation

M. Pulvirenti[1] , W. Wagner[2] , M.B. Zavelani Rossi[1]

submitted: 3rd June 1993

[1] Dipartimento di Matematica
Università degli Studi di Roma "La Sapienza"
Piazzale Aldo Moro, 2
I–00185 Roma
Italy

[2] Institute of Applied Analysis
and Stochastics
Mohrenstraße 39
D – O 1086 Berlin
Germany

Preprint No. 49
Berlin 1993

1991 Mathematics Subject Classification. 60 K 35, 76 P 05, 82 C 40.
Key words and phrases. Stochastic particle schemes, Boltzmann equation, rate of convergence.

Herausgegeben vom
Institut für Angewandte Analysis und Stochastik
Mohrenstraße 39
D – O 1086 Berlin

Fax: + 49 30 2004975
e-Mail (X.400): c=de;a=dbp;p=iaas-berlin;s=preprint
e-Mail (Internet): preprint@iaas-berlin.dbp.de

Convergence of Particle Schemes for the Boltzmann Equation

Mario Pulvirenti*, Wolfgang Wagner and Maria Beatrice Zavelani Rossi***

* Dipartimento di Matematica
Università degli Studi di Roma "La Sapienza"
Piazzale Aldo Moro, 2
I–00185 Roma, Italy

** Institute of Applied Analysis and Stochastics
Hausvogteiplatz 5–7
D–10117 Berlin, Germany

June 3, 1993

ABSTRACT. We show the convergence of a certain family of Markov chains, defined on the state space of a N–particle system (as the Bird's method), to the solutions of the (regularized) Boltzmann equation.

1. INTRODUCTION

Particle methods are widely used to simulate the Boltzmann dynamics of a rarefied gas (cf. [9], [5], [1], [10]). Among them, Bird's method [2], and many of its variants, is based on the implementation of a Markov chain, defined on the state space of a particle system. The convergence of such a scheme was proved by one of the authors of the present paper by using martingale techniques [11]. However this approach, based on compactness arguments, is not constructive and cannot provide an explicit rate of convergence.

In this paper we prove the convergence of a class of Markov chains, with state space given by a particle system, in the limit as the number of particles tends to infinity, by an explicit control of the marginal distributions of the process. This method is inspired by previous results (see in [6], [7] the analysis of the Kac model, and also [3], [8]), where problems of propagation of chaos were approached.

2. Preliminary considerations

We consider the Boltzmann equation in $\mathbb{R}^d$ (cf. [4])

$$\frac{\partial}{\partial t} f(t,x,v) + \langle v, \nabla_x \rangle f(t,x,v) = Q(f)(x,v)\,, \tag{2.1}$$

where $f(t,x,v)$, $x \in \mathbb{R}^d$, $v \in \mathbb{R}^d$ is the distribution function which will be normalized to one:

$$\int dx \int dv\, f(t,x,v) = 1\,. \tag{2.2}$$

We could also consider bounded domains with reasonable boundary conditions with minor modifications in what follows.

The collision operator is given by

$$\begin{aligned} Q(f)(x,v) = \int_{\mathbb{R}^d} dw \int_{\mathbb{S}^{d-1}} de\, q(v,w,e) \times \\ \times \Big[f(t,x,v^\star)\, f(t,x,w^\star) - f(t,x,v)\, f(t,x,w) \Big]\,, \end{aligned} \tag{2.3}$$

where

$$v^\star = v + e\langle e, w - v \rangle\,, \quad w^\star = w + e\langle e, v - w \rangle \tag{2.4}$$

are the postcollisional velocities, and $q(v,w,e)$ is the collision kernel which, for hard spheres, takes the form

$$\langle e, w - v \rangle\, \chi(\langle e, w - v \rangle \geq 0)\,, \tag{2.5}$$

where $\chi(A)$ is the indicator of the set A and $\langle .,. \rangle$ denotes the scalar product.

Together with Eq. (2.1) we consider also a regularized version of it:

$$\frac{\partial}{\partial t} f(t,x,v) + \langle v, \nabla_x \rangle f(t,x,v) = Q_\delta(f)(x,v)\,. \tag{2.6}$$

To define Q_δ we partition $\mathbb{R}^d$ into a union of identical, disjoint square cells of side δ. The generic cell will be denoted by Δ. Consider the function

$$h_\delta(x,y) = \sum_\Delta \chi(x \in \Delta)\, \chi(y \in \Delta)\, \frac{1}{\delta^d}\,. \tag{2.7}$$

Then $\int h_\delta(x,y)\, dx = \int h_\delta(x,y)\, dy = 1$. Finally, setting

$$q_\delta(v,w,e) = \chi(|\, v - w \,| < \frac{1}{\delta})\, q(v,w,e) \tag{2.8}$$

we define

$$\begin{aligned} Q_\delta(f)(x,v) = \int_{\mathbb{R}^d} dy \int_{\mathbb{R}^d} dw \int_{\mathbb{S}^{d-1}} de\, h_\delta(x,y)\, q_\delta(v,w,e) \times \\ \times \Big[f(t,x,v^\star)\, f(t,y,w^\star) - f(t,x,v)\, f(t,y,w) \Big]\,. \end{aligned} \tag{2.9}$$

Eq. (2.9) is much better, from a mathematical point of view, than Eq. (2.1). Indeed it is easy to prove the following Lipschitz condition in $L_1(dx, dv)$:

$$\| Q_\delta(f) - Q_\delta(g) \|_1 \leq C_\delta \; \| f + g \|_1 \, \| f - g \|_1 \,, \tag{2.10}$$

which allows us to formulate an L_1–theory for the initial value problem associated with Eq. (2.6).

