

Brownian Approximation and Monte Carlo Simulation of the Non-Cutoff Kac Equation

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Abstract The non-cutoff Boltzmann equation can be simulated using the DSMC method, by a truncation of the collision term. However, even for computing stationary solutions this may be very time consuming, in particular in situations far from equilibrium. By adding an appropriate diffusion, to the DSMC-method, the rate of convergence when the truncation is removed, may be greatly improved. We illustrate the technique on a toy model, the Kac equation, as well as on the full Boltzmann equation in a special case.

Keywords Kac equation · Direct simulation Monte Carlo · Diffusion approximation · Thermostat · Non-equilibrium stationary state · Markov jump process

The Boltzmann equation describes the evolution of the phase space density of a gas. It is a nonlinear equation in many dimensions, which makes it difficult to treat by e.g. finite difference methods. The classical way of solving the Boltzmann equation numerically is by means of Monte Carlo simulation. The method was first described by Bird (see the book [4]), but since then many variations on the theme have been published [2, 23, 25, 29].

Very briefly, the DSMC-method can be described as follows: The gas is represented by a finite (although sometimes rather large) number of particles. The time evolution is then carried out by alternating a transport step, in which the particles move independently with their own velocity, and a collision step. The spatial domain of calculation is divided into cells which should be large enough that it typically contains a not too small number of particles, but still small enough to take into account the spatial gradients in the problem.

The collision step is then carried out in each cell separately as a jump process in \mathbb{R}^{3n} , where n is the number of particles, and the jumps occur as the velocity change in classical collisions between randomly chosen pairs of particles. The collisions conserve en-

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ergy and momentum, so the jump process actually takes place on $\{(v_1, \dots, v_n) \in \mathbb{R}^{3n} \mid \sum v_k = u \in \mathbb{R}^3, \sum v_k^2 = W\}$.

The simulation can be understood as a sampling of the solution of a Poisson driven stochastic differential equation. In the original DSMC methods, the rate of the underlying Poisson process was always taken to be finite, but there are at least two reasons for considering infinite (or very large) collision rates. The first one occurs when the density of the gas is very large in a cell, i.e. when n is very large. One way of handling that situation is to sample the velocity distribution at the end of a collision step as a suitable mixture of a distribution as the one that results from a moderate number of collisions and the equilibrium distribution, which is a Maxwellian [25–27].

The other case derives from the fact that many realistic collision models correspond to long-range potentials, which effectively gives rise to an infinite collision rate. The vast majority of collisions only change the velocities marginally, and so the rate of change of momentum due to collisions is finite.

To carry out a Monte Carlo simulation in this situation, one may truncate the jump process so as to obtain a finite collision rate. It has been proven [10, 13, 14] that truncated Monte Carlo methods converge as the truncation is lifted, and this has also been illustrated by numerical experiments. However, we have found that in certain cases, in particular when the stationary solutions are far from equilibrium, the jump rate must be truncated at a very high (and so, costly) level to get an acceptable accuracy.

We propose here a method to replace the small jumps by an appropriate diffusion, and show by example that this gives an important improvement of the accuracy compared to just ignoring the small jumps. This has been inspired by the works [1, 30], where this technique is proposed for simulating Lévy processes in \mathbb{R}^n .

There are, of course, other methods than the Monte Carlo methods, for solving the Boltzmann equation, and in particular there are fast methods based on the Fourier transform, that have been used successfully for the non-cutoff situation [11, 12, 22].

This study was motivated by the difficulty of obtaining accurate estimations of the non-equilibrium stationary state for a non-cutoff collision kernel, and of the theoretical results in [5], where the one-dimensional Kac equation with a Gaussian thermostat was studied. Also in this paper, the main part is devoted to the Kac equation. The diffusion term is then a Brownian motion on the sphere S^{n-1} , and the approximation is very straight forward. We describe the method in some detail for this case. However, from a conceptual point of view, the method is not restricted to one-dimensional models, and we have also carried out numerical calculations for the Boltzmann equation with a thermostat and Maxwellian non-cutoff collisions. In that case, the diffusion model is more complicated (it is essentially the Balescu-Prigogine model for Maxwellian molecules [18, 33]), and the actual calculation is carried out somewhat differently, as described in Sect. 3.

In [34, 36], it is shown that, contrary to the Kac equation, the Boltzmann equation with a thermostatted force field only has trivial stationary states, and hence it is only interesting to compare the evolution of the solutions. At the end of the paper, we present some numerical results for this model.

