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Monte Carlo Methods and Numerical Solutions

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Abstract

The purpose of this paper is to illustrate that direct simulation Monte Carlo methods can often be considered as rigorous mathematical tools for solving nonlinear kinetic equations numerically. First a convergence result for Bird's DSMC method is recalled. Then some sketch of the history of stochastic models related to rarefied gas dynamics is given. The model introduced by Leontovich in 1935 provides the basis for a rigorous derivation of the Boltzmann equation from a stochastic particle system. The last part of the paper is concerned with some recent directions of study in the field of Monte Carlo methods for nonlinear kinetic equations. Models with general particle interactions and the corresponding limiting equations are discussed in some detail. In particular, these models cover rarefied granular gases (inelastic Boltzmann equation) and ideal quantum gases (Uehling-Uhlenbeck-Boltzmann equation). Problems related to the order of convergence, to the approximation of the steady state solution, and to variance reduction are briefly mentioned.

Contents

[0]Invited lecture at the 24th International Symposium on Rarefied Gas Dynamics, Bari, Italy, July 10-16, 2004

1 DSMC and the Boltzmann equation

Direct simulation Monte Carlo (DSMC) has been the most widely used numerical algorithm in kinetic theory. We refer to G.A. Bird's monograph [Bir94, 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 volume.

The method is based on systems of particles

$$\Big(x_1(t), v_1(t); \ldots; x_n(t), v_n(t)\Big), \qquad t \geq 0\,, \qquad n \geq 1\,, \tag{1}$$

imitating the behaviour of gas molecules in a probabilistic way. It includes several numerically motivated approximations. 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. In each cell a certain amount of binary collisions between particles is performed,

$$v_i, v_j \quad \Rightarrow \quad v_i^*, v_j^*\,.$$

The probabilistic rules of these transformations depend on the interaction potential between gas molecules.

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 [Nan86], [IN87]). Convergence for the Nanbu scheme and its modifications was studied in [Bab89] (spatially homogeneous case) and [BI89] (spatially inhomogeneous case). Convergence for Bird's method was proved in [Wag92]. It was established that the empirical measures related to the particle system (1),

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

converge (as $n \to \infty$) to a deterministic measure with some density $\hat{f}$, which is defined as follows.

Consider the time discretization $t_k = k\,\Delta t$, $k = 0, 1, \ldots$, and auxiliary functions

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

These functions are determined by two systems of equations coupled via their initial conditions. The first system, corresponding to the free flow simulation steps, has the form

$$\frac{\partial}{\partial t} f^{(1,k)}(t,x,v) + (v, \nabla_x) f^{(1,k)}(t,x,v) = 0\,, \tag{2}$$

with appropriate boundary conditions. Here ∇ denotes the vector of partial derivatives and $(\,.\,,\,.\,)$ is the scalar product in the Euclidean space $\mathcal{R}^3$. The initial conditions are

$$f^{(1,k)}(t_k,x,v) = f^{(2,k-1)}(t_k,v)\,, \qquad k = 1,2,\ldots\,, \qquad f^{(1,0)}(0,x,v) = f_0(x,v)\,,$$

where f_0 is some density function related to the initial state of the particle system (1). The second system of equations, corresponding to the collision simulation steps, has the form

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

where

$$h(x,y) = \frac{1}{|D_l|} \sum_{l=1}^{l_c} \chi_{D_l}(x)\, \chi_{D_l}(y)\,, \tag{4}$$

$|.|$ denotes the volume, χ_A is the indicator function of a set A and $\mathcal{S}^2$ is the unit sphere in $\mathcal{R}^3$. The collision kernel B is determined by the interaction potential between gas molecules. The initial conditions are

$$f^{(2,k)}(t_k,x,v) = f^{(1,k)}(t_{k+1},x,v)\,, \qquad k = 0,1,\ldots\,.$$

The limiting density $\hat{f}$ is defined as

$$\hat{f}(t_k,x,v) = f^{(2,k-1)}(t_k,x,v)\,, \qquad k = 1,2,\ldots\,, \qquad \hat{f}(0,x,v) = f_0(x,v)\,.$$