On the other hand it is rather straightforward to prove that "if one assumes" the existence of a sufficiently smooth solution of Eq. (2.1), this can be approximated, in the limit $\delta \to 0$, by solutions f^δ of Eq. (2.6) with the same initial datum. Therefore, for our approximation problem we shall consider solutions to Eq. (2.6).

3. The basic Markov chain

We first introduce the following quantities:

$$\tilde{\alpha}(z, i, j, e) = h_\delta(x_i, x_j)\, q_\delta(v_i, v_j, e)\,, \tag{3.1}$$

$$\bar{\alpha}(e) = \sup_{z,i,j} \tilde{\alpha}(z, i, j, e)\,, \tag{3.2}$$

$$\alpha = \int_{\mathbb{S}^{d-1}} de\, \bar{\alpha}(e)\,. \tag{3.3}$$

We consider a time discretization (τ_n), $n=0,1,...$, where $\tau_0=0$, $\tau_n=\tau_{n-1}+\Delta\tau$, and

$$\Delta\tau = \frac{2}{\alpha\,(N-1)}\,. \tag{3.4}$$

The simulation of our random particle system

$$z(t) = \Big\{(x_i(t), v_i(t))\Big\}_{i=1}^N\,, \quad (x_i(t), v_i(t)) \in \mathbb{R}^d \times \mathbb{R}^d\,,$$

in the time interval $[\tau_{n-1}, \tau_n)$ is splitted into free flow simulation and collision simulation. The system resulting from the free flow simulation is the starting point for the collision simulation. We define the collision simulation according to the following rules:

i) the indices i and j of the colliding particles are generated according to the uniform distribution among all indices;

ii) an element $e \in \mathbb{S}^{d-1}$ is generated according to the probability density $\alpha^{-1}\,\bar{\alpha}(e)$;

iii) a random number η is sampled in $[0,1]$ with the uniform distribution;

iv) if

$$\eta < \frac{\tilde{\alpha}(z, i, j, e)}{\bar{\alpha}(e)} \tag{3.5}$$

the new state is obtained from the old one by replacing v_i and v_j by

$$v_i^\star = v_i + e\langle e, v_j - v_i\rangle\,, \quad v_j^\star = v_j + e\langle e, v_i - v_j\rangle\,.$$

If (3.5) is not fulfilled, then the system does not change and the collision is called fictitious.

Notice that, if x_i and x_j are not in the same cell the collision is always fictitious.

Let us now consider the time evolution of the probability density $\mu = \mu(\tau_n, z)$ defined on the state space of our particle system, which is symmetric in the exchange of any pair of particles. It is easy to realize that

$$\mu(\tau_n) = T\, S\, \mu(\tau_{n-1})\,, \tag{3.6}$$

where

$$(S\,\mu)(x_1, v_1, \ldots, x_N, v_N) = \mu(x_1 - v_1\,\Delta\tau, v_1, \ldots, x_N - v_N\,\Delta\tau, v_N) \tag{3.7}$$

is the free–stream operator and

$$(T\,\mu)(z) = \frac{1}{N\,\Delta\tau} \sum_{1\le i<j\le N} \int_{\mathbb{S}^{d-1}} de \int_0^1 d\eta\, \bar{\alpha}(e)\, \mu(z + \psi(z, i, j, e, \eta))\,, \tag{3.8}$$

where

$$\psi(z, i, j, e, \eta) = \begin{cases} \zeta(z, i, j, e) & , \text{ if } \quad \eta < \frac{\bar{\alpha}(z,i,j,e)}{\bar{\alpha}(e)}\,, \\ 0 & , \text{ otherwise}\,. \end{cases} \tag{3.9}$$

and

$$\zeta(z, i, j, e)_m = \begin{cases} (0, 0) & , \text{ if } \quad m \ne i, j\,, \\ (0, v_m^\star - v_m) & , \text{ if } \quad m = i, j\,. \end{cases} \tag{3.10}$$

In what follows it will be convenient to write Eq. (3.6) in the form

$$\mu(\tau_n) = S\,\mu(\tau_{n-1}) + \Delta\tau\, \mathcal{A}_N\, S\,\mu(\tau_{n-1}) \tag{3.11}$$

where

$$(\mathcal{A}_N\,\mu)(z) = \frac{1}{N} \sum_{1\le i<j\le N} \int_{\mathbb{S}^{d-1}} de \int_0^1 d\eta\, \bar{\alpha}(e)\, \{\mu(z + \psi(z, i, j, e, \eta)) - \mu(z)\}\,. \tag{3.12}$$

The advantage of the formulation (3.11) is to make more transparent the meaning of our Markov chain. Indeed we have

$$(\mathcal{A}_N\,\mu)(z) = \frac{1}{N} \sum_{\substack{i,j=1 \\ i<j}}^{N} \int_{\mathbb{S}^{d-1}} de\, h_\delta(x_i, x_j)\, q_\delta(v_i, v_j, e) \{\mu(z + \zeta(z, i, j, e)) - \mu(z)\}\,. \tag{3.13}$$

Notice that $\mathcal{A}_N$ is the generator of a (continuous in time) Markov process for which the particles are moving freely and collide (whenever they are in the same cell, with random impact parameter e) with an intensity depending on the state of the system.

