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**A VECTORIZABLE SIMULATION METHOD
 FOR THE BOLTZMANN EQUATION (*)**

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Abstract — This paper deals with a conservative Monte Carlo method for the Boltzmann equation, which allows to take into account long time steps as well as small ones. Numerical results for the Boltzmann equation and for the Kac model are compared with those of the classical Direct Simulation Monte Carlo (DSMC) method.

Résumé. — On propose dans cet article une méthode de Monte Carlo conservative pour l'équation de Boltzmann. Cette méthode permet de prendre en compte des pas de temps plus longs que ceux usuellement utilisés. Les résultats numériques calculés par cette méthode pour l'équation de Boltzmann et de Kac sont ensuite comparés à ceux obtenus avec la méthode DSMC habituelle.

1. INTRODUCTION

There has been lately a growing interest in numerical computations for rarefied gases. In the upper atmosphere, the Navier-Stokes model becomes physically irrelevant, and one has to come back to a kinetic description of the gas. In this theory the unknown quantity is the nonnegative density $f(t, x, v)$, representing the gas molecules which at time t and point x move with velocity v . This density satisfies the Boltzmann equation :

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = Q(f), \tag{1}$$

where $Q(f)$ is a quadratic kernel acting only on the velocity variable v :

$$Q(f)(v) = \int_{v_1 \in \mathbb{R}^3} \int_{\sigma \in S^2} \{f(v'_1) f(v') - f(v_1) f(v)\} \times \\ \times B(v, v_1, \sigma) dv_1 d\sigma, \tag{2}$$

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and

$$v' = \frac{v + v_1}{2} + \frac{|v - v_1|}{2} \sigma, \quad (3)$$

$$v'_1 = \frac{v + v_1}{2} - \frac{|v - v_1|}{2} \sigma. \quad (4)$$

The cross section B is nonnegative and depends only upon $|v - v_1|$ and $(v - v_1) \cdot \sigma$. The assumption of hard potentials is often made by physicists (*cf.* [Ce]). However, in an upper atmosphere context, engineers often use the « Variable Hard Spheres » model, noted VHS, where

$$B(v, v_1, \sigma) = K |v - v_1|^\alpha, \quad (5)$$

and the parameters $K \in \mathbb{R}^+$ and $\alpha \in]0, 1]$ depend on the considered gas. The examples in this paper are given for $K = 1$ and $\alpha = 0.5$.

The dimension of the phase space for the Boltzmann equation is 6. Therefore, in order to solve numerically equation (1), one generally uses a *particle* method (*cf.* [Na]), where the density $f(t, x, v)$ is discretized as

$$f(t, x, v) \approx \sum_{i=1}^N r_i(t) \delta_{x_i(t), v_i(t)}. \quad (6)$$

Then, it is usual to split equation (1) into its free transport part

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = 0, \quad (7)$$

and its collisional part

$$\frac{\partial f}{\partial t} = Q(f). \quad (8)$$

At each time step Δt , equations (7), (8) are solved one after another. Classical methods of trajectography are used to solve equation (7), i.e. particles which are at time t at $(x_i(t), v_i(t))$ in the phase space, will be at time $t + \Delta t$ at $(x_i(t) + \Delta t v_i(t), v_i(t))$, except if they have encountered a boundary (*cf.* [Il, Ne]). Note that this method is vectorizable. Then, the computational domain is divided into small cells and equation (8) is solved in each cell.

However, the time step Δt is fixed by constraints independent of equation (8). It must be small enough for the splitting to hold, but an average particle must cross at least one cell per time step, lest the convergence to the steady state be too slow. Moreover, Δt will be the same for every cell, and therefore in some cells it will be very small in front of a characteristic time of equation (8) (for example at the rear of a body), or very large (for example at the front of a body).

Note also that in equation (8), the macroscopic quantities $\int_{v \in \mathbb{R}^3} f(t, v) dv$, $\int_{v \in \mathbb{R}^3} v f(t, v) dv$, and $\int_{v \in \mathbb{R}^3} \frac{v^2}{2} f(t, v) dv$, representing the mass, momentum and kinetic energy are conserved.