2 History of stochastic models in RGD

2.1 Statistical description

The basis for the statistical theory of gases 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,

$$f_{eq}(v) = \frac{1}{[2\pi\, T]^{3/2}} \exp\left(-\frac{\|v\|^2}{2\, T} \right), \qquad v \in \mathcal{R}^3\,. \tag{5}$$

The positive 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 (5). In [Bol72] he established the equation

$$\frac{\partial}{\partial t} f(t,x,v) + (v, \nabla_x) f(t,x,v) = \tag{6}$$
$$\int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, B(v,w,e) \Big[f(t,x,v^*)\, f(t,x,w^*) - f(t,x,v)\, f(t,x,w) \Big]$$

governing the time evolution of the distribution function

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

This function represents the relative amount of gas particles at time t having a position close to x and a velocity close to v. The collision transformation is

$$v^* = v + e\,(e, w - v)\,, \qquad w^* = w + e\,(e, v - w)\,. \tag{7}$$

For the hard sphere model (billiard balls) the collision kernel takes the form

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

2.2 Leontovich model

Consider a stochastic particle system

$$Z^{(n)}(t) = \Big(X_1(t), V_1(t); \ldots; X_n(t), V_n(t) \Big), \qquad t \geq 0\,, \tag{8}$$

determined by an infinitesimal generator of the form

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

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

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

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 (8), 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

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

where

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

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 (7).

The study of the relationship between the process (8) and the Boltzmann equation (6) was started by M. A. Leontovich (1903-1981) in the paper [Leo35] in 1935. Let $p^{(n)}(t, z)$ denote the n–particle distribution function of the process. Applying properties of the collision transformation (7) and some symmetry assumptions on $q^{(n)}$, the equation

$$\begin{aligned} &\frac{\partial}{\partial t}\,p^{(n)}(t, z) + \sum_{i=1}^{n} \big(v_i, \nabla_{x_i}\big)\,p^{(n)}(t, z) = \\ &\qquad \frac{1}{2\,n} \sum_{1 \leq i \neq j \leq n} \int_{S^2} \Big[p^{(n)}(t, J(z, i, j, e)) - p^{(n)}(t, z)\Big]\,q^{(n)}(x_i, v_i, x_j, v_j, e)\,de \end{aligned} \tag{10}$$

is obtained from Kolmogorov's forward equation. 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 (10) (even including a boundary condition of specular reflection). Concerning the asymptotic behaviour of the process, 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. However, he pointed out the following. Let $p_k^{(n)}$ denote the marginal distributions corresponding to the density $p^{(n)}$. If

$$\lim_{n\to\infty} p_2^{(n)}(t,x_1,v_1,x_2,v_2) = \lim_{n\to\infty} p_1^{(n)}(t,x_1,v_1) \lim_{n\to\infty} p_1^{(n)}(t,x_2,v_2) \tag{11}$$

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

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

solves the Boltzmann equation. For example, (12) is satisfied for

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

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 a ball with 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 stochastic approach to the Boltzmann equation was developed by M. Kac (1914-1984) in the paper [Kac56a] in 1956 (see also the books [Kac56b] and [Kac59]). The spatially homogeneous version of equation (10) is called "master equation" referring to [NLU40]. The factorization property (11) is called "chaos property" (indicating asymptotic independence) and the statement of the basic theorem is "propagation of chaos". 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 mollified Boltzmann equation (cf. [Cer88, Section VIII.3])

$$\frac{\partial}{\partial t} f(t,x,v) + (v, \nabla_x)\, f(t,x,v) = \tag{13}$$
$$\int_D \int_{\mathcal{R}^3} \int_{\mathcal{S}^2} h(x,y)\, B(v,w,e) \Big[f(t,x,v^*)\, f(t,y,w^*) - f(t,x,v)\, f(t,y,w) \Big] de\, dw\, dy\,,$$

which reduces to the Boltzmann equation (6) if the "mollifier" h is a delta-function. Further references concerning the spatially inhomogeneous case are [Sko88], [Fun86], [NT89], [LP90], [Wag96], [GM97], [Rez03].