The introduction of the formulation (3.12) (and hence the concept of fictitious collisions) allows us to consider the same process with a constant intensity given by $\frac{N-1}{2}\,\alpha = (\Delta\tau)^{-1}$. Therefore Eq. (3.11) can be interpreted as the time discretization of this process (with fictitious collisions) in which the exponential waiting time is replaced by its expectation.

Now define the marginal distributions of the density μ:

$$f_s^N = \int \mu \, dz_{s+1} \dots dz_N \,, \quad s = 1, \dots, N \,. \tag{3.14}$$

Starting from Eq. (3.11), one can show that f_s^N satisfies the following hierarchy of equations

$$f_s^N(\tau_n) = S\, f_s^N(\tau_{n-1}) + \Delta\tau \, \frac{s}{N} \, \mathcal{A}_s \, S\, f_s^N(\tau_{n-1}) + \Delta\tau \, \frac{N-s}{N} \, \mathcal{C}_{s,s+1} \, S\, f_{s+1}^N(\tau_{n-1}) \,, \tag{3.15}$$

where

$$\mathcal{C}_{s,s+1} \, S\, f_{s+1}^N(\tau_{n-1}) = \sum_{i=1}^{s} \int_{\mathbb{R}^d \times \mathbb{R}^d} \int_{\mathbb{S}^{d-1}} \int_0^1 \bar{\alpha}(e) \tag{3.16}$$
$$\{S\, f_{s+1}^N(\tau_{n-1}, z + \psi(z,i,s+1,e,\eta)) - S\, f_{s+1}^N(\tau_{n-1}, z)\} \, d\eta \, de \, dz_{s+1} \,.$$

The hierarchy is derived from the evolution equation for densities (3.11) by integrating with respect to the last $(N-s)$ variables $z_{s+1} \dots z_N$:

$$f_s^N(\tau_n) = S\, f_s^N(\tau_{n-1}) + \Delta\tau \int \mathcal{A}_N \, S\, \mu(\tau_{n-1}) \, dz_{s+1} \dots dz_N \,. \tag{3.17}$$

(Here we used the identity $\int S\, \mu \, dz_{s+1} \dots dz_N = S \int \mu \, dz_{s+1} \dots dz_N$). The last term of (3.17) can be considerably simplified and expressed in terms of f_s^N by making the following distinctions among the terms of the sum (3.12):

i) case $i > s$: these terms do not contribute to the integral;

ii) case $i \le s$ and $j \le s$: these terms form the s–particle operator $\mathcal{A}_s$;

iii) case $i \le s$ and $j > s$: these terms form the following sum

$$\frac{1}{N} \sum_{\substack{i=1,\dots,s \\ j=s+1,\dots,N}} \int_{\mathbb{S}^{d-1}} \int_0^1 \bar{\alpha}(e) [S\, \mu(z + \psi(z,i,j,e,\eta)) - S\, \mu(z)] \, d\eta \, de \,.$$

Because of the symmetry of μ, each term in the sum over j makes the same contribution. Hence we have $(N-s)$ terms equal to the term with $j = s+1$. By integrating we find

$$\int \frac{N-s}{N} \sum_{i=1}^{s} \int_{\mathbb{S}^{d-1}} \int_0^1 \bar{\alpha}(e) \{S\, \mu(z + \psi(z,i,s+1,e,\eta)) - S\, \mu(z)\} \, d\eta \, de \, dz_{s+1} \dots dz_N$$
$$= \frac{N-s}{N} \, \mathcal{C}_{s,s+1} \, S\, f_{s+1}^N(\tau_{n-1}) \,.$$

4. Convergence

Let us come back now to the regularized Boltzmann equation (2.6). We formulate the following time discretization:

$$g^N(\tau_n) = S\, g^N(\tau_{n-1}) + \Delta\tau\, Q_\delta(S\, g^N(\tau_{n-1}))\,. \tag{4.1}$$

Notice that $g^N(\tau_n)$ is positive, if $g^N(\tau_0) = g_0 \geq 0$. Indeed,

$$g^N(\tau_n) \geq S\, g^N(\tau_{n-1}) - \Delta\tau\, \alpha\, S\, g^N(\tau_{n-1})\,, \tag{4.2}$$

and since $\Delta\tau\, \alpha < 1$ if $N \geq 4$, under such hypothesis we prove the non–negativity by induction.

