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► **To cite this version:**

| Benoît Perthame. Introduction to the theory of random particle methods for Boltzmann equation.
| [Research Report] RR-2218, INRIA. 1994. <inria-00074452>

HAL Id: inria-00074452

<https://hal.inria.fr/inria-00074452>

Submitted on 24 May 2006

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INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

*Introduction to the Theory
of Random Particle Methods
for Boltzmann Equation*

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N° 2218

Mars 1994

PROGRAMME 6

Calcul scientifique,
modélisation et
logiciels numériques

*R*apport
de recherche

1994

Introduction to the Theory of Random Particle Methods for Boltzmann Equation

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Abstract :

We present theoretical derivations of several random particle methods for solving the Boltzmann equation, including Direct Simulation Monte Carlo methods and a method derived directly from Boltzmann equation. The DSMC methods are presented as discretizations of the master equations.

Introduction à la Théorie des Méthodes Particulières Aléatoires pour les Equations de Boltzmann

Résumé :

Nous présentons des dérivations théoriques de plusieurs méthodes particulières aléatoires pour la résolution des équations de Boltzmann, y compris les méthodes DSMC de simulation directe par Monte-Carlo et une méthode directement dérivée des équations de Boltzmann. Les méthodes DSMC sont introduites comme discrétisations des équations Master.

1 Introduction

The object of this text is to present how several classical resolution methods for the Boltzmann equation can be derived theoretically. We focus on the methods based on a particle approximation of the density which means as a sum of Dirac masses, and where the integrations resulting from Boltzmann kernel are numerically performed using a random method.

We will derive these methods either from the master equations or from the Boltzmann equation directly.

Due to the large number of variables in the Boltzmann equation (t for time, two three-dimensional vectors x for space and v for velocity, also a one-dimensional internal energy parameter is needed for polyatomic gases), much of the methods are based on a Monte Carlo procedure, or at least random integrations, at several levels. This is the case of those methods developed departing from the master equations and called Direct Simulation Monte Carlo methods (DSMC in short), see Bird [5], Koura [15], Nanbu [17], Ivanov and Rogasinsky [14]. Since the master equations are linear, like in neutron transport, the solution can be represented with the help of a jump markov process and the DSMC methods mimic this process. After Nanbu's method [16], the tendency has been to relate more closely to Boltzmann equations (see Babovsky [2], Babovsky and Illner [3], Neunzert et al. [18]) but random methods are still used.

These methods relying on particle approximations have the general advantage to put discretization points where they are needed (see also the other papers in this issue). For instance, for hypersonic flows in a rarefied atmosphere, the average flow velocity away from the obstacle can be around a Mach number of 25, but is zero close to the obstacle (see figure 1). This problem would require a huge number of grid points in v for a finite difference method with a fixed grid. On the other hand, particle methods always provide fluctuating results. This is due of course to the Monte Carlo procedure used to solve the collision operator, but also because the transport operator is solved exactly. Hence no numerical diffusion is present to smooth out the results. Compare for instance finite volume schemes for the Euler limit of the Boltzmann equation with particle-based schemes (Pullin [22], Coron and Perthame [8], Perthame [20] : so many particles are needed that particle methods are not competitive in the fluid regime.

In order to avoid fluctuations, several authors proposed different approaches based on finite volumes, finite elements or finite differences, especially to compute transitory regimes or problems where fluctuations are costly to avoid (low mach numbers for instance, or small variations of the flow velocity). Let us give some very incomplete set of references for such methods. Aristov and Tcheremissine [1] have developed an important effort in computing Boltzmann

equation with a finite volume discretization in v , which preserves conservation laws, Frezzotti [12], see also the references therein, extended and compared variants of this method, in the context of the evaporation of binary mixtures which arise in metallurgy processes for instance. Notice that in these papers a Monte-Carlo method is still used to calculate the eight-fold integral arising in Boltzmann equation. Further, a fully deterministic finite volume in v , finite elements in x method has been proposed recently by Rogier and Schneider [24] (and the references therein). Since it is directly deduced from an approximation of the Boltzmann kernel, this method preserves naturally the conservation laws, and Boltzmann's H-theorem at a semi-discrete level. Also, purely deterministic particle methods are presented in Niclot and Degond [19], Russo [25]. Another class of schemes, based on the theory of branching random processes, an exact algorithm for solving the Boltzmann equation is proposed in Ermakov and al. [11], Chauvun [7]. However this method has not been tested intensively and is costly.