We note, finally, that for non-Maxwellian molecules the situation is rather different, and then it may in some cases be more appropriate to go the other way around and to approximate the diffusion process by a non-cutoff collision process [7].

1 The Kac Equation, the Master Equation and Monte Carlo Simulations

We consider a system of n particles that are entirely characterized by their one-dimensional velocities v_i , $i = 1, \dots, n$. These velocities undergo random jumps,

$$\begin{aligned}
 &(v_1, \dots, v_j, \dots, v_k, \dots, v_n) \\
 &\mapsto R_{j,k,\theta}(v_1, \dots, v_j, \dots, v_k, \dots, v_n) \\
 &= (v_1, \dots, v_j \cos \theta - v_k \sin \theta, \dots, v_j \sin \theta + v_k \cos \theta, \dots, v_n), \\
 &1 \leq j, k \leq n, \theta \in] - \pi, \pi].
 \end{aligned}
 \tag{1}$$

These jumps occur independently with a rate proportional to

$$n^{-1}b(\theta)d\theta. \tag{2}$$

This is the Kac model of a dilute gas [17]. In the original paper, $b(\theta) = (2\pi)^{-1}$, i.e. all rotation angles θ are equally probable.

We note that the jumps are rigid rotations in a plane spanned by a pair of velocities, and hence it is clear that the kinetic energy, $W = \frac{1}{2} \sum_{j=1}^n v_j^2$ is preserved, and therefore this describes a jump process with values in $S^{n-1}(\sqrt{2W})$. It is convenient to choose $2W = n$.

Another important thing to notice is the factor n^{-1} in (2); this implies that for the rate of jumps that involve a particular velocity, e.g. v_1 , asymptotically does not depend on the number of velocities, n . However, in many physically realistic cases, the rate of jumps depend on the rotation angle, approximately as $|\theta|^{-(1+\alpha)}$, where $\alpha \in [0, 2[$. This implies that the total jump rate for the vector $\mathbf{v} = (v_1, \dots, v_j, \dots, v_k, \dots, v_n)$ is infinite. We speak about non-cutoff models as opposed to the cutoff models where b is replaced by some function \tilde{b} such that $\int_{-\pi}^{\pi} \tilde{b}(\theta) d\theta < \infty$.

This jump process may equally well be defined by the master equation, which describes the evolution of a phase space density under the process. We let $\Psi(t, \cdot) \in C([0, \infty[, L^1(S^{n-1}(\sqrt{n})))$, and assume that $\Psi(0, \cdot)$ is a non negative density on $S^{n-1}(\sqrt{n})$. Then Ψ satisfies the equation

$$\partial_t \Psi^n(t, \mathbf{v}) = \frac{2}{n} \sum_{1 \leq j < k \leq n} \int_{-\pi}^{\pi} (\Psi^n(t, R_{j,k,-\theta} \mathbf{v}) - \Psi^n(t, \mathbf{v})) b(\theta) d\theta, \tag{3}$$

which is known as Kac’s master equation. The superscript n denotes the number of variables in the model, and this corresponds to the number of particles in a cell. Kac proved that if one considers the family of master equations for $\Psi_n, n = 0, \dots, \infty$, with initial data Ψ_0^n that is symmetric with respect to permutation of the variables, and such that the marginal densities $\Psi_{k,0}^n(v_1, \dots, v_k)$ satisfy

$$\lim_{n \rightarrow \infty} \Psi_{k,0}^n(v_1, \dots, v_k) = \lim_{n \rightarrow \infty} \prod_{j=1, \dots, k} \Psi_{1,0}^n(v_j). \tag{4}$$

Then also the time evolved density $\Psi^n(t, \mathbf{v})$ factories into a product of one-particle marginals $f(t, v) \equiv \Psi_1^n(t, v)$, and that $f(t, v)$ satisfies the so-called Kac equation

$$\partial_t f = Q(f, f), \tag{5}$$

where the collision operator Q

$$Q(g, g)(v) = \int_{\mathbb{R}} \int_{-\pi}^{\pi} (g(v')g(v'_*) - g(v)g(v_*))b(\theta) d\theta dv_*, \tag{6}$$

and where

$$(v', v'_*) = (v \cos \theta - v_* \sin \theta, v \sin \theta + v_* \cos \theta). \tag{7}$$

Compared to the real Boltzmann equation, the Kac equation is very easy to analyze mathematically, and we refer to [9, 21] for some of the basic results concerning existence and uniqueness of solutions, trend to equilibrium, etc.