We look in this work for a method conserving exactly the above quantities. It means that the collisional process has to be symmetric. Therefore in the discretization of f , the mathematical representativity $r_i(t)$ of the particles is assumed to be constant in each cell and at a given time step. Accordingly, in each cell, we write

$$f(t, v) = \sum_{i=1}^N r \delta_{v_i(t)}. \quad (9)$$

Now classical methods (conserving momentum and energy) are based on the fact that if Δt is small enough, the probability of a particle of velocity v_i to collide with a particle of velocity v_j during the time interval $[t, t + \Delta t]$ is

$$P_{i,j} = r \Delta t K [v_i - v_j]^\alpha. \quad (10)$$

In Bird's method (*cf.* [Bi]), collisions are performed sequentially and a time counter is advanced after each collision, therefore the time step Δt can become very large without problem, but the process is not vectorizable. On the other hand, in the classical DSMC method, an upper bound q_* of $|v_i - v_j|^\alpha$ is generally taken, and

$$\mathcal{N} = N^2 r \Delta t K q_* \quad (11)$$

particles are selected. The particles belonging to this set are taken by pairs, and for each pair of particles with velocities v_i and v_j the collision is made with probability $|v_i - v_j|^\alpha / q_*$.

Therefore, all collisions can be made at the same time, but the time step Δt must be small enough for the linearization implied by equations (10), (11) to hold (in particular one needs at least the estimate $N r \Delta t q_* < 1$). Since in most regions of the domain of computation the time step Δt will be too large, it is necessary to divide it in smaller time steps δt (typically $\delta t = \frac{\Delta t}{5}$). This is of course a penalization to the vectorization rate.

Our goal is to present here a method which enables to consider time steps Δt larger than in the DSMC method, having a good vectorization rate and conserving the mass, momentum and energy. This method retains some ideas used in non-conservative schemes (*cf.* [Na]).

The organization of the paper is as follows : in section 2, we present Kac model, the classical DSMC model for Kac and Boltzmann equations, and the

method we propose for those equations Section 3 is devoted to the discussion of the numerical results

The reader can find explanations on DSMC methods in the context of the reentry of a space vehicle in the upper atmosphere in [Ba] for example

2. DSMC METHODS FOR KAC AND BOLTZMANN EQUATIONS

2.1. The Kac model

Let us introduce Kac’s model in which the method we propose has a simple interpretation In this model a one-dimensional gas is characterized by a density $f(t, v)$ of molecules which at time t , move with velocity v This distribution satisfies Kac’s equation

$$\frac{\partial f}{\partial t}(t, v) = \int_{v_1 \in \mathbb{R}} \int_{\theta \in [-\pi, \pi]} \times \{f(t, v^*) f(t, v_1^*) - f(t, v) f(t, v_1)\} \frac{d\theta}{2\pi} dv_1, \quad (12)$$

where

$$v^* = v \cos \theta - v_1 \sin \theta, \quad (13)$$

$$v_1^* = v \sin \theta + v_1 \cos \theta \quad (14)$$

The mass $\int_{v \in \mathbb{R}} f(t, v) dv$ and the kinetic energy $\int_{v \in \mathbb{R}} f(t, v) \frac{v^2}{2} dv$ are conserved, but not the momentum $\int_{v \in \mathbb{R}} f(t, v) v dv$ (though if f is even at time $t = 0$, then it remains even for $t > 0$) As in the case of the Boltzmann equation, f is discretized under the form

$$f(t, v) = \sum_{i=1}^N r_i \delta_{v(t)} \quad (15)$$

2.2. The classical DSMC method.

For Kac’s model, the probability of a given particle to collide during the (small) time interval $[t, t + \Delta t]$ is given by

$$P_c = Nr \Delta t \quad (16)$$

Therefore $\lfloor NP_c/2 \rfloor$ pairs of particles are selected (in a stochastic way, with a uniform probability) to collide, and for each pair i, j of particles, an angle

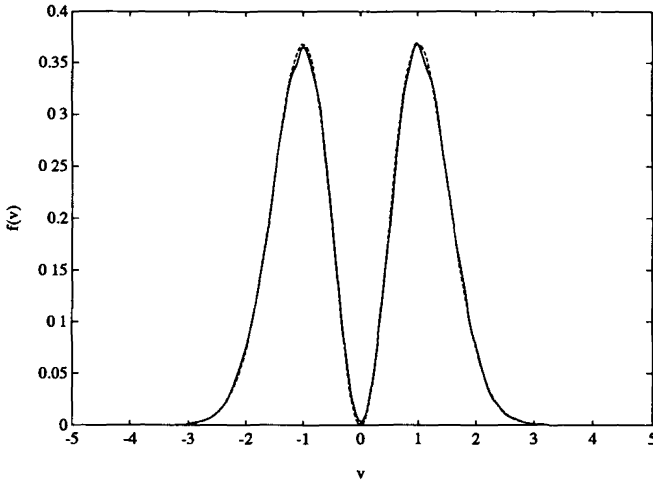


Figure 1. — Initial condition $f_0(v)$ given by equation (34) for the Kac equation versus velocity v . The dashed line represents the analytical solution and the full line the Monte Carlo simulation of this initial datum with 5 000 particles.