This paper is organized as follows. In the first section, we introduce the main notations. In section II, we present the theoretical bases of the original DSMC method and of an improvement : the majorant frequency collision method. The last section is devoted to a direct derivation of a random particle method from the Boltzmann equation. In [2, 13, 18], this method, combined with low discrepancy random choices, is called Finite Pointset Method.

2 The Boltzmann equation

The Boltzmann equation describes the evolution of a continuum of particles by mean of three variables : the time t , the position x and the velocity v of particles. In this model, the density of particles follows the equation

$$\frac{\partial f}{\partial t} + v \cdot \frac{\partial f}{\partial x} = Q(f) = \int_{\mathbb{R}^3 \times S^2} [f' f'_* - f f_*] B dv_* d\sigma, \quad (1)$$

where $f = f(t, x, v)$, $f_* = f(t, x, v_*)$, $f' = f(t, x, v')$ and $f'_* = f(t, x, v'_*)$. Given (v, v_*, σ) in (1), we obtain the post-collisional velocities

$$v' = \frac{v + v_*}{2} + \frac{|g|}{2} \sigma, v'_* = \frac{v + v_*}{2} - \frac{|g|}{2} \sigma, \quad (2)$$

$$g = v - v_*, \quad (3)$$

$$B := B(|g|, |g \cdot \sigma|), B(0, a) = 0. \quad (4)$$

Boltzmann's collision operator $Q(f)$ has the fundamental properties that it conserves mass, momentum, energy which means

$$\int Q(f)(v)(1, v, |v|^2) dv = (0, 0, 0). \quad (5)$$

This follows from a more general symmetry identity ; for any function φ

$$\begin{aligned}\int Q(f)(v)\varphi(v)dv &= \frac{1}{4} \int Q(f)[\varphi + \varphi_* - \varphi' - \varphi'_*]dv \\ &= \frac{1}{2} \int Q(f)[\varphi + \varphi_*]dv.\end{aligned}\quad (6)$$

The deviation of (6) uses the particular form of B in (4). Finally, a consequence of (6) is Boltzmann's H-theorem

$$\int Q(f)(v)\ln f(v)dv \leq 0. \quad (7)$$

We refer to Cercignani [6], Truesdell and Muncaster [27] for a complete proof of these results. Notice that we have used in (2) a parametrization of the sphere which is adapted to the numerical methods. A more frequent presentation is to use a vector w of the sphere, related to (1) by

$$\begin{aligned}g' &:= v' - v'_* = |g|\sigma = g - 2(g, w)w, \\ d\sigma &= 4 \frac{|(g, w)|}{|g|} dw.\end{aligned}$$

This reduces the classical Very Hard Spheres model used for hypersonic flows in the upper atmosphere to

$$B(|g|, |g \cdot \sigma|) = K|g|^\alpha, 0 \leq \alpha < 1.$$

Nowadays, the methods based on splitting the physical processes are widely used. A free transport is evaluated first, for a time interval Δt_f . Next, a spatially homogeneous collision step is performed, which is

$$\frac{\partial f}{\partial t} = Q(f), 0 \leq t \leq \Delta t_f. \quad (8)$$

Recently Desvillettes and Mischler [29] have proved that this splitting converge, as Δt_f tends to zero, to the Di Perna-Lions [10] solution of Boltzmann equation.