From a numerical point of view, the connection between the jump process described in (1) and (2) and the Kac equation, is that one may regard

$$\frac{1}{n} \sum_{j=1}^n \delta_{v_j(t)} \tag{8}$$

as an approximation of the probability density $f(t, v)$, and it has been proven for many different cases that (8) does indeed converge to $f(t, v)$ (see [3, 28]).

The solutions of (5) converge to equilibrium exponentially as t increases to infinity, the equilibrium solution being a Gaussian function with mean zero. It is of interest to study situations where the stationary solution is not an equilibrium state. This is the case e.g. in kinetic models for dissipative systems (see e.g. [6, 8, 15]).

Another example comes from molecular dynamics and the introduction of thermostats, and which is used here as a test case for the Monte Carlo method with Brownian approximation.

The basic model is the one described in the beginning of this section, with a vector $\mathbf{v} \in \mathbb{R}^n$, that jumps according to (1). The difference in the thermostat model is that the velocity field is accelerated by a constant force field $\mathbf{E} = E(1, \dots, 1)$, which is projected on the tangent plane to the sphere $S^{n-1}(\sqrt{n})$. This means that between jumps, the a velocity component v_j satisfies

$$\frac{d}{dt} v_j(t) = E \left(1 - \frac{\sum v_k}{\sum v_k^2} v_j \right). \tag{9}$$

The physical interpretation is that each particle is accelerated by the same, constant, force field of strength E , but that a force field depending on the whole system of particles keeps the total kinetic energy fixed. The model is described more in details in [34, 36], where also the corresponding Kac equation is derived and analyzed. This Kac equation takes the form

$$\frac{\partial}{\partial t} f + E \frac{\partial}{\partial v} ((1 - \zeta(t)v)f) = Q(f, f), \tag{10}$$

where

$$\zeta(t) = \int_{\mathbb{R}} v f(v, t) dv. \tag{11}$$

The collision operator, Q is defined as before, in (6). The stationary states to this equation are far from Gaussian. One can show that for an integrable kernel, $\int_{-\pi}^{\pi} b(\theta) d\theta$, the stationary state becomes singular for sufficiently large values of E (see [35]), whereas in the non-cutoff case, the stationary state is C^∞ (see [5]). The latter case is really the motivation for the work presented in this paper, because it proved very difficult to get accurate numerical results using a truncated kernel.

2 Brownian Approximation

The evolution of the n -particle system (including a thermostatted force field of strength E) can be described by a stochastic differential equation driven by a Poisson random measure:

$$\begin{aligned} \mathbf{v}(t) = \mathbf{v}(0) + E \int_0^t \left(\mathbf{e} - \frac{\mathbf{e} \cdot \mathbf{v}(s)}{|\mathbf{v}(s)|^2} \mathbf{v}(s) \right) ds \\ + \sum_{1 \leq j < k \leq n} \int_0^t \int_{-\pi}^{\pi} A_{j,k}(\theta_{j,k}) \mathbf{v}(s_-) N(ds, d\theta_{j,k}). \end{aligned} \tag{12}$$

Here $A_{j,k}(\theta)$ is the $n \times n$ -matrix

$$A_{j,k}(\theta) = \begin{pmatrix} 1 & 0 & \dots & 0 & \dots & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & \dots & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & \cos \theta - 1 & \dots & -\sin \theta & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & \sin \theta & \dots & \cos \theta - 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & \dots & 0 & \dots & 1 & 0 \\ 0 & 0 & \dots & 0 & \dots & 0 & \dots & 0 & 1 \end{pmatrix}, \tag{13}$$

$\mathbf{e} = (1, 1, \dots, 1) \in \mathbb{R}^n$, and $N(ds, d\theta)$ is a Poisson random measure with intensity measure $n^{-1}b(\theta) d\theta dt$. In the non-cutoff case,

$$b(\theta) \sim |\theta|^{-(1+\alpha)} \tag{14}$$

near $\theta = 0$, and with $0 < \alpha < 2$, this implies that the total jump rate is infinite.