θ_{ij} is determined with a uniform probability on $[0, 2\pi]$. Then, new velocities

$$v_i^* = v_i \cos(\theta_{ij}) - v_j \sin(\theta_{ij}), \tag{17}$$

$$v_j^* = v_i \sin(\theta_{ij}) + v_j \cos(\theta_{ij}), \tag{18}$$

are assigned to the particles i, j .

The case of the Boltzmann equation is slightly more complex, and the *dummy collision* method is used. In this method a number q_i is determined, such that

$$q_i \geq \max_{i,j} K |v_i - v_j|^\alpha, \tag{19}$$

and $\lfloor N^2 r q_i \Delta t / 2 \rfloor$ pairs of particles are selected to collide in a fictitious way. For each selected pair i, j , the collision is said to be « real » with the probability

$$P_{i,j}^{f \rightarrow r} = K |v_i - v_j|^\alpha / q_i. \tag{20}$$

When the collision is real, an angle σ_{ij} is determined uniformly on S^2 , and new velocities

$$v_i' = \frac{v_i + v_j}{2} + \frac{|v_i - v_j|}{2} \sigma_{ij}, \tag{21}$$

$$v_j' = \frac{v_i + v_j}{2} - \frac{|v_i - v_j|}{2} \sigma_{ij}, \tag{22}$$

are assigned to the particles i, j .

Of course, this algorithm is precise only if $Nr \Delta t \ll 1$ in the case of the Kac equation, and if $Nrq_* \Delta t \ll 1$ for the Boltzmann equation. Note that when $Nrq_* \Delta t > 1$, the algorithms cannot work. Therefore, the time step Δt imposed by the trajectography is often divided, and a new time step $\delta t = \Delta t/5$ for example is taken.

2.3 The modified DSMC method : the case of Kac equation

Because of the conservation of mass, the loss term in Kac equation is

$$\begin{aligned} Lf(v) &= -\frac{1}{2\pi} \int_{v_1 \in \mathbb{R}} \int_{\theta \in [0, 2\pi]} f(t, v_1) f(t, v) d\theta dv_1 \\ &= -\left(\int_{v_1 \in \mathbb{R}} f(0, v_1) dv_1 \right) f(t, v). \end{aligned} \tag{23}$$

It is therefore the same as in a linear transport equation (cf. [Pa]). Accordingly, the number of collisions for the particles involved in equation (12) follows a Poisson's law with possible repetition.

The probability for each particle to be involved in exactly k collisions is

$$\mathcal{P}_k^K = \exp(-Nr \Delta t) \frac{(Nr \Delta t)^k}{k!}, \tag{24}$$

therefore, the probability for a particle to be involved in at least k collisions is

$$\mathcal{Q}_k^K = 1 - \exp(-Nr \Delta t) \sum_{s=0}^{k-1} \frac{(Nr \Delta t)^s}{s!}. \tag{25}$$

Thus, to model Kac's equation, we make in a first step $\lfloor N\mathcal{Q}_1^K/2 \rfloor$ collisions, then in a second step $\lfloor N\mathcal{Q}_2^K/2 \rfloor$, then $\lfloor N\mathcal{Q}_3^K/2 \rfloor$, etc... But of course, the sequence \mathcal{Q}_k^K is rapidly decreasing and it is not necessary in a realistic simulation to consider \mathcal{Q}_k^K for $k \geq 4$.

Therefore, we state the algorithm of our methods as follows :

For each time step, we make three rounds of collisions,

1. In the first round, we select $\lfloor N\mathcal{Q}_1^K/2 \rfloor$ pairs of particles, such that a given particle can be in at most one pair. This selection is made in a stochastic way. For each pair, the particles collide as in the DSMC method.

2. Then, in the second round, we select $\lfloor N\mathcal{Q}_2^K/2 \rfloor$ pairs of colliding particles.

3. Finally, in the third round, we select $[N \mathcal{Q}_3^K/2]$ pairs of colliding particles.

Remark : Indeed the above algorithm take into account a bigger number of collisions for each prescribed particle and therefore it leads naturally to a larger time step.