Next, particle approximations of kinetic equations are based on the approximation of the density f by a sum of Dirac masses

$$f(t, x, v) \simeq \frac{1}{n_\infty} \sum_{i=1}^N \delta(x - x_i(t))\delta(v - v_i(t)). \quad (9)$$

The positions $x_i(t)$ change during the free flow only, the velocities $v_i(t)$ change during the collision step only. N denotes the total number of particles, n_∞ is a reference number. Covering the computational domain with cells C_j (say of uniform volume to simplify), this allows to define a local density ρ_j in the cell C_j by

$$\rho_j(t) = n_j(t)/n_\infty$$

where n_j is the number of $x_i(t)$ which belong to C_j . Sampling a maxwellian distribution, for instance, is now possible.

Using particles, the main difficulty in the numerical resolution of (1) is the collision step. From (9), a local distribution in the cells C_j is deduced, still denoted f ,

$$f(t, v) = \frac{1}{n_\infty} \sum_{i=1}^n \delta(v - v_i(t)), \rho = \frac{n}{n_\infty} \quad (10)$$

where n stands for n_j and new indices for v have been introduced compared to (9). And the question is to solve (8) with a distribution like (10).

3 Direct Simulation Monte-Carlo

Although the numerical techniques for simulating (8) are often obtained using heuristic arguments based on physical ideas, it seems possible to relate a large class of methods to the master equation, associated with (8). This class contains Bird's original algorithm [5], and variants are compared in Koura [15]. A very good description of these variants can be found in Ivanov and Rogasinsky [14] as well as relations with the master equation, and we will follow his presentation in this section. But these relations are frequently quoted : Nanbu [17], Belotserkovsky, Erofeyev and Yanitsky [4]. Also this approach gave rise to mathematical convergence proofs for small initial data (Wagner [28]) or for delocalized collisions (Pulvirenti, Wagner and Zavelani-Rossi [23]), or for simplified models up to the fluid limit (Perthame and Pulvirenti [21]).

The homogeneous master equation for the n -particle distribution function has the form (see Cercignani [6])

$$\frac{\partial}{\partial t} h_n(t, V) = \frac{\rho}{n} \sum_{1 \leq i < j \leq n} \int_{S^2} [h_n(t, V'_{ij}) - h_n(t, V)], B_{ij}(\sigma) d\sigma, \quad (11)$$

$$B_{ij}(\sigma) := B(|g_{ij}|, |g_{ij} \cdot \sigma|), g_{ij} = v_i - v_j, \quad (12)$$

where ρ is the local density in the cell (see (10)), V and V'_{ij} are $3n$ -dimensional vectors, $V = (v_1, \dots, v_n)$, $V'_{ij} = (v_1, \dots, v'_i, \dots, v'_j, \dots, v_n)$, and (v'_i, v'_j) are the post-collisional velocities obtained colliding (v_i, v_j, σ) according to (2) with $g_{ij} = v_i - v_j$. The relation between (9) and (11) is as follows. Integrating (11) against $dv_2 \dots dv_n$ and using the symmetry of h in (v_1, \dots, v_N) when the initial data is symmetric, we obtain

$$\frac{\partial}{\partial t} h_n^{(1)}(t, v_1) = \rho \frac{n-1}{n} \int_{S^2} [h_n^{(2)}(t, v'_1, v'_2) - h_n^{(2)}(t, v_1, v_2)] B_{12}(\sigma) d\sigma dv_2, \quad (13)$$

$h_n^{(j)}(t, v_1, \dots, v_j) = \int h_n(t, V) dv_{j+1} \dots dv_n$. Now, we take the initial date

$$h_n(0, V) = \prod_{i=1}^n f(0, v_i) / \rho, \quad (14)$$

and we expect from the propagation of chaos that h_n factorizes as N tends to infinity, which means that

$$h_n^{(2)}(t, v_1, v_2) \simeq h_n^{(1)}(t, v_1)h_n^{(1)}(t, v_2). \quad (15)$$

Then, (13) exactly yields (8) with $f = \rho h = \lim \rho h_n^{(1)}$ as N tends to infinity.