2.3 Stochastic numerics

Stochastic numerical procedures in rarefied gas dynamics go back to the papers [Bir63] (homogeneous gas relaxation problem) and [Bir65] (shock structure problem) by G.A. Bird in 1963 and 1965, respectively. An interesting development of the DSMC method was related to the "time counter" – the mechanism that determines the number of collisions during a time step. Several similar modifications were introduced under different names in [Kou86] (null-collision technique), [IR88] (majorant frequency scheme), [Bir89] (no time counter scheme). The basic idea of "fictitious jumps" is applicable in general situations (cf. [EK86, Section 4.2]). In [Nan80] K. Nanbu derived a stochastic particle scheme starting directly from the Boltzmann equation. However, the original method suffered from certain deficiencies (quadratic effort in the number of particles, conservation of momentum and energy only on average). Later this approach was considerably improved (cf. [Bab86], [Bab89]) so that it did successfully work in applications like the reentry problem (cf. [NGS91], [Bab98]). Among the numerous Russian sources on stochastic algorithms for the Boltzmann equation we mention papers related to the Leontovich-Kac-process [BY75], [Kon86], [Khi86], [IR89], papers using branching processes [ENS89], [EM87] and papers following Skorokhod's approach via stochastic differential equations with respect to Poisson measures [Ars87], [LS89].

2.4 Comments

Boltzmann's equation (6) was derived from a model with deterministic interaction between particles. The origin of stochasticity (necessary for the interpretation of the solution) remained unclear. Statistical mechanics solves this problem via a random initial state of the system. Leontovich's motivation for introducing his model was to provide a stochastic process such that the Boltzmann equation describes the limit (for the particle number going to infinity) of rigorously defined mathematical expectations. Moreover, this approach allows one to study fluctuations. He did not address the problem of the relationship between the stochastic process and the description of the system by quantum (or classical) mechanics. The main new point in this model are the stochastic interactions. Billiard balls can penetrate each other colliding only with a certain probability. This is a conceptual barrier, which Kac was not able to overcome. In 1959 he wrote [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." In 1973 the message was the same [Kac73, p.385]: "The master equation approach suffers from a major deficiency. It is limited to the spatially homogeneous case. It seems impossible to bring in streaming terms while at the same time treating collisions as random events." Bird's DSMC algorithm can be derived from the Leontovich model by introducing certain numerical approximations (splitting, cells). The problem of combining free flow with stochastic collisions is avoided (hidden) by the splitting procedure. Nevertheless, all particles in a cell collide according to some probabilistic rules and not according to

their actual trajectories.

3 Some recent directions of study

3.1 General interactions

Consider particles with types from a locally compact separable metric space $\mathcal{Z}$. Any event in the system consists in the interaction of at most R particles and produces as a result a finite number of particles. This includes, for example, the generation of new particles from a source, the extinction or transformation of single particles, the collision of two particles, as well as more complicated chemical reactions. Formally, we introduce the state space of the particle system as

$$E = \left\{ \sum_{i=1}^{n} \delta_{z_i} : \quad n \geq 0\,, \quad z_i \in \mathcal{Z}\,, \quad i = 1, \ldots, n \right\},$$

where δ_a denotes the delta-measure concentrated at a. The admissible subsequent states of $\nu \in E$ are denoted by

$$J_0(\nu, \xi) = \nu + \xi\,, \qquad J_r(\nu, i_1, \ldots, i_r, \xi) = \nu + \xi - \delta_{z_{i_1}} - \ldots - \delta_{z_{i_r}}\,, \qquad r = 1, \ldots, R,$$