The Brownian approximation consists in replacing $N(ds, d\theta)$ in (12) by a truncated measure $\tilde{N}_\epsilon(ds, d\theta)$ with intensity measure $n^{-1}\tilde{b}_\epsilon(\theta) d\theta dt$, where \tilde{b} is defined by

$$\tilde{b}_\epsilon(\theta) = \min(b(\theta), b(\epsilon)), \tag{15}$$

and adding a Brownian term to compensate for the truncated part.

The explicit form of a stochastic differential equation whose solution is a Brownian motion on an n -dimensional sphere $S^{n-1}(r)$ can be found e.g. in [31], or in Øksendal’s book [24]:

$$X(t) = X(0) + \int_0^t \lambda r_W(X(s)) ds + \int_0^t \sqrt{\lambda} \sigma(X(s)) dW(s), \tag{16}$$

where $\{W(t)\}$ is a standard Wiener process in \mathbb{R}^n with mean zero and whose covariance is the identity matrix. The matrix σ projects the dW onto the tangent plane to $S^{n-1}(\sqrt{n})$ at X , its elements being given by

$$\sigma_{j,k}(\mathbf{x}) = \delta_{j,k} - \frac{x_j x_k}{|\mathbf{x}|^2}. \tag{17}$$

The drift term r_W is

$$r_W(x) = -\frac{n-1}{2} \frac{x}{|x|^2}. \tag{18}$$

The diffusion rate μ is computed so as to match the second moment of the truncated part of the jump measure:

$$\mu = \mu_\epsilon = \frac{2n}{n-1} \frac{1}{2} \int_{-\epsilon}^\epsilon (b(\theta) - b(\epsilon)) \theta^2 d\theta. \tag{19}$$

When $b(\theta) = |\theta|^{-(1+\alpha)}$, we find

$$\mu_\epsilon = \frac{2n}{n-1} \frac{1+\alpha}{3(2-\alpha)} \epsilon^{2-\alpha}. \tag{20}$$

Details of this calculation will be found in [32], where also the rate of convergence is analysed. One result is that while the generators of the processes corresponding to (14) with a truncated kernel converges with rate $\epsilon^{2-\alpha}$, the convergence rate is $\epsilon^{3-\alpha}$ when the Brownian term is added. When α is close to 2, the improvement is significant.

Adding the force term, like in (12), gives

$$\begin{aligned} \mathbf{v}(t) = & \mathbf{v}(0) + \int_0^t (r_{Th}(\mathbf{v}(s)) + r_W(\mathbf{v}(s))) ds + \int_0^t \sigma(\mathbf{v}(s)) dW(s) \\ & + \sum_{1 \leq j < k \leq N} \int_0^t \int_{-\pi}^\pi A_{j,k}(\theta_{j,k}) \mathbf{v}(s_-) N_\epsilon(ds, d\theta_{j,k}), \end{aligned} \tag{21}$$

where $r_{Th}(\mathbf{v}(t)) = \mathbf{e} - \frac{\mathbf{e} \cdot \mathbf{v}(s)}{|\mathbf{v}(s)|^2} \mathbf{v}(t) = \Gamma(\mathbf{v})\mathbf{e}$, Γ being the matrix with elements $\Gamma_{j,k} = \delta_{j,k} - v_j(t)v_k(t)/|\mathbf{v}|^2$, and where N_ϵ is a Poisson random measure with intensity measure $n^{-1} \tilde{b}_\epsilon(\theta) d\theta dt$.

3 The 3n Dimensional Master Equation and the Boltzmann Equation

The master equation that corresponds to the full Boltzmann equation and with an added thermostatted force term is [36]

$$\begin{aligned} \partial_t \Psi^n(t, \mathbf{v}) + \sum_{i=1}^n \frac{\partial}{\partial v_i} ([F - F \cdot \mathbf{j} - v_i] \Psi^n(t, \mathbf{v})) \\ = \frac{2}{n} \sum_{1 \leq j < k \leq n} \int_{S^2} (\Psi^n(t, R_{j,k,\omega} \mathbf{v}) - \Psi^n(t, \mathbf{v})) b(\theta) d\omega, \end{aligned} \tag{22}$$

where in this case, $\mathbf{v} \in \mathbb{R}^{3n}$, and where $R_{j,k,\omega}$ is an operator that models the collision of two particles,

$$(v_j, v_k) \mapsto \left(\frac{v_j + v_k}{2} + \frac{|v_j - v_k|}{2} \omega, \frac{v_j + v_k}{2} - \frac{|v_j - v_k|}{2} \omega \right).$$