The DSMC method aims to solve the equation (11), which is linear, rather than the nonlinear equation (8). This assumes that we have a large number of particles in each cell, but all methods do so. Also, due to the linearity of (11), its solution is represented by a Markov process, which leads the numerical procedure.

Let us describe one algorithm, details, variants, improvements can be found in [5, 14, 15, 17, 4].

The collision frequency is defined as

$$\nu(V) = \frac{\rho}{n} \sum_{i < j} B_{T,ij} \quad (16)$$

$$B_{T,ij} = \int_{S^2} B_{ij}(\sigma) d\sigma. \quad (17)$$

Then, (11) can be written also

$$\partial_t h_n(t, V) + \nu(V)h_n(t, V) = \frac{\rho}{n} \sum_{i < j} \int_{S^2} h_n(t, V'_{ij}) B_{ij}(\sigma) d\sigma. \quad (18)$$

The probabilistic representation of the solution to (11) is

$$h_n(t, V) = E[h_n(0, V(t))], \quad (19)$$

where the expectation is taken according to a probability space on which the jump process $V(t)$ is built with generator in (11) (see Iketa and Watanabe [13]).

The DSMC method is just to sample this Markov process. Its initial state V_o is assumed to be known or sampled according to the initial distribution (14) at time $t_o = 0$. Then, the DSMC method generates a sequence of random times $t_1, t_2, \dots, t_k, \dots$ and at each time t_k a new $3n$ -dimensional state V_k is computed, until we reach $t_k = \Delta t_f$ the final time. From (t_k, V_k) we compute (t_{k+1}, V_{k+1}) as follows :

First step : The times t_k are sampled according to a Poisson law of parameter $\nu(V_k)$ i.e.

$$t_{k+1} - t_k = -\nu^{-1}(V_k) \ln(\text{rand})$$

where rand is random number uniformly distributed on the interval $(0, 1)$.

Second step : A collisional pair (v_i^o, v_j^o) with $i < j$ and a collision parameter $\sigma \in S^2$ are sampled with the probability

$$p(i, j, \sigma) = \frac{B_{ij}(\sigma)}{\nu(V)} \quad (20)$$

Once (i, j, σ) are known (from the current value V_k of V) we just choose $V_{k+1} = V'_{ij}$, using the rule (2), (12).

In practice, the second step is performed so as to decouple the choice of the pair (i, j) and the choice of σ . (i, j) is sampled with the probability

$$q(i, j) = \frac{B_{T,ij}}{\nu(V)}, \quad (21)$$

using this pair, σ is sampled with the probability

$$q'(\sigma) = \frac{B_{ij}(\sigma)}{B_{T,ij}}. \quad (22)$$

This method, usually called "time counter", is rather expensive (of order n per time step using a fast algorithm to sample (21)). A classical cost reduction to 1 per time step can be achieved using the "majorant collision frequency" technique where an upper bound λ of B_T is supposed to be known

$$B_{T,ij} \leq \lambda, \text{ for all } i, j. \quad (23)$$

Then, (11) is rewritten again as

$$\partial_t h_n + \rho(n-1)\lambda h_n = \frac{\rho}{n} \sum_{i < j} [(\lambda - B_{T,ij})h_n + \int_{S^2} h_n(V'_{ij}) B_{ij}(\sigma) d\sigma] \quad (24)$$

The Markov process consists now in

First step : $t_{k+1} - t_k = -[\rho(n-1)\lambda]^{-1} \ln(\text{rand})$.

Second step : A pair (v_i, v_j) is uniformly chosen in V_k , and a new random number, rand' too. If

$$\lambda \text{rand}' \geq B_{T,ij}$$

the collision is "fictitious" and we keep $V_{k+1} = V_k$ (no collision occurs). In the other case, we can perform the

Third step : (v_i, v_j) is chosen as the collisional pair and σ is sampled following (21). The new V_{k+1} is computed as before using (2).