We want to compare f_s^N introduced in the previous section with the products

$$g_s^N(\tau_n, z_s) = \prod_{i=1}^{s} g^N(\tau_n, x_i, v_i)\,, \qquad z_s = (x_1, v_1, \ldots x_s, v_s)\,. \tag{4.3}$$

To this end we derive a recursive formula from (4.1) and (4.3):

$$\begin{aligned} g_s^N(\tau_n, z_s) &= \prod_{i=1}^{s} [S\, g^N(\tau_{n-1})(x_i, v_i) + \Delta\tau\, Q_\delta(S\, g^N(\tau_{n-1}))(x_i, v_i)] = \\ &= \ S\, g_s^N(\tau_{n-1})(z_s) + \sum_{k=1}^{s} \Delta\tau\, Q_\delta(S\, g^N(\tau_{n-1}))(x_k, v_k) \prod_{i\neq k} S\, g^N(\tau_{n-1})(x_i, v_i) \\ &\quad + R^s(\tau_{n-1})\,, \end{aligned} \tag{4.4}$$

where $R^s(\tau_{n-1})$ denotes the remaining terms. From (3.16) and (2.9) we obtain

$$g_s^N(\tau_n) = S\, g_s^N(\tau_{n-1}) + \Delta\tau\, \mathcal{C}_{s,s+1}\, S\, g_{s+1}^N(\tau_{n-1}) + R^s(\tau_{n-1})\,. \tag{4.5}$$

Comparing (3.15) and (4.5) one obtains

$$\begin{aligned} & f_s^N(\tau_n) - g_s^N(\tau_n) = \\ & \quad S\, [f_s^N(\tau_{n-1}) - g_s^N(\tau_{n-1})] + \Delta\tau\, \mathcal{C}_{s,s+1}\, S\, [f_{s+1}^N(\tau_{n-1}) - g_{s+1}^N(\tau_{n-1})] \\ & \quad + \Delta\tau\, \frac{s}{N}\, \mathcal{A}_s\, S\, f_s^N(\tau_{n-1}) - \Delta\tau\, \frac{s}{N}\, \mathcal{C}_{s,s+1}\, S\, f_{s+1}^N(\tau_{n-1}) - R^s(\tau_{n-1})\,. \end{aligned} \tag{4.6}$$

Let us now establish some preliminary estimates which will be useful in the convergence proof. We have

$$\|\, Q_\delta(f)\,\|_1 \leq\ 2\,\alpha\ \|\, f\,\|_1^2\,, \tag{4.7}$$

$$\|\, \mathcal{C}_{s,s+1}\, f_{s+1}\,\|_1 \leq\ 2\, s\, \alpha\ \|\, f_{s+1}\,\|_1\,, \tag{4.8}$$

$$\|\, S\, f_s\,\|_1 \leq \|\, f_s\,\|_1\,, \tag{4.9}$$

$$\|\, \mathcal{A}_s\, f_s\,\|_1 \leq\ (s-1)\,\alpha\ \|\, f_s\,\|_1\,, \tag{4.10}$$

$$\| R^s(\tau_n) \|_1 \leq const \, \frac{s^2}{N^2} \, . \tag{4.11}$$

Inequalities (4.7)–(4.10) are obvious consequences of the definitions of the corresponding operators. To prove (4.11) we observe that by the positivity of g^N we have $\|g_s^N\|_1 = 1$. Therefore, from (4.4) and (4.7) we obtain

$$\begin{aligned} \| R^s(\tau_n) \|_1 &\leq \sum_{k=2}^{s} \binom{s}{k} \, (2\,\alpha\,\Delta\tau)^k = \left(1 + \frac{4}{N-1}\right)^s - \left(1 + \frac{4\,s}{N-1}\right) \\ &\leq \frac{s\,(s-1)}{2} \left(1 + \frac{4}{N-1}\right)^{s-2} \left(\frac{4}{N-1}\right)^2 \leq \frac{s^2}{2} \, \frac{16}{(N-1)^2} \, e^4 \, , \end{aligned}$$

where (3.4) has been used.

With the notation

$$\Delta_s^N(\tau_n) = \|f_s^N(\tau_n) - g_s^N(\tau_n)\|_1 \, ,$$

we obtain from (4.6), (4.8)–(4.11),

$$\begin{aligned} \Delta_s^N(\tau_{n+1}) \; &\leq \; \Delta_s^N(\tau_n) + \Delta\tau \, 2\,s\,\alpha \, \Delta_{s+1}^N(\tau_n) \\ &\quad + \Delta\tau \, \frac{s}{N} \, (s-1)\,\alpha + \Delta\tau \, \frac{s}{N} \, 2\,s\,\alpha + const \, \frac{s^2}{N^2} \, . \end{aligned} \tag{4.12}$$

Using (3.4) we derive from (4.12) the following basic inequality

$$\Delta_s^N(\tau_{n+1}) \leq \Delta_s^N(\tau_n) + c_1 \, \frac{s}{N} \, \Delta_{s+1}^N(\tau_n) + c_2 \, \frac{s^2}{N^2} \, , \tag{4.13}$$

where c_1 and c_2 are appropriate constants.