where $i_1, \ldots, i_r$ are pairwise distinct indices from $\{1, \ldots, n\}$ and $\xi \in E$. The intensity of these events is determined by some compactly bounded kernels $q_0, q_1, \ldots, q_R$ depending on a corresponding number of arguments. The asymptotic behaviour of such systems has been studied under appropriate assumptions in [EW03]. It turned out that they approximate the deterministic measure-valued solution of the equation

$$\frac{d}{dt} \langle \varphi, \mu(t) \rangle = \mathcal{G}(\varphi, \mu(t))\,, \qquad t > 0\,. \tag{14}$$

The nonlinear operator is defined as

$$\mathcal{G}(\varphi, \mu) = \int_E \langle \varphi, \xi \rangle \, q_0(d\xi) + \sum_{r=1}^{R} \int_{\mathcal{Z}} \ldots \int_{\mathcal{Z}} \int_E \Big[\langle \varphi, \xi \rangle - \varphi(z_1) - \ldots - \varphi(z_r) \Big] q_r(z_1, \ldots, z_r, d\xi) \, \mu(dz_1) \ldots \mu(dz_r)\,,$$

for continuous test functions φ with compact support and measures μ on $\mathcal{Z}$, where the notation $\langle \varphi, \nu \rangle = \int_{\mathcal{Z}} \varphi(z)\, \nu(dz)$ is used. As an example we consider the spatially homogeneous Boltzmann equation with dissipative collisions. Let $\mathcal{Z} = \mathcal{R}^d$, $d \geq 1$, and denote

$$\begin{aligned} v'(v, w, e, \theta) &= \frac{v + w}{2} + \varepsilon(v, w, \theta) \, \frac{\|v - w\| \, e}{2} \\ w'(v, w, e, \theta) &= \frac{v + w}{2} - \varepsilon(v, w, \theta) \, \frac{\|v - w\| \, e}{2}\,, \end{aligned}$$

where $v, w \in \mathcal{R}^d$, $e \in \mathcal{S}^{d-1}$ (unit sphere), $\theta \in \Theta$ (measurable space) and ε is some measurable function. Note that

$$\|v'\|^2 + \|w'\|^2 \;=\; \|v\|^2 + \|w\|^2 - \frac{1-\varepsilon(v,w,\theta)^2}{2}\,\|v-w\|^2\,,$$

i.e. energy is dissipated if $\varepsilon^2 < 1$, conserved if $\varepsilon^2 = 1$, and created if $\varepsilon^2 > 1$. Assuming

$$q_2(v,w,A) = \frac{1}{2}\int_\Theta \int_{\mathcal{S}^{d-1}} \chi_A(\delta_{v'(v,w,e,\theta)} + \delta_{w'(v,w,e,\theta)})\, B(v,w,e)\, de\, \pi(d\theta)\,,$$

where A is a measurable subset of E and π is some probability measure on Θ, equation (14) takes the form

$$\begin{aligned}\frac{d}{dt}\,\langle\varphi,\mu(t)\rangle = \frac{1}{2}\int_{\mathcal{R}^d}\int_{\mathcal{R}^d}\int_\Theta\int_{\mathcal{S}^{d-1}} \Big[\varphi(v'(v,w,e,\theta))+ \\ \varphi(w'(v,w,e,\theta)) - \varphi(v) - \varphi(w)\Big] B(v,w,e)\, de\, \pi(d\theta)\, \mu(t,dv)\, \mu(t,dw)\end{aligned}$$

and reduces to the weak form of the spatially homogeneous Boltzmann equation in the case $\varepsilon \equiv 1$.