The "majorant collision frequency" reduces the computational cost to the order

1 per time step-compare to the original "time counter". On the other hand, it is nothing but a rejection method and thus its variance is worse in particular when λ is too large.

Further variants are possible, introducing fixed time steps for instance. This makes it possible to relate these methods directly to the Boltzmann equation (1) rather than to the master equation.

4 Random particle methods

The first algorithm which relies directly on the Boltzmann equation seems to be due to Nanbu [16]. A first theoretical investigation of this method can be found in Babovski [2] and Babovski-Illner [3]. Further research in this direction led Illner and Neunzert [30], Neunzert, Gropengiesser and Struckmeier [18] to introduce the Finite Pointset Method where low discrepancy methods are used to sample the random variables.

Here, we just derive a simulation scheme directly from (8), (10) and we send the reader to the above references for practical details and further variants.

First, a smaller timestep Δt is chosen to reach Δt_f , the timestep for free flow. The homogeneous Boltzmann equation is approximated by Euler scheme

$$f^{k+1}(v) = f^k(v) + \Delta t Q(f^k)(v), \quad (25)$$

where $f^k(v)$ is an approximation of $f(k\Delta t, v)$. We assume that f^k is given by a sum of Dirac masses

$$f^k(v) = \frac{1}{n_\infty} \sum_{i=1}^n \delta(v - v_i), \quad v_i := v_i^k, \quad (26)$$

and the method approximates f^{k+1} in (20) by another combination of exactly n new Dirac masses at the points v_i^{k+1} . To do so, we first notice that Q acts on measures. Indeed, for any continuous test function φ , (25) is equivalent, using (6) to

$$\begin{aligned} \int f^{k+1}(v) \varphi(v) dv &= \int f^k(v) \varphi(v) dv \\ &- \frac{\Delta t}{2} \int f^k f_*^k (\varphi + \varphi_*) B_T(|g|) dv dv_* \\ &+ \frac{\Delta t}{2} \int f^k f_*^k (\varphi' + \varphi'_*) B(|g|, |g \cdot \sigma|) dv dv_* d\sigma. \end{aligned} \quad (27)$$

Inserting the distribution (26) in this relation, we obtain using the notation (12), (17) and after straightforward calculations

$$\int f^{k+1}(v) \varphi(v) dv =$$

$$\frac{1}{2n_\infty(n-1)} \sum_{\substack{i,j=1 \\ i \neq j}}^n \{(\varphi(v_i) + \varphi(v_j))(1 - \rho\Delta t B_{T,i,j}) \\ + \int_{S^2} \rho\Delta t B_{ij}(\sigma)(\varphi(v'_i) + \varphi(v'_j))d\sigma\}, \quad (28)$$

where $\rho = (n-1)/n_\infty$ and (v'_i, v'_j) is obtained as a collision of (v_i, v_j) with the parameter σ as in (2). Notice that, due to the assumption (4) the sum in (28) is indeed on $i \neq j$.

Next, and following the above reference, we assume that the number of particles is even

$$n = 2p, \quad (29)$$

and we denote by P the set of all possible pairings of $E = \{v_1, \dots, v_n\}$ i.e. P is the set of all possible covering of E by p pairs $\{(v_1, w_1), (v_2, w_2), \dots, (v_p, w_p)\}$. Now for any function q , we have

$$\frac{1}{2(n-1)} \sum_{i \neq j} \varphi(v_i, v_j) = \frac{1}{|P|} \sum_P \sum_{i=1}^p \varphi(v_i, w_i), \quad (30)$$

where $|P|$ is the number of all possible pairings of E . Therefore, (28) can also be written