In $b(\theta)$, $\theta = \arccos(\omega \cdot \frac{v_j - v_k}{|v_j - v_k|})$. To keep the notation similar to the one-dimensional case, we let $\mathbf{v} = (v_1, \dots, v_n)$, where $v_j \in \mathbb{R}^3$, $j = 1, \dots, n$. The non-cutoff case again corresponds to allowing $\int_{S^2} b(\theta) d\omega$ to diverge. The force field is $F = (E, 0, 0)$, and $\mathbf{j} = \frac{1}{n} \sum_{j=1}^n v_j$. At the level of the master equation, the Brownian approximation corresponds to truncating the non-cutoff jump rate, and replacing the truncated part by a suitable diffusion term. For the Kac equation, the diffusion is just the one given by the Laplace-Beltrami operator on the sphere S^{n-1} , but here it is rather the Balescu-Prigogine operator for Maxwellian interactions (see [18, 33]),

$$\frac{\mu}{n} \sum_{j \neq k} (\partial_{v_j} - \partial_{v_k}) |v_j - v_k|^2 P_{v_j - v_k}^\perp (\partial_{v_j} - \partial_{v_k}), \tag{23}$$

where P_z^\perp is the 3×3 -matrix $I - \frac{zz^{\text{tr}}}{|z|^2}$, and μ is a constant depending on the level of truncation.

Given this expression, one can write a stochastic equation much like (21). However, from a computational point of view, it does not seem to be efficient, because of the effort needed to compute σdW . An alternative, that gives good results at much lower computational cost, is to replace (23) by

$$\frac{\mu}{n} \sum_{j \neq k} \partial_{v_j} |v_j - v_k|^2 P_{v_j - v_k}^\perp \partial_{v_j}, \tag{24}$$

which corresponds to adding a Brownian motion $R_j dW_j \in \mathbb{R}^3$ to each velocity, where $R_j^{\text{tr}} R_j = \mu \sum_{j \neq k} (|v_j - v_k|^2 I - (v_j - v_k)(v_j - v_k)^{\text{tr}})$. The matrices R_j can be expressed in terms of moments and v_j , and hence the computational cost is proportional to the number of particles. The increments $(R_1 dW_1, \dots, R_n dW_n)$ still need to be projected onto the tangent space of the manifold of constant energy and momentum, but that is an operation that can be carried out in time proportional to the number of particles. Some numerical results are given in the following section.

4 Numerical Experiments

The numerical experiments have been carried out in the most direct way, with no large effort to make the code efficient. The large jumps have been simulated by computing exponentially distributed time intervals with rate proportional to $n \int_{-\pi}^\pi \tilde{b}(\theta) d\theta$. At the end of such an interval, a random pair (j, k) is chosen and the jump is effectuated by rotating the vector (v_j, v_k) by a random angle θ distributed according to $\tilde{b}(\theta) / \int_{-\pi}^\pi \tilde{b}(\theta) d\theta$.

In the intervals between the large jumps, we solve (21) using a simple explicit Euler method with a step size that depends on μ_ϵ . The step size is taken to be a given fraction of the typical rate for the truncated jump process. We have not made a rigorous analysis that would help in choosing the step size, rather we have numerically tested that the choice gives relevant answers.

We have computed uniformly distributed pseudo-random variables using the routine DLARAN from the LAPACK package [19] and to compute normally distributed random variables, we have used the ziggurat method of Marsaglia and Tsang [20].