An even more general class of stochastic models is obtained when the intensity of an individual interaction depends on the state of the whole system, e.g. via the particle density. Such systems approximate certain generalized Boltzmann equations. One example is the Uehling-Uhlenbeck-Boltzmann equation [UU33] related to ideal quantum gases. In the spatially homogeneous case this equation reads

$$\begin{aligned}\frac{\partial}{\partial t}\, f(t,v) \;=\; \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, B(v,w,e)\Big[[1+\theta f(t,v)]\,[1+\theta f(t,w)]\, f(t,v^*)\, f(t,w^*) - \\ [1+\theta f(t,v^*)]\,[1+\theta f(t,w^*)]\, f(t,v)\, f(t,w)\Big]. \qquad (15)\end{aligned}$$

It reduces to the Boltzmann equation in the case $\theta = 0$. Bose-Einstein statistics and Fermi-Dirac statistics are equilibrium distributions of equation (15) with $\theta = +1$ and $\theta = -1$, respectively. A DSMC method for this equation was studied in [GW03], where more details and further references can be found. A second example is the limiting equation for the Consistent Boltzmann Algorithm [AGA95], a DSMC modification for dense gases. This equation takes the form

$$\begin{aligned}\frac{\partial}{\partial t}\, f(t,x,v) + (v, \nabla_x)\, f(t,x,v) = \int_{\mathcal{R}^3} dw \int_{\mathcal{S}^2} de\, B(v,w,e)\times \qquad (16) \\ \Big[Y(\varrho(t,x^*))\, f(t,x^*,v^*)\, f(t,x^*,w^*) - Y(\varrho(t,x))\, f(t,x,v)\, f(t,x,w)\Big].\end{aligned}$$

Here $\varrho(t,x) = \int_{\mathcal{R}^3} f(t,x,v)\, dv$ is the density and x^* denotes an appropriate displacement during collisions. The positive continuous function Y is going to infinity as the density reaches its close-packing value. Equation (16), which is closely related to the Enskog equation, has been studied in [GW00a], [GW02], where more details and further references can be found. The derivation of equations (15) and (16) from corresponding particle systems was rather formal, and rigorous results would be of considerable interest.

3.2 Convergence order

The DSMC algorithm mentioned above depends on three main approximation parameters – the number of particles n, the splitting time step Δt and the cell size Δx. By taking the limit $n \to \infty$ one obtains the system of equations (2), (3), which depends on the remaining two parameters. In the limit $\Delta t \to 0$ this system transforms into equation (13) with h defined in (4). Finally, the Boltzmann equation (6) is obtained in the limit $\Delta x \to 0$. For numerical purposes the order of convergence with respect to the various parameters is important. The order with respect to n has been established in the context of general Markov processes in [NT89], [GM97]. Cell size dependence was studied in [AGA98]. Second order with respect to time step was predicted in [Bog88]. However, in [Ohw98], [Ohw00] the author noticed a mistake in the derivations of [Bog88] and gave some specific example illustrating first order behaviour. On the other hand, rather thorough numerical experiments in [GW00b] showed second order behaviour in many test cases (see also the derivation in [Had00]). So this problem still needs some further investigations (see, e.g., the contribution by M.A. Gallis and co-authors in these proceedings).

3.3 Steady state problems

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. Some result concerning the factorization of the equilibrium distribution was obtained in [CPW98]. But in this field the state of the theory is rather unsatisfactory.

3.4 Variance reduction

A serious problem in many applications of DSMC (flows with high density gradients, or low Mach number flows) are large statistical fluctuations. For the purpose of variance reduction, a modification of DSMC called SWPM (stochastic weighted particle method) 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]). A convergence proof for SWPM has recently been

proposed in [MW03]. Further references related to weighted particles are [Sch93], [Boy96]. An "information preservation method" (cf. [FS01], [SB02]) has been developed for low Mach number flows occurring in micro-electro-mechanical systems (MEMS). Here the convergence issue is open.

References

[AGA95] F. J. Alexander, A. L. Garcia, and B. J. Alder. A consistent Boltzmann algorithm. *Phys. Rev. Lett.*, 74(26):5212–5215, 1995.