2.4. The modified DSMC method : the case of the Boltzmann equation

In this section, we extend the method proposed in subsection 2.3 to the Boltzmann equation (with the VHS cross section) :

$$\frac{\partial f}{\partial t} + \left(\int_{v_1 \in \mathbb{R}^3} f(v_1) K |v - v_1|^\alpha dv_1 \right) f(v) = \int_{v_1 \in \mathbb{R}^3} \int_{\sigma \in S^2} f(v'_1) f(v') K |v - v_1|^\alpha d\sigma dv_1. \quad (26)$$

The quantity $\int_{v_1 \in \mathbb{R}^3} f(v_1) K |v - v_1|^\alpha dv_1$ is not conserved any more, but $\alpha \in]0, 1[$ and therefore we hope that this quantity does not change too much in the interval $[t, t + \Delta t]$.

The *dummy collision* technique is still used. A number q_* such that

$$q_* \geq \max_{i,j} K |v_i - v_j|^\alpha \quad (27)$$

is computed.

The probability for each particle to be involved in exactly k fictitious collisions is now

$$\mathcal{P}_k^B = \exp(-Nr q_* \Delta t) \frac{(Nr q_* \Delta t)^k}{k!}. \quad (28)$$

Therefore, the probability for a particle to be involved in at least k fictitious collisions is

$$\mathcal{Q}_k^B = 1 - \exp(-Nr q_* \Delta t) \sum_{s=0}^{k-1} \frac{(Nr q_* \Delta t)^s}{s!}. \quad (29)$$

Let us define the quantity q_k^B as

$$q_k^B = 1 - \exp(-Nr K |v_i - v_j|^\alpha \Delta t) \sum_{s=0}^{k-1} \frac{(Nr K |v_i - v_j|^\alpha \Delta t)^s}{s!}. \quad (30)$$

Once again, we perform three rounds of collisions.

1 In the first round, $\lfloor N \mathcal{Q}_1^B/2 \rfloor$ pairs of particles are selected in a stochastic way, such that a given particle can belong to at most one pair. Then for each pair i, j of particles, the collision is said to be real with a probability

$$P_{i \rightarrow j}^f = \frac{q_1^B}{\mathcal{Q}_1^B} \quad (31)$$

Then, each real collision is made as in the classical DSMC method, according to equations (21), (22)

2 In the second round, $\lfloor N \mathcal{Q}_2^B/2 \rfloor$ pairs are selected, and for each pair i, j , the collision is said to be real with a probability

$$P_{i \rightarrow j}^f = \frac{q_2^B}{\mathcal{Q}_2^B}, \quad (32)$$

and each real collision is performed

3 Finally, in the third round, $\lfloor N \mathcal{Q}_3^B/2 \rfloor$ pairs are selected, and for each pair i, j , the collision is made with a probability

$$P_{i \rightarrow j}^f = \frac{q_3^B}{\mathcal{Q}_3^B}, \quad (33)$$

and, once again, each real collision is performed

Note that a given particle can be part of a colliding pair in either of the three rounds. Accordingly, the algorithm is vectorizable within each of the three rounds, but the rounds must be made consecutively

3 NUMERICAL RESULTS

3.1. Kac equation

For the Kac equation, the initial condition

$$f_0(v) = v^2 \exp(-v^2) \quad (34)$$

leads to an explicit solution

$$f(t, v) = \left(\frac{3}{4} (1 - c(t)) \sqrt{c(t)} + \frac{1}{2} (3c(t) - 1) c(t)^{3/2} v^2 \right) \exp(-c(t)v^2), \quad (35)$$

with

$$c(t) = \frac{1}{3 - 2 \exp(-\sqrt{\pi} t/16)} \quad (36)$$

We compare in this section the numerical results of the classical and the modified DSMC methods for the Kac equation with initial condition equation (34) All the simulations are made with 5 000 particles

We have chosen to compare the classical DSMC method with a time step $\delta t_C = 0.5$ and the modified DSMC method with a time step $\Delta t_M = 2.5$ The quantity $\delta t_C = 0.5$ corresponds to a probability of collision for a particle in the classical DSMC method of $Nr\delta t_C \approx 0.4$, which is reasonable (remember that $Nr\delta t_C$ must be less than 1) Since the original time step is typically divided by 5 for the classical DSMC method, we have taken $\Delta t_M = 2.5$ for the modified DSMC method (where the original time step is not divided)