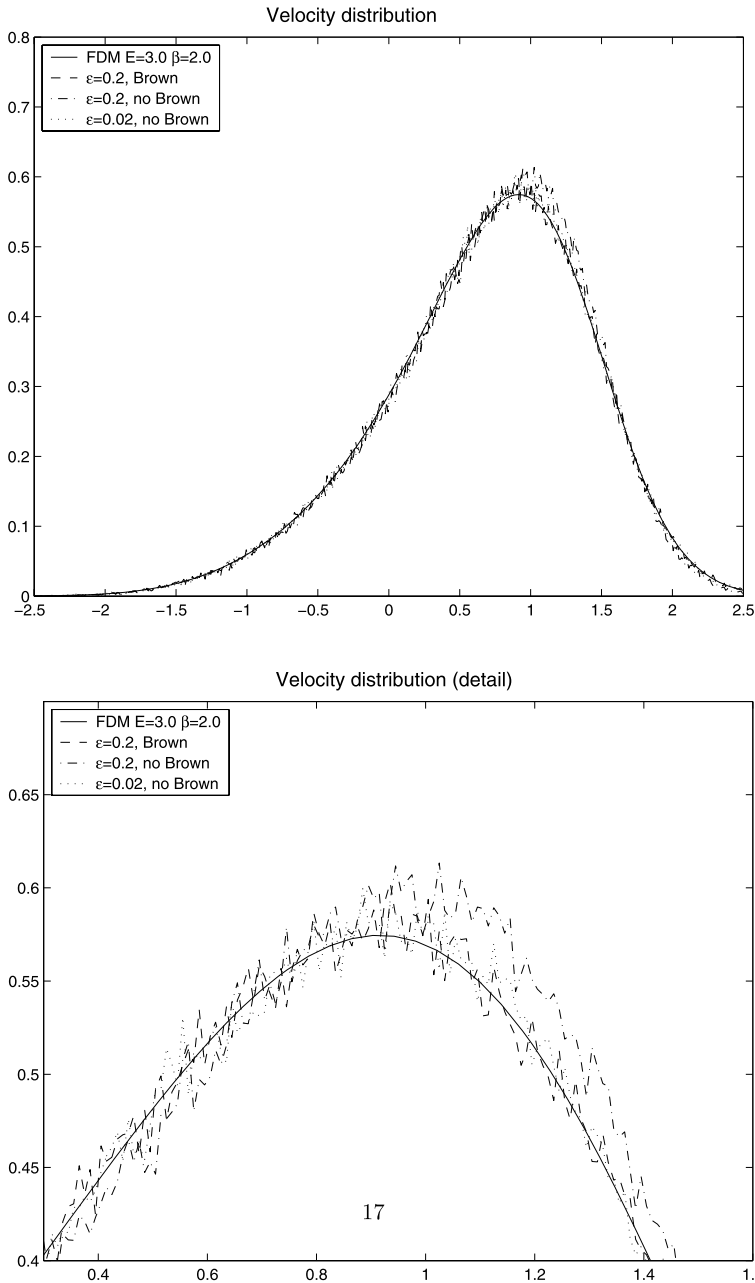


Fig. 1 Simulation results using different values of truncation: the velocity distribution, and an enlargement

As initial data, we have taken $\frac{1}{2}(\delta_{v=1} + \delta_{v=-1})$.

We have no exact solutions to compare the results with. However, taking the Fourier transform of the time independent Kac equation, i.e. (10) considered without t , gives