[AGA98] F. J. Alexander, A. L. Garcia, and B. J. Alder. Cell size dependence of transport coefficients in stochastic particle algorithms. *Phys. Fluids*, 10(6):1540–1542, 1998.

[Ars87] A. A. Arsenev. Approximation of the solution of the Boltzmann equation by solutions of Ito stochastic differential equations. *Zh. Vychisl. Mat. i Mat. Fiz.*, 27(3):400–410, 1987. In Russian.

[Bab86] H. Babovsky. On a simulation scheme for the Boltzmann equation. *Math. Methods Appl. Sci.*, 8:223–233, 1986.

[Bab89] H. Babovsky. A convergence proof for Nanbu's Boltzmann simulation scheme. *European J. Mech. B Fluids*, 8(1):41–55, 1989.

[Bab98] H. Babovsky. *Die Boltzmann-Gleichung: Modellbildung–Numerik–Anwendungen.* B. G. Teubner, Stuttgart, 1998.

[BI89] 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.

[Bir63] G. A. Bird. Approach to translational equilibrium in a rigid sphere gas. *Phys. Fluids*, 6:1518–1519, 1963.

[Bir65] G. A. Bird. Shock wave structure in a rigid sphere gas. In J.H. de Leeuw, editor, *Rarefied Gas Dynamics*, volume 1, pages 216–222. Academic Press, New York, 1965.

[Bir89] G. A. Bird. Perception of numerical methods in rarefied gas dynamics. *Progr. Astronaut. Aeronaut.*, 118:211–226, 1989.

[Bir94] G. A. Bird. *Molecular Gas Dynamics and the Direct Simulation of Gas Flows.* Clarendon Press, Oxford, 1994.

[Bog88] S. V. Bogomolov. Convergence of the method of summary approximation for the Boltzmann equation. *Zh. Vychisl. Mat. i Mat. Fiz.*, 28(1):119–126, 1988. In Russian.

[Bol72] L. Boltzmann. Weitere Studien über das Wärmegleichgewicht unter Gasmolekülen. *Sitzungsber. Akad. Wiss. Wien*, 66:275–370, 1872.

[Boy96] I. D. Boyd. Conservative species weighting scheme for the direct simulation Monte Carlo method. *J. of Thermophysics and Heat Transfer*, 10(4):579–585, 1996.

[BY75] O. M. Belotserkovskij and V. E. Yanitskij. Statistical particle in cell method for problems in rarefied gas dynamics. I. Construction of the method. *Zh. Vychisl. Mat. i Mat. Fiz.*, 15(5):1195–1209, 1975. In Russian.

[Cer83] C. Cercignani. The Grad limit for a system of soft spheres. *Comm. Pure Appl. Math.*, 36(4):479–494, 1983.

[Cer88] C. Cercignani. *The Boltzmann Equation and its Applications*. Springer, New York, 1988.

[CPW98] S. Caprino, M. Pulvirenti, and W. Wagner. Stationary particle systems approximating stationary solutions to the Boltzmann equation. *SIAM J. Math. Anal.*, 29(4):913–934, 1998.

[Dav93] M. H. A. Davis. *Markov Models and Optimization*. Chapman & Hall, London, 1993.

[EK86] S. N. Ethier and T. G. Kurtz. *Markov Processes, Characterization and Convergence*. Wiley, New York, 1986.

[EM87] S. M. Ermakov and N. M. Moskaleva. Branching processes and the Boltzmann equation. Numerical aspects. *Vestnik Leningrad Univ. Ser. 1*, 3:38–43, 1987. In Russian.

[ENS89] S. M. Ermakov, V. V. Nekrutkin, and A. S. Sipin. *Random Processes for Classical Equations of Mathematical Physics*, volume 34 of *Mathematics and its Applications (Soviet Series)*. Kluwer Academic Publishers Group, Dordrecht, 1989.