We have selected the following criterions to compare the results If f is the explicit solution, f_C the solution obtained by the classical DSMC method and f_M the solution obtained by the modified DSMC method, we calculate the solution f_C and f_M from the particle representation by means of a convolution formula

$$\tilde{f}(v) = \sum_1^N rW_H(v_i - v), \tag{37}$$

where

$$W_H(v) = \begin{cases} (3/4 - (|v|/H)^2)/H & \text{if } |v| \leq H/2, \\ (1/2 - (|v|/H)^2)/2H & \text{if } H/2 \leq |v| \leq 3H/2, \\ 0 & \text{otherwise} \end{cases} \tag{38}$$

We compute

- 1 the L^2 norms $\int_{v \in \mathbb{R}} |f_C - f|^2 dv(t)$ and $\int_{v \in \mathbb{R}} |f_M - f|^2 dv(t)$,
- 2 the first moments $a_1 = \int_{v \in \mathbb{R}} |v| f(t, v) dv$, $\int_{v \in \mathbb{R}} |v| f_M(t, v) dv$ and $\int_{v \in \mathbb{R}} |v| f_C(t, v) dv$, and
- 3 the fourth moments $a_4 = \int_{v \in \mathbb{R}} |v|^4 f(t, v) dv$, $\int_{v \in \mathbb{R}} |v|^4 f_M(t, v) dv$ and $\int_{v \in \mathbb{R}} |v|^4 f_C(t, v) dv$

The results concerning the L^2 -norms are given in table 1, those concerning the first and fourth moments in figure 3 and figure 4 respectively Note that the moments are more important than the L^2 -norms in a realistic situation (even in the case of the Boltzmann equation, since they represent macroscopic quantities), moreover the *particle* discretization is well adapted to their computation

We comment now the results of table 1, figure 3 and figure 4

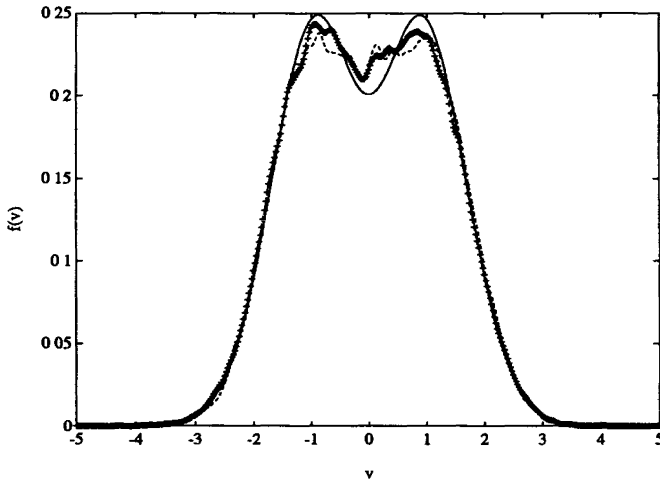


Figure 2. — Solution $f(v)$ of the Kac equation versus velocity v , at time $t = 2.5$. The full line represents the analytical solution, the crosses correspond to the numerical solution obtained with the classical DSMC method for $\delta t_C = 0.5$, and the dashed line to the numerical solution obtained with the modified DSMC method for $\Delta t_M = 2.5$.

Table 1. — L_2 norms of the difference between the analytical solution and the Monte Carlo solutions for Kac equation. The first column corresponds to the classical DSMC method with $\delta t_C = 0.5$, and the second column corresponds to the modified DSMC method with $\Delta t_M = 2.5$.

Time	Norm L_2 , $\delta t_C = 0.5$	Norm L_2 , $\Delta t_M = 2.5$
0.0	0.003192	0.003192
0.5	0.008876	
1.0	0.014177	
1.5	0.017159	
2.0	0.016740	
2.5	0.012189	0.020704
3.0	0.019144	
3.5	0.015511	
4.0	0.008882	
4.5	0.006343	
5.0	0.007669	0.005947
5.5	0.008094	
6.0	0.004198	
6.5	0.004018	
7.0	0.003972	
7.5	0.004398	0.002278