Iterating the first term on the right–hand side of (4.13) we obtain

$$\begin{aligned} \Delta_s^N(\tau_{n+k}) \; &\leq \; \Delta_s^N(\tau_n) + \sum_{j=0}^{k-1} \left[c_1 \, \frac{s}{N} \, \Delta_{s+1}^N(\tau_{n+j}) + c_2 \, \frac{s^2}{N^2} \right] \\ &= \; \varepsilon_{s,k} + c_1 \, \frac{s}{N} \sum_{j=0}^{k-1} \Delta_{s+1}^N(\tau_{n+j}) \, , \end{aligned} \tag{4.14}$$

where

$$\varepsilon_{s,k} = \Delta_s^N(\tau_n) + c_2 \, k \, \frac{s^2}{N^2} \, . \tag{4.15}$$

Now we iterate the term under the sum on the right–hand side of (4.14) with respect to s and obtain

$$\Delta_s^N(\tau_{n+k}) \le \varepsilon_{s,k} + \frac{c_1}{N}\, s \sum_{j_1=0}^{k-1} \varepsilon_{s+1,j_1} + \dots \tag{4.16}$$
$$+ \left(\frac{c_1}{N}\right)^{l-1} s\,(s+1)\dots(s+l-2) \sum_{j_1=0}^{k-1} \dots \sum_{j_{l-1}=0}^{j_{l-2}-1} \varepsilon_{s+l-1,j_{l-1}}$$
$$+ \left(\frac{c_1}{N}\right)^{l} s\,(s+1)\dots(s+l-1) \sum_{j_1=0}^{k-1} \dots \sum_{j_l=0}^{j_{l-1}-1} \Delta_{s+l}^N(\tau_{n+j_l})\,.$$

Notice that $\varepsilon_{s,k}$ increases with k and $\Delta_s^N(\tau_n) \le 2$. Hence, one derives from (4.16)

$$\Delta_s^N(\tau_{n+k}) \le \varepsilon_{s,k} + \frac{c_1}{N}\, s\, \varepsilon_{s+1,k}\, \sigma_{k,1} + \dots \tag{4.17}$$
$$+ \left(\frac{c_1}{N}\right)^{l-1} s\,(s+1)\dots(s+l-2)\, \varepsilon_{s+l-1,k}\, \sigma_{k,l-1}$$
$$+ 2\left(\frac{c_1}{N}\right)^{l} s\,(s+1)\dots(s+l-1)\, \sigma_{k,l}\,,$$

where

$$\sigma_{k,l} = \sum_{j_1=0}^{k-1} \dots \sum_{j_l=0}^{j_{l-1}-1} 1\,.$$

Using the estimate $\sigma_{k,l} \le \frac{k^l}{l!}$ we obtain from (4.17)

$$\Delta_s^N(\tau_{n+k}) \le \varepsilon_{s,k} + \frac{k\,c_1}{N}\,\frac{s}{1!}\,\varepsilon_{s+1,k} + \dots \tag{4.18}$$
$$+ \left(\frac{k\,c_1}{N}\right)^{l-1} \frac{s\,(s+1)\dots(s+l-2)}{(l-1)!}\, \varepsilon_{s+l-1,k}$$
$$+ 2\left(\frac{k\,c_1}{N}\right)^{l} \frac{s\,(s+1)\dots(s+l-1)}{l!}\,.$$

With the estimate

$$\frac{s\,(s+1)\dots(s+l-1)}{l!} \le 2^{s+l-1}\,,$$

(4.18) implies

$$\Delta_s^N(\tau_{n+k}) \le \sum_{j=0}^{l-1} \varepsilon_{s+j,k}\, 2^{s-1} \left(\frac{2\,k\,c_1}{N}\right)^{j} + 2^s \left(\frac{2\,k\,c_1}{N}\right)^{l}. \tag{4.19}$$

Using the explicit form (4.15) of $\varepsilon_{s,k}$, we derive from (4.19)

$$\Delta_s^N(\tau_{n+k}) \;\leq\; \sum_{j=0}^{l-1} \Delta_{s+j}^N(\tau_n)\, 2^{s-1} \left(\frac{2\,k\,c_1}{N}\right)^j + \tag{4.20}$$
$$+\sum_{j=0}^{l-1} c_2\, k\, \frac{(s+j)^2}{N^2}\, 2^{s-1} \left(\frac{2\,k\,c_1}{N}\right)^j + 2^s \left(\frac{2\,k\,c_1}{N}\right)^l .$$

Consider a number $\Delta N \in \left(\frac{N}{4\,c_1} - 1, \frac{N}{4\,c_1}\right]$ and introduce moments of time $t_i = \tau_{i\,\Delta N}$. Notice that $\lim_{N\to\infty} t_i = i\,\Delta t$, with $\Delta t = \frac{1}{2\,\alpha\,c_1}$.

It follows from (4.20) that

$$\Delta_s^N(t_{i+1}) \leq \sum_{j=0}^{l-1} \Delta_{s+j}^N(t_i)\, 2^{s-1} \left(\frac{1}{2}\right)^j + \sum_{j=0}^{l-1} \frac{c_2}{4\,c_1}\, \frac{(s+j)^2}{N}\, 2^{s-1} \left(\frac{1}{2}\right)^j + 2^s \left(\frac{1}{2}\right)^l . \tag{4.21}$$

Now we suppose that

$$\Delta_s^N(t_i) \leq \beta_i^N, \quad \forall s \leq \gamma_i^N, \tag{4.22}$$

and show that

$$\Delta_s^N(t_{i+1}) \leq \beta_{i+1}^N, \quad \forall s \leq \gamma_{i+1}^N, \tag{4.23}$$

for some appropriately defined bounds β_i^N and γ_i^N such that $\lim_{N\to\infty} \beta_i^N = 0$ and $\lim_{N\to\infty} \gamma_i^N = \infty$.