[EW03] A. Eibeck and W. Wagner. Stochastic interacting particle systems and nonlinear kinetic equations. *Ann. Appl. Probab.*, 13(3):845–889, 2003.

[FS01] J. Fan and C. Shen. Statistical simulation of low-speed rarefied gas flows. *J. Comput. Phys.*, 167:393–412, 2001.

[Fun86] T. Funaki. Construction of stochastic processes associated with the Boltzmann equation and its applications. In K. Ito and T. Hida, editors, *Stochastic processes and their applications*, volume 1203 of *Lecture Notes in Mathematics*, pages 51–65. Springer, Berlin/Heidelberg, 1986.

[GM97] C. Graham and S. Méléard. Stochastic particle approximations for generalized Boltzmann models and convergence estimates. *Ann. Probab.*, 25(1):115–132, 1997.

[GW00a] A. L. Garcia and W. Wagner. The limiting kinetic equation of the consistent Boltzmann algorithm for dense gases. *J. Statist. Phys.*, 101(5-6):1065–1086, 2000.

[GW00b] A. L. Garcia and W. Wagner. Time step truncation error in direct simulation Monte Carlo. *Phys. Fluids*, 12(10):2621–2633, 2000.

[GW02] A. L. Garcia and W. Wagner. Some new properties of the kinetic equation for the Consistent Boltzmann Algorithm. *Transport Theory Statist. Phys.*, 31(4-6):579–594, 2002.

[GW03] A. L. Garcia and W. Wagner. Direct simulation Monte Carlo method for the Uehling-Uhlenbeck-Boltzmann equation. *Physical Review E*, 68:056703, 2003.

[Had00] N. G. Hadjiconstantinou. Analysis of discretization in direct simulation Monte Carlo. *Phys. Fluids*, 12(10):2634–2638, 2000.

[IN87] R. Illner and H. Neunzert. On simulation methods for the Boltzmann equation. *Transport Theory Statist. Phys.*, 16(2&3):141–154, 1987.

[IR88] M. S. Ivanov and S. V. Rogazinskij. Comparative analysis of algorithms of the direct statistical modeling method in rarefied gas dynamics. *Zh. Vychisl. Mat. i Mat. Fiz.*, 28(7):1058–1070, 1988. In Russian.

[IR89] M. S. Ivanov and S. V. Rogazinskij. Efficient schemes for direct statistical modeling of rarefied gas flows. *Mat. Model.*, 1(7):130–145, 1989. In Russian.

[Kac56a] M. Kac. Foundations of kinetic theory. In *Third Berkeley Symposium on Mathematical Statistics and Probability Theory*, volume 3, pages 171–197, 1956.

[Kac56b] M. Kac. *Some Stochastic Problems in Physics and Mathematics*. Magnolia Petroleum Co., 1956.

[Kac59] M. Kac. *Probability and Related Topics in Physical Sciences*. Interscience, London, 1959.

[Kac73] M. Kac. Some probabilistic aspects of the Boltzmann equation. *Acta Phys. Austriaca*, Suppl. X:379–400, 1973.

[Khi86] A. I. Khisamutdinov. A simulation method for statistical modeling of rarefied gases. *Dokl. Akad. Nauk SSSR*, 291(6):1300–1304, 1986. In Russian.

[Kon86] Yu. N. Kondyurin. A statistical approach to the solution of the Boltzmann equation. *Zh. Vychisl. Mat. i Mat. Fiz.*, 26(10):1527–1534, 1986. In Russian.

[Kou86] K. Koura. Null–collision technique in the direct–simulation Monte Carlo method. *Phys. Fluids*, 29(11):3509–3511, 1986.

[Leo35] M. A. Leontovich. Basic equations of the kinetic gas theory from the point of view of the theory of random processes. *Zhurnal Teoret. Ehksper. Fiziki*, 5(3-4):211–231, 1935. In Russian.