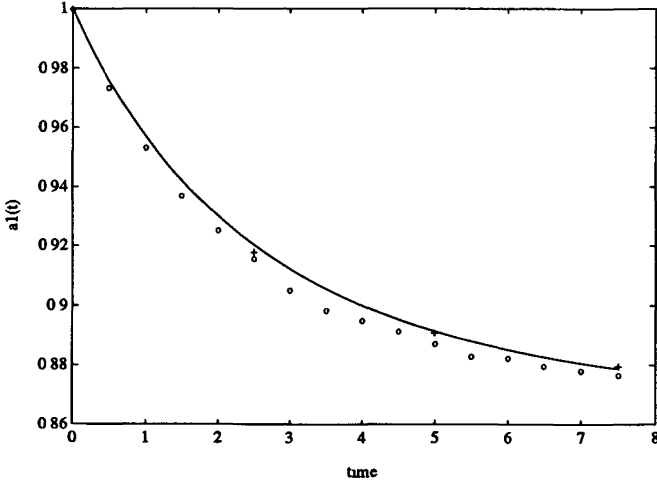


Figure 3. — First moment a_1 of the Kac equation versus time. The full line represents the analytical solution, the circles correspond to the numerical solution obtained by the classical DSMC method for $\delta t_C = 0.5$, and the crosses to the numerical solution obtained by the modified DSMC method for $\Delta t_M = 2.5$.

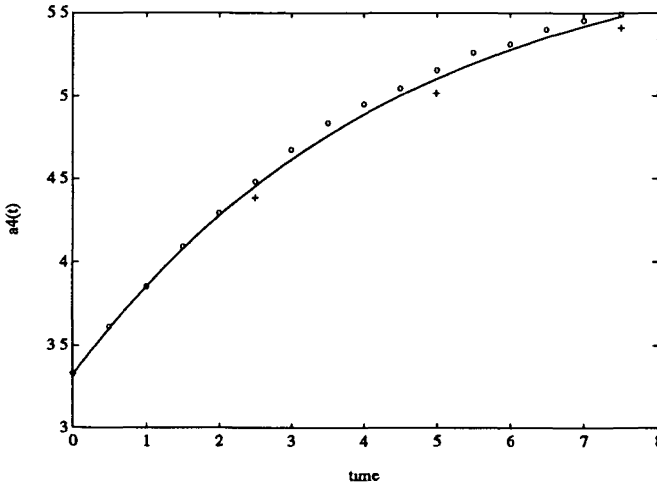


Figure 4. — Fourth moment a_4 of the Kac equation versus time. The full line represents the analytical solution, the circles correspond to the numerical solution obtained with the classical DSMC method for $\delta t_C = 0.5$, and the crosses to the numerical solution obtained with the modified DSMC method for $\Delta t_M = 2.5$.

1 The mean value of the norm $\|f - f_C\|_{L^2}$ between the times 1.5 and 3.5 is about 0.016, whereas $\|f - f_M\|_{L^2}(2.5) \approx 0.020$. However, the mean value of $\|f - f_C\|_{L^2}$ between the times 4.0 and 6.0 is about 0.007, whereas $\|f - f_M\|_{L^2}(5.0) \approx 0.006$. One can say that the precision of the two methods with respect to the norm is about the same.

2 The precision of the modified DSMC method with respect to the first moment a_1 is slightly better than that of the classical DSMC method. However, it is just the opposite for the fourth moment a_4 . (Note that in the computation of this moment, only large velocities are taken into account, and therefore the statistical error can become important.)

We can conclude that the precisions of the two methods are almost the same.

We compare now the number of collisions. The classical DSMC method needs about 55 300 collisions for a time interval of 2.5. The modified DSMC method needs about 22 300 collisions for the first round, 16 200 collisions for the second round and 2 500 collisions for the third and last round. Therefore a total 48 000 collisions is needed. The gain of 15%, which is sensible for the Kac's equation, becomes far more important in the case of the Boltzmann equation (where some collisions are fictitious).

Note that the number of collisions need not be the same in different methods, since the effect of one collision depends on whether one is near the equilibrium or not (at the limit, when the equilibrium is reached, the collisions have no effects at all).

Note also that the vectorization rate is better in the modified method, since three consecutive rounds of collisions are necessary, whereas in the classical method, it needs five consecutive sessions of collisions.

Finally, we put the stress on another advantage of the modified method. If Δt becomes so large that even for $\delta t = \Delta t/5$, one has $Nr\delta t > 1$, the classical method cannot work, whereas the modified method still works with a reasonable precision as is shown in figure 5 and figure 6. (These figures show the first and fourth moments of the Kac equation for the modified DSMC method with the time step $\delta t = 5.0$).

In figure 2 we can see the analytical solution, the classical DSMC solution, and the solution calculated with the modified DSMC method at the time $t = 2.5$. We can observe that both Monte Carlo simulations follow the behavior of the analytical solution. This figure must be compared with figure 1, where the initial datum is drawn, together with its particle discretization.