Let $l \in (\gamma_i^N - \gamma_{i+1}^N, \gamma_i^N - \gamma_{i+1}^N + 1]$ so that $s+l-1 \leq \gamma_i^N$ if $s \leq \gamma_{i+1}^N$. Hence, we obtain from (4.21) that

$$\Delta_s^N(t_{i+1}) \;\leq\; \beta_i^N\, 2^s + \frac{c_2}{4\,c_1}\, \frac{(\gamma_i^N)^2}{N}\, 2^s + 2^{s-l}$$
$$\leq\; \beta_i^N\, 2^{\gamma_{i+1}^N} + \frac{c_2}{4\,c_1}\, \frac{(\gamma_i^N)^2}{N}\, 2^{\gamma_{i+1}^N} + 2^{2\,\gamma_{i+1}^N - \gamma_i^N} . \tag{4.24}$$

We denote the terms on the right–hand side of (4.24) by $T_{i,N}^{(1)}$, $T_{i,N}^{(2)}$, and $T_{i,N}^{(3)}$, respectively. In order to establish (4.23) it remains to assure

$$T_{i,N}^{(1)} + T_{i,N}^{(2)} + T_{i,N}^{(3)} \leq \beta_{i+1}^N . \tag{4.25}$$

To this end, we introduce the following explicit expressions for the bounds γ_i^N and β_i^N:

$$\gamma_i^N = a^i\, \bar{\gamma}\, log_2 N , \tag{4.26}$$

$$\beta_i^N = \bar{\beta}_i\, 2^{-b\,a^i\, log_2 N} = \bar{\beta}_i \left(\frac{1}{N}\right)^{b\,a^i} . \tag{4.27}$$

Using (4.26) and (4.27) we obtain

$$T^{(1)}_{i,N} = \bar{\beta}_i \, 2^{-b\, a^i \, log_2 N} \, 2^{a^{i+1}\, \bar{\gamma}\, log_2 N} = \bar{\beta}_i \, 2^{-(b-a\,\bar{\gamma})\, a^i \, log_2 N} \,,$$

$$\begin{aligned} T^{(2)}_{i,N} &= \frac{c_2}{4\, c_1} (a^i \,\bar{\gamma})^2 \, (log_2 N)^2 \, 2^{-log_2 N} \, 2^{a^{i+1}\, \bar{\gamma}\, log_2 N} \\ &\le \frac{c_2}{c_1} \left(\frac{a^i \,\bar{\gamma}}{\varepsilon_i} \right)^2 \, 2^{-(1-\varepsilon_i - a^{i+1}\,\bar{\gamma})\, log_2 N} \,, \end{aligned}$$

(Here we used the estimate $x^2 \, 2^{-\varepsilon\, x} \le \left(\frac{2}{\varepsilon}\right)^2$, $x \ge 0$, $\varepsilon > 0$), and

$$T^{(3)}_{i,N} = 2^{2\, a^{i+1}\, \bar{\gamma}\, log_2 N - a^i\, \bar{\gamma}\, log_2 N} = 2^{-(1-2\,a)\, a^i \,\bar{\gamma}\, log_2 N} \,.$$

Consequently, to assure (4.25), the following inequalities are sufficient:

$$(b - a\,\bar{\gamma})\, a^i \ge b\, a^{i+1} \,, \tag{4.28}$$

$$(1 - \varepsilon_i - a^{i+1}\,\bar{\gamma}) \ge b\, a^{i+1} \,, \tag{4.29}$$

$$(1 - 2\,a)\, a^i \,\bar{\gamma} \ge b\, a^{i+1} \,, \tag{4.30}$$

$$\bar{\beta}_i + \frac{c_2}{c_1} \left(\frac{a^i \,\bar{\gamma}}{\varepsilon_i} \right)^2 + 1 \le \bar{\beta}_{i+1} \,. \tag{4.31}$$

In order to simplify the above inequalities, we choose

$$\varepsilon_i = \varepsilon\, a^i \,, \quad \varepsilon \in (0,1) \,, \quad a \in (0, \frac{1}{2}) \,,$$

and define

$$\bar{\beta}_i = \bar{\beta}_0 + i \left[\frac{c_2}{c_1} \left(\frac{\bar{\gamma}}{\varepsilon} \right)^2 + 1 \right] . \tag{4.32}$$

Thus, (4.31) is fulfilled, and (4.28)–(4.30) reduce to

$$b - a\,\bar{\gamma} \ge b\, a \,, \tag{4.33}$$

$$1 - \varepsilon \ge (b + \bar{\gamma})\, a \,, \tag{4.34}$$

$$(1 - 2\,a)\,\bar{\gamma} \ge b\, a \,. \tag{4.35}$$

After replacing the constants c_1 and c_2 by their maximum (cf. (4.13)) the corresponding quotient in (4.32) disappears.

The parameters $\bar{\gamma}$, $\bar{\beta}_0$ and b are determined by the assumption concerning the initial chaos. The parameter a is an arbitrary positive number such that

$$a \leq min\left(\frac{b}{b+\bar{\gamma}}, \frac{1-\varepsilon}{b+\bar{\gamma}}, \frac{\bar{\gamma}}{b+2\bar{\gamma}}\right).$$

Thus, we have proved the following theorem.