$$\int f^{k+1}(v)\varphi(v)dv = \\ \frac{1}{n_\infty} \frac{1}{|P|} \sum_P \int_0^1 \left\{ \sum_{i=1}^p \chi(\rho\Delta t B_{T,i} \leq s \leq 1)(\varphi(v_i) + \varphi(w_i)) \right. \\ \left. + \chi(0 \leq s \leq \rho\Delta t B_{T,i}) \int_{S^2} (\varphi(v'_i) + \varphi(w'_i))d\mu_i(\sigma) \right\} ds \quad (31)$$

where (v'_i, w'_i) is obtained as a collision of (v_i, w_i) with the parameter σ , χ is the indicator function and

$$B_i(\sigma) = B(|v_i - w_i|, |(v_i - w_i) \cdot \sigma|), \quad B_{T,i} = \int_{S^2} B_i(\sigma)d\sigma, \quad (32)$$

$$d\mu_i(\sigma) = \frac{B_i(\sigma)}{B_{T,i}} d\sigma. \quad (33)$$

At this level a restriction on the time step has to be imposed

$$\rho\Delta t \max_{1 \leq i \leq p} B_{T,i} \leq 1. \quad (34)$$

Finally, a Monte-Carlo procedure is used to evaluate integral in (31) against the probability measures

$$\frac{1}{|P|} \sum_P \int_0^1 (\dots) ds, \text{ and } \int_{S^2} (\dots) d\mu_i(\sigma).$$

This means that a special pairing $(v_1, w_1), \dots, (v_p, w_p)$ is chosen with an uniform law in P , a random number $s \in (0, 1)$ is chosen with a uniform law as well and a unit vector σ_i , for each i , is finally chosen with the probability $d\mu_i(\sigma)$. This replaces (31) by a random approximation

$$\begin{aligned} \int f^{k+1}(v)\varphi(v)dv = \\ \frac{1}{n_\infty} \sum_{i=1}^p \{ \chi(\rho\Delta t B_{T,i} \leq s \leq 1)(\varphi(v_i) + \varphi(w_i)) \\ + \chi(0 \leq s \leq \rho\Delta t B_{T,i})(\varphi(v'_i) + \varphi(w'_i)) \}, \end{aligned} \quad (35)$$

which completely identifies f^{k+1} as a sum of $n = 2p$ Dirac masses,

$$f^{k+1}(v) = \frac{1}{n_\infty} \sum_{i=1}^p [\delta(v - v_i^{k+1}) + \delta(v - w_i^{k+1})]. \quad (36)$$

when $\rho\Delta t B_{T,i} \leq s$ then $(v_i^{k+1}, w_i^{k+1}) = (v_i^k, w_i^k)$, no collision is performed. When $s \leq \rho\Delta t B_{T,i}$ then $(v_i^{k+1}, w_i^{k+1}) = (v'_i, w'_i)$, the collision is performed between (v_i, w_i) with the parameter σ_i .

Notice that when the number of particles n is odd, a systematic error is done. It can be corrected by choosing s uniformly on $(0, \frac{n-1}{n})$ rather than $(0, 1)$ for n odd.

Also, variants are possible : one can choose s_i for each i rather than a global s ; this is equivalent to inverting \int_0^1 and \sum_i in (31). Another variant consists in using a majorant collision frequency as described in section II ; the advantage is to use the same number of cycles for each cell which is better for vectorization. In order to avoid the restriction (34) on the timestep, L. Desvilletes [9] proposed also a variant where Δt can be as large as necessary. His method is also very close to the DSMC method and works pretty well on practical examples.

Finally, we would like to point out that the DSMC method and this random particle method are very similar. In some sense the DSMC method uses a time step n time smaller and performs one collision per timestep. Here the timestep is n time larger and n possible collisions are done at once so that the computational time between the majorant frequency technique and the present method are comparable. Comparisons can be found in Struckmeier and Steiner [26]. Recall that the Monte-Carlo method is now reduced to the generation of independant variables with a specified repartition law. This is a whole problem in itself.

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ISSN 0249 - 6399



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