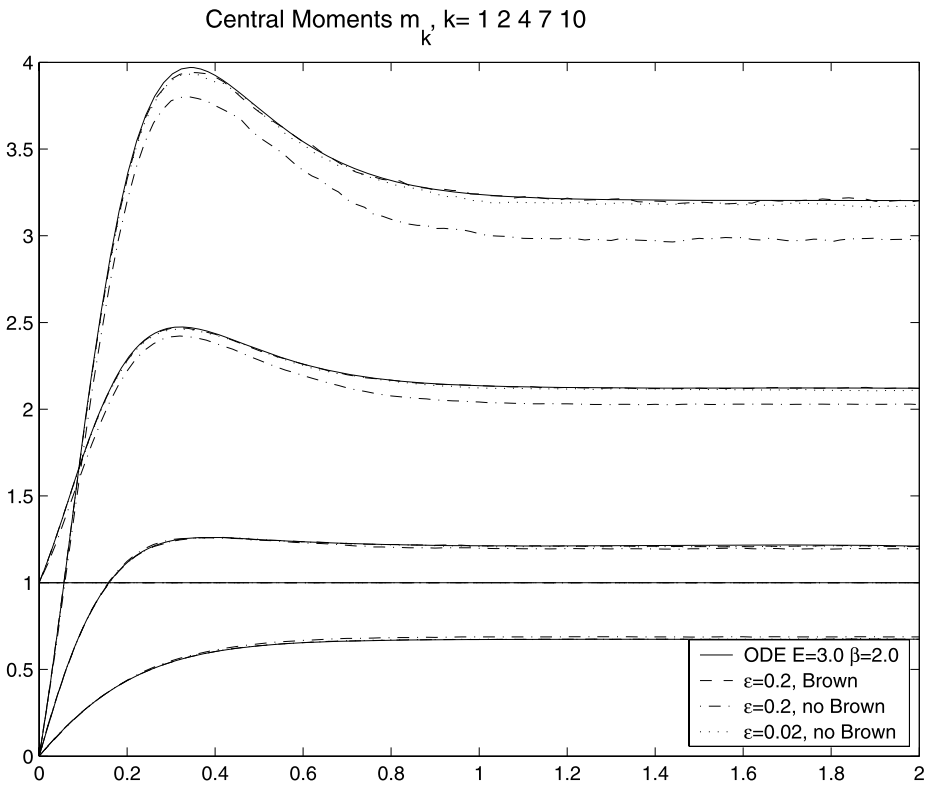


Fig. 2 Simulation results using different values of truncation: time evolution of some of the moments

equation

$$\hat{f}'(\xi) + \frac{i}{\gamma\xi} \hat{f}(\xi) = \frac{1}{E\gamma\xi} \int_{-\pi}^{\pi} (\hat{f}(\xi \cos\theta)\hat{f}(\xi \sin\theta) - \hat{f}(0)\hat{f}(\xi))b(\theta) d\theta, \quad (25)$$

where γ is the stationary current, which can be explicitly computed. Equation (25) can be solved accurately numerically using a finite difference method, combined with the built-in ODE-solvers of Matlab™. Numerical results obtained in this way were presented in [5], where also a detailed mathematical analysis of the non-cutoff Kac equation with a thermostat can be found. Although no rigorous error analysis has been carried out, we consider this finite-difference solution to be an accurate solution to the stationary problem: a fine discretization was used, and the method was found to converge well.

Another test for the accuracy is to compare the evolution of moments. Also here we do not have any exact results to compare with, but as with other Boltzmann like equations of Maxwell type (i.e. models where the collision rate does not depend on the relative velocity of the colliding particles), one can write a closed system of ordinary differential equations for the first moments $m_k = \int f(v, t)v^k dv$, and this system can then be solved accurately with a numerical ODE-solver. We have used Matlab™ to solve the following