Theorem 4.1. *Suppose that*

$$\|f_s^N(t_0) - g_s^N(t_0)\|_1 \leq \bar{\beta}_0 \left(\frac{1}{N}\right)^b, \quad \forall s \leq \bar{\gamma}\, log_2 N,$$

for some positive parameters $\bar{\beta}_0$, $\bar{\gamma}$ and b.

Then, for $i = 1, 2, \dots$,

$$\|f_s^N(t_i) - g_s^N(t_i)\|_1 \leq \bar{\beta}_i \left(\frac{1}{N}\right)^{a^i b}, \quad \forall s \leq a^i \bar{\gamma}\, log_2 N,$$

where

$$\bar{\beta}_i = \bar{\beta}_0 + i\left[\left(\frac{\bar{\gamma}}{\varepsilon}\right)^2 + 1\right], \quad 0 < a \leq min\left(\frac{b}{b+\bar{\gamma}}, \frac{1-\varepsilon}{b+\bar{\gamma}}, \frac{\bar{\gamma}}{b+2\bar{\gamma}}\right),$$

and $\varepsilon \in (0,1)$ is an arbitrary parameter.

It is interesting to consider the special case, when the initial values factorize, i.e.

$$f_s^N(t_0) = g_s^N(t_0).$$

In this case, one can choose the parameters $\bar{\beta}_0$, $\bar{\gamma}$ and b arbitrarily.

Example 4.2. *First we look for the largest possible value $\bar{a}$ of the parameter a. It follows from* (4.33) *and* (4.35) *that*

$$a \leq min\left(\frac{b/\bar{\gamma}}{b/\bar{\gamma}+1}, \frac{1}{b/\bar{\gamma}+2}\right).$$

Thus, we find $\bar{a} = \frac{3-\sqrt{5}}{2}$, when $b/\bar{\gamma} = \frac{\sqrt{5}-1}{2}$. Choosing $b = 1-\varepsilon$ and $\bar{\gamma} = (1-\varepsilon)\frac{\sqrt{5}+1}{2}$, one obtains the estimate

$$\|f_s^N(t_i) - g_s^N(t_i)\|_1 \leq i\left[\frac{3}{\varepsilon^2} + 1\right]\left(\frac{1}{N}\right)^{\bar{a}^i(1-\varepsilon)}, \quad \forall s \leq \bar{a}^i(1-\varepsilon)\frac{\sqrt{5}+1}{2}\, log_2 N.$$

Example 4.3. *Now we look for the best possible order of convergence after one time step. Thus, we want to maximize the value of the product* $a\,b$. *For this purpose, we choose* $a=\varepsilon\,,\, b=\frac{1-2\varepsilon}{\varepsilon}\,,\ \bar{\gamma}=1$. *Inequalities* (4.33)–(4.35) *are fulfilled for sufficiently small* ε, *and one obtains the estimate*

$$\|f_s^N(t_i)-g_s^N(t_i)\|_1 \le i\left[\frac{1}{\varepsilon^2}+1\right]\left(\frac{1}{N}\right)^{\varepsilon^{i-1}(1-2\varepsilon)}\,, \quad \forall s\le \varepsilon^i\, log_2 N\,.$$

Thus, in this case the rate of convergence is arbitrarily close to 1 *after one time step, but later it becomes much worse than in Example* 4.2.

From Theorem 4.1 we show that f_s^N converges, in the limit $N\to\infty$, to the product $\prod_{i=1}^{s} f(t,x_i,v_i)$, where $f(t)$ solves Eq. (2.6). Indeed it is straightforward to prove the L_1 convergence of $g^N(t)$ (given by Eq. (4.1)) to $f(t)$ when $N\to\infty$ (and hence $\Delta\tau\to 0$, according to (3.4)).

Remark. In our scheme we alternate the free stream with a (maybe fictitious) collision. Obviously one can perform more than one collision for each time step. This is actually one variant of the Bird scheme (cf. [2]). It is clear that our convergence argument can work as well in that case.

References

1. 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).
2. G.A. Bird, Molecular Gas Dynamics, Clarendon Press, Oxford, 1976.
3. C. Cercignani, The Grad limit for a system of soft spheres, Comm. Pure Appl. Math. 36, 479–494 (1983).
4. C. Cercignani, The Boltzmann Equation and its Applications, Springer, New York, 1988.
5. R. Illner and H. Neunzert, On simulation methods for the Boltzmann equation, Transport Theory and Statistical Physics 16, 2&3, 141–154 (1987).
6. M. Kac, Foundations of kinetic theory, Proc. Third Berkeley Symp. Math. Stat. Prob. 3, 171–197 (1955).
7. M. Kac, Probability and Related Topics in the Physical Sciences, Interscience, New York, 1959.
8. M. Lachowicz and M. Pulvirenti, A stochastic system of particles modelling the Euler equation, Arch. Rational Mech. Anal. 109, 1, 81–93 (1990).
9. K. Nanbu, Interrelations between various direct simulation methods for solving the Boltzmann equation, J. Phys. Soc. Japan 52, 10, 3382–3388 (1983).
10. H. Neunzert, F. Gropengiesser, and J. Struckmeier, Computational methods for the Boltzmann equation, in: Applied and Industrial Mathematics (Ed. R. Spigler), Kluwer Acad. Publ., Dordrecht, 111–140 (1991).
11. 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).