3.2. Boltzmann equation

As announced in the introduction, we take for the cross section the parameters $K = 1$ and $\alpha = 0.5$. Since the only known explicit solutions for

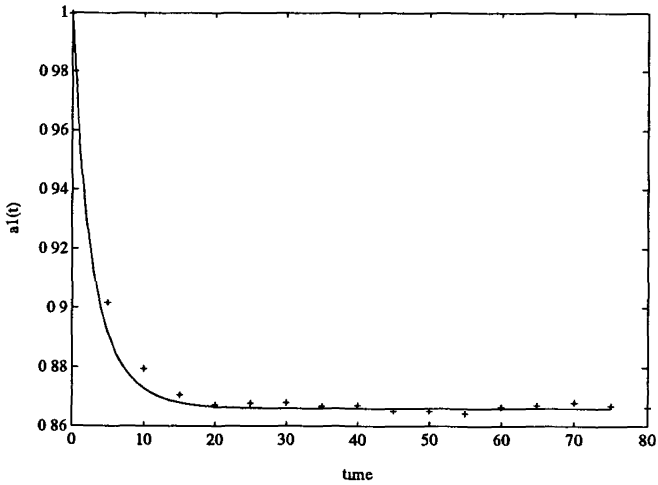


Figure 5. — First moment a_1 of the Kac equation versus time. The full line represents the analytical solution, the crosses correspond to the numerical solution obtained with the modified DSMC method for $\Delta t_M = 5.0$.

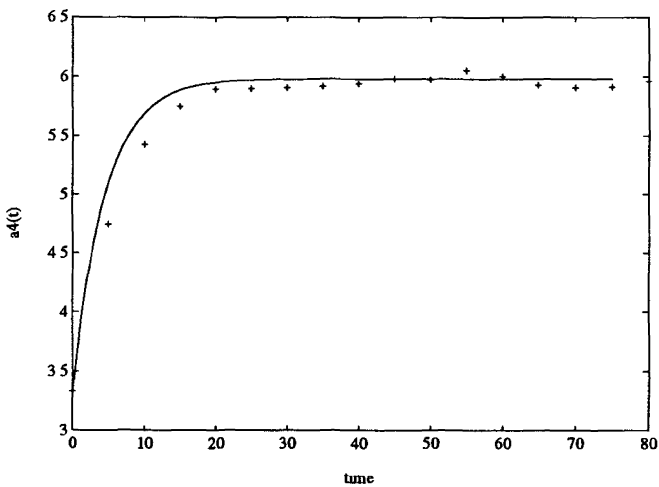


Figure 6. — Fourth moment a_4 of the Kac equation versus time. The full line represents the analytical solution, the crosses correspond to the numerical solution obtained with the modified DSMC method for $\Delta t_M = 5.0$.

the Boltzmann equation are with $\alpha = 0$, we cannot compare our numerical simulations with an analytical curve. We compute however a reference solution $f_r(t, v)$ for the initial condition

$$f_0(v) = \mathbf{1}_{v_x \in [-1, 1]} (\mathbf{1}_{v_x \in [-1, 1]} \mathbf{1}_{v_y \in [1, 3]} + \mathbf{1}_{v_x \in [2, 4]} \mathbf{1}_{v_y \in [0, 2]}), \quad (39)$$

and it is computed with a very small time step $\Delta t = 0.00005$ and 40 000 particles (with the classical DSMC method). Next, we compute the function f_C with the classical DSMC method with a time step $\delta t_C = 0.0143$ and the function f_M with the modified DSMC method with a time step $\Delta t_M = 5 \delta t_C = 0.0714$.

Two criterions are selected

1. The second moments $m_2^r = \int_{v \in \mathbb{R}^3} f_r(v) v_x v_y dv$, $m_2^C = \int_{v \in \mathbb{R}^3} f_C(v) v_x v_y dv$, and $m_2^M = \int_{v \in \mathbb{R}^3} f_M(v) v_x v_y dv$ are given in figure 7.
2. The fourth moments $m_4^r = \int_{v \in \mathbb{R}^3} f_r(v) (v_x^4 + v_y^4 + v_z^4) dv$, $m_4^C = \int_{v \in \mathbb{R}^3} f_C(v) (v_x^4 + v_y^4 + v_z^4) dv$, and $m_4^M = \int_{v \in \mathbb{R}^3} f_M(v) (v_x^4 + v_y^4 + v_z^4) dv$ are given in figure 8.