[LP90] M. Lachowicz and M. Pulvirenti. A stochastic system of particles modelling the Euler equation. *Arch. Rational Mech. Anal.*, 109(1):81–93, 1990.

[LS89] A. V. Lukshin and S. N. Smirnov. An efficient stochastic algorithm for solving the Boltzmann equation. *Zh. Vychisl. Mat. i Mat. Fiz.*, 29(1):118–124, 1989. In Russian.

[MW03] I. Matheis and W. Wagner. Convergence of the stochastic weighted particle method for the Boltzmann equation. *SIAM J. Sci. Comput.*, 24(5):1589–1609, 2003.

[Nan80] K. Nanbu. Direct simulation scheme derived from the Boltzmann equation. I. Monocomponent gases. *J. Phys. Soc. Japan*, 49(5):2042–2049, 1980.

[Nan86] K. Nanbu. Theoretical basis of the direct simulation Monte Carlo method. In V. Boffi and C. Cercignani, editors, *Rarefied Gas Dynamics*, volume 1, pages 369–383. Teubner, Stuttgart, 1986.

[NGS91] H. Neunzert, F. Gropengiesser, and J. Struckmeier. Computational methods for the Boltzmann equation. In *Applied and industrial mathematics (Venice, 1989)*, volume 56 of *Math. Appl.*, pages 111–140. Kluwer Acad. Publ., Dordrecht, 1991.

[NLU40] A. Nordsieck, W. E. Lamb, Jr., and G. E. Uhlenbeck. On the theory of cosmic–ray showers. I. The furry model and the fluctuation problem. *Physica*, 7(4):344–360, 1940.

[NT89] V. V. Nekrutkin and N. I. Tur. On the justification of a scheme of direct modelling of flows of rarefied gases. *Zh. Vychisl. Mat. i Mat. Fiz.*, 29(9):1380–1392, 1989. In Russian.

[Ohw98] T. Ohwada. Higher order approximation methods for the Boltzmann equation. *J. Comput. Phys.*, 139:1–14, 1998.

[Ohw00] T. Ohwada. Higher order time integration of spatially nonhomogeneous Boltzmann equation: deterministic and stochastic computations. *Transport Theory Statist. Phys.*, 29(3-5):495–508, 2000.

[Rez03] F. Rezakhanlou. A stochastic model associated with Enskog equation and its kinetic limit. *Comm. Math. Phys.*, 232(2):327–375, 2003.

[RGD60] *Rarefied gas dynamics: Proceedings of the First International Symposium held at Nice*, International Series on Aeronautical Sciences and Space Flight, Division IX, Vol. 3, Pergamon Press, New York, 1960.

[RW96] S. Rjasanow and W. Wagner. A stochastic weighted particle method for the Boltzmann equation. *J. Comput. Phys.*, 124(2):243–253, 1996.

[RW01] S. Rjasanow and W. Wagner. Simulation of rare events by the stochastic weighted particle method for the Boltzmann equation. *Math. Comput. Modelling*, 33(8-9):907–926, 2001.

[SB02] Q. Sun and I.D. Boyd. A direct simulation method for subsonic, microscale gas flows. *J. Comput. Phys.*, 179:400–425, 2002.

[Sch93] M. Schreiner. Weighted particles in the finite pointset method. *Transport Theory Statist. Phys.*, 22(6):793–817, 1993.

[Sko88] A. V. Skorokhod. *Stochastic Equations for Complex Systems*, volume 13 of *Mathematics and its Applications (Soviet Series)*. D. Reidel Publishing Co., Dordrecht, 1988.

[UU33] E. A. Uehling and G. E. Uhlenbeck. Transport phenomena in Einstein-Bose and Fermi-Dirac gases. I. *Phys. Rev.*, 43:552–561, 1933.

[Wag92] 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.

[Wag96] W. Wagner. A functional law of large numbers for Boltzmann type stochastic particle systems. *Stochastic Anal. Appl.*, 14(5):591–636, 1996.