Veröffentlichungen des Instituts für Angewandte Analysis und Stochastik

Preprints 1992

1. D.A. Dawson, J. Gärtner: Multilevel large deviations.
2. H. Gajewski: On uniqueness of solutions to the drift–diffusion–model of semiconductor devices.
3. J. Fuhrmann: On the convergence of algebraically defined multigrid methods.
4. A. Bovier, J.-M. Ghez: Spectral properties of one–dimensional Schrödinger operators with potentials generated by substitutions.
5. D.A. Dawson, K. Fleischmann: A super–Brownian motion with a single point catalyst.
6. A. Bovier, V. Gayrard: The thermodynamics of the Curie–Weiss model with random couplings.
7. W. Dahmen, S. Prößdorf, R. Schneider: Wavelet approximation methods for pseudodifferential equations I: stability and convergence.
8. A. Rathsfeld: Piecewise polynomial collocation for the double layer potential equation over polyhedral boundaries. Part I: The wedge, Part II: The cube.
9. G. Schmidt: Boundary element discretization of Poincaré–Steklov operators.
10. K. Fleischmann, F.I. Kaj: Large deviation probability for some rescaled superprocesses.
11. P. Mathé: Random approximation of finite sums.
12. C.J. van Duijn, P. Knabner: Flow and reactive transport in porous media induced by well injection: similarity solution.
13. G.B. Di Masi, E. Platen, W.J. Runggaldier: Hedging of options under discrete observation on assets with stochastic volatility.
14. J. Schmeling, R. Siegmund–Schultze: The singularity spectrum of self-affine fractals with a Bernoulli measure.
15. A. Koshelev: About some coercive inequalities for elementary elliptic and parabolic operators.
16. P.E. Kloeden, E. Platen, H. Schurz: Higher order approximate Markov chain filters.

17. H.M. Dietz, Y. Kutoyants: A minimum–distance estimator for diffusion processes with ergodic properties.

18. I. Schmelzer: Quantization and measurability in gauge theory and gravity.

19. A. Bovier, V. Gayrard: Rigorous results on the thermodynamics of the dilute Hopfield model.

20. K. Gröger: Free energy estimates and asymptotic behaviour of reaction–diffusion processes.

21. E. Platen (ed.): Proceedings of the 1^{st} workshop on stochastic numerics.

22. S. Prößdorf (ed.): International Symposium "Operator Equations and Numerical Analysis" September 28 – October 2, 1992 Gosen (nearby Berlin).

23. K. Fleischmann, A. Greven: Diffusive clustering in an infinite system of hierarchically interacting diffusions.

24. P. Knabner, I. Kögel–Knabner, K.U. Totsche: The modeling of reactive solute transport with sorption to mobile and immobile sorbents.

25. S. Seifarth: The discrete spectrum of the Dirac operators on certain symmetric spaces.

26. J. Schmeling: Hölder continuity of the holonomy maps for hyperbolic basic sets II.

27. P. Mathé: On optimal random nets.

28. W. Wagner: Stochastic systems of particles with weights and approximation of the Boltzmann equation. The Markov process in the spatially homogeneous case.

29. A. Glitzky, K. Gröger, R. Hünlich: Existence and uniqueness results for equations modelling transport of dopants in semiconductors.

30. J. Elschner: The h-p–version of spline approximation methods for Mellin convolution equations.

31. R. Schlundt: Iterative Verfahren für lineare Gleichungssysteme mit schwach besetzten Koeffizientenmatrizen.

32. G. Hebermehl: Zur direkten Lösung linearer Gleichungssysteme auf Shared und Distributed Memory Systemen.

33. G.N. Milstein, E. Platen, H. Schurz: Balanced implicit methods for stiff stochastic systems: An introduction and numerical experiments.

34. M.H. Neumann: Pointwise confidence intervals in nonparametric regression with heteroscedastic error structure.

35. M. Nussbaum: Asymptotic equivalence of density estimation and white noise.

Preprints 1993

36. B. Kleemann, A. Rathsfeld: Nyström's method and iterative solvers for the solution of the double layer potential equation over polyhedral boundaries.

37. W. Dahmen, S. Prössdorf, R. Schneider: Wavelet approximation methods for pseudodifferential equations II: matrix compression and fast solution.

38. N. Hofmann, E. Platen, M. Schweizer: Option pricing under incompleteness and stochastic volatility.

39. N. Hofmann: Stability of numerical schemes for stochastic differential equations with multiplicative noise.

40. E. Platen, R. Rebolledo: On bond price dynamics.

41. E. Platen: An approach to bond pricing.

42. E. Platen, R. Rebolledo: Pricing via anticipative stochastic calculus.

43. P.E. Kloeden, E. Platen: Numerical methods for stochastic differential equations.

44. L. Brehmer, A. Liemant, I. Müller: Ladungstransport und Oberflächenpotentialkinetik in ungeordneten dünnen Schichten.

45. A. Bovier, C. Külske: A rigorous renormalization group method for interfaces in random media.

46. G. Bruckner: On the regularization of the ill–posed logarithmic kernel integral equation of the first kind.

47. H. Schurz: Asymptotical mean stability of numerical solutions with multiplicative noise.

48. J.W. Barrett, P. Knabner: Finite element approximation of transport of reactive solutes in porous media. Part I: Error estimates for non–equilibrium adsorption processes.