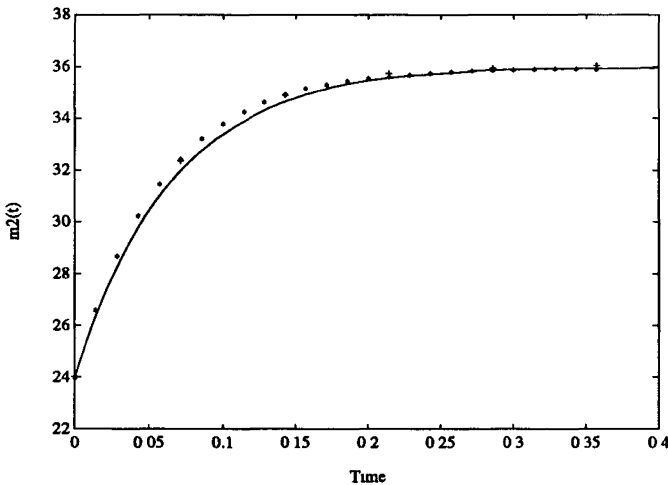


Figure 7. — Second moment m_2 of the Boltzmann equation versus time. The full line represents the reference solution obtained with $\Delta t = 0.00005$, the stars represent the numerical solution obtained with the classical DSMC method for $\delta t_C = 0.0143$ and the crosses correspond to the numerical solution obtained by the modified DSMC method for $\Delta t_M = 0.0714$.

We can see that the modified DSMC method gives slightly better results for the second moment m_2 , see figure 7, and that the two considered methods are equivalent for the fourth moment m_4 , see figure 8. We can make the same observation (about the importance of statistical errors) as in the case of the Kac equation for the fourth moment.

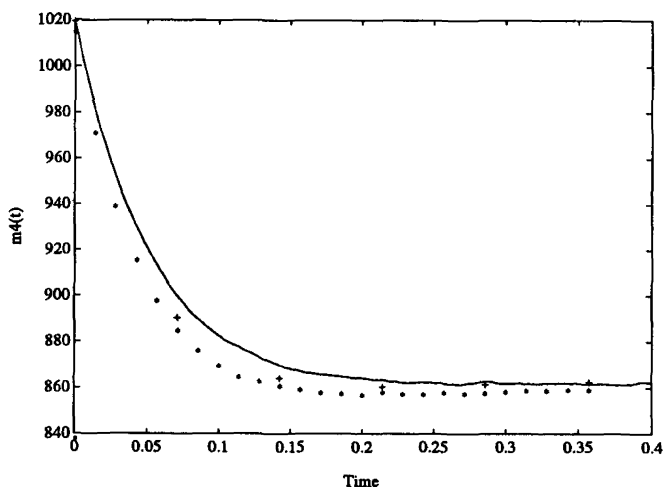


Figure 8. — Fourth moment m_4 of the Boltzmann equation versus time. The full line represents the reference solution obtained with $\Delta t = 0.00005$, the stars represent the numerical solution obtained with the classical DSMC method for $\delta t_C = 0.0143$, and the crosses correspond to the numerical solution obtained by the modified DSMC method for $\Delta t_M = 0.0714$.

The number of collisions for a time interval of 0.0714 is about 42 000 for the classical DSMC method, whereas for the modified DSMC method, the number of collisions is 9 800 for the first round, 9 100 for the second and 7 600 for the third, which gives a total number of 26 600, and the gain in the number of collisions is about 35 %.

Finally, the remarks about the number of collisions, the vectorization rate and the case when $Nr q_* \delta t > 1$ that we made for Kac equation are still valid in the more realistic case of the Boltzmann equation.

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REFERENCES

- [Ba] H. BABOVSKI, 1986, On a simulation scheme for the Boltzmann equation, *Math. Med. Appl. Sc.*, **8**, 223-233.
- [Bi] G. A. BIRD, 1976, *Molecular gas dynamics*, Clar. Press, Oxford.
- [Ce] C. CERCIGNANI, 1988, *The Boltzmann equation and its applications*, Springer, Berlin.
- [Il, Ne] R. ILLNER, H. NEUNZERT, 1987, On simulation methods for the Boltzmann equation, *Tr. Th. Stat. Phys.*, **16**, 141-154.
- [Ba] K. NAMBU, 1983, Interrelations between various direct simulations methods for solving the Boltzmann equation, *J. Phys. Soc. Jap.*, **52**, 3382-3388.
- [Pa] G. C. PAPANICOLAOU, 1975, Asymptotic analysis of transport processes, *Bull. A.M.S.*, **81**, 330-392.