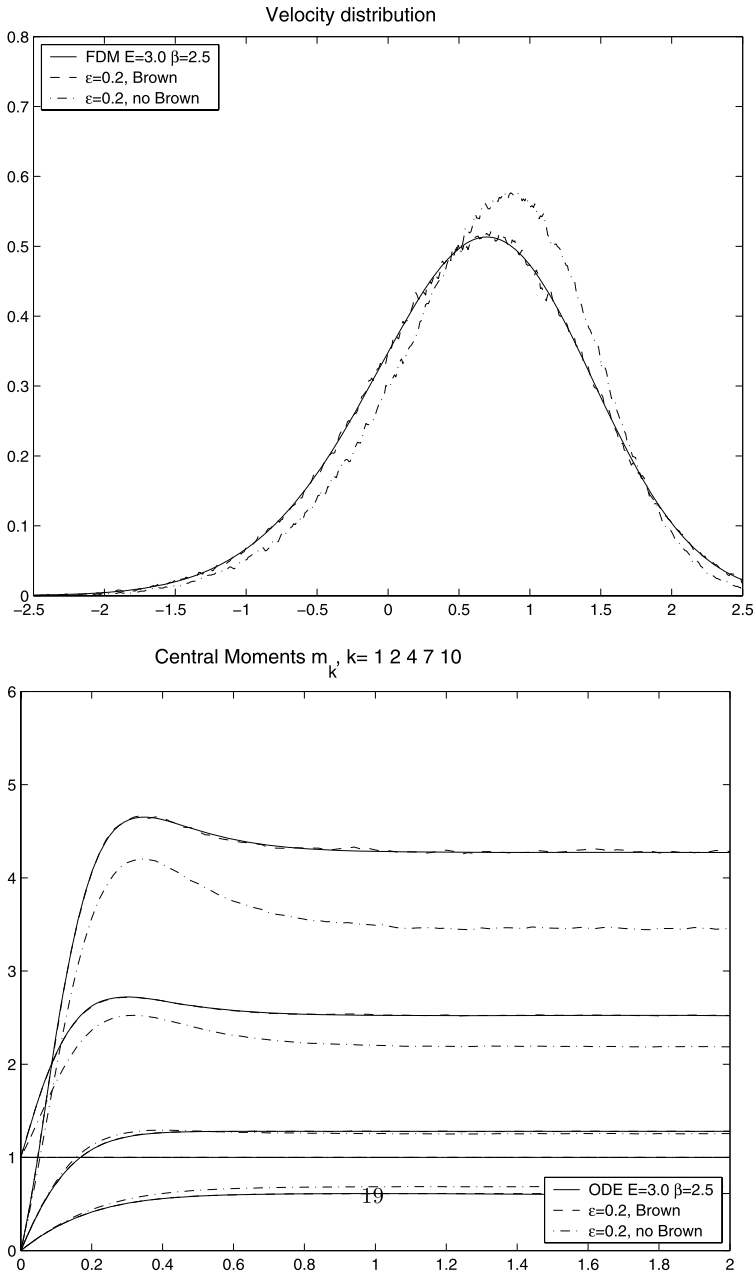


Fig. 3 Simulation results using different values of truncation for a stronger singularity: the velocity distribution, and the evolution of moments. Here the effect of the Brownian correction is more evident

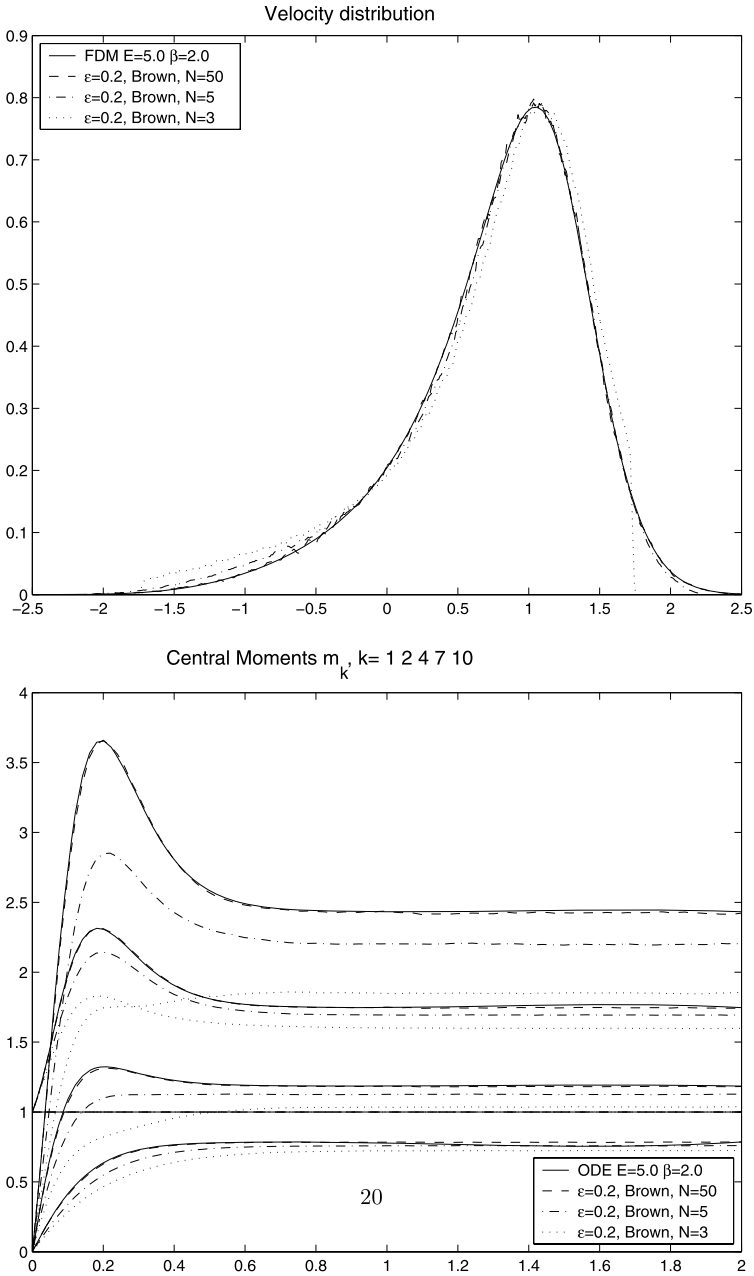


Fig. 4 Simulation results using different values of the number of particles. The simulation is repeated more times to get comparable results. As few as 50 particles gives a rather good agreement, but as few as five or even three particles are clearly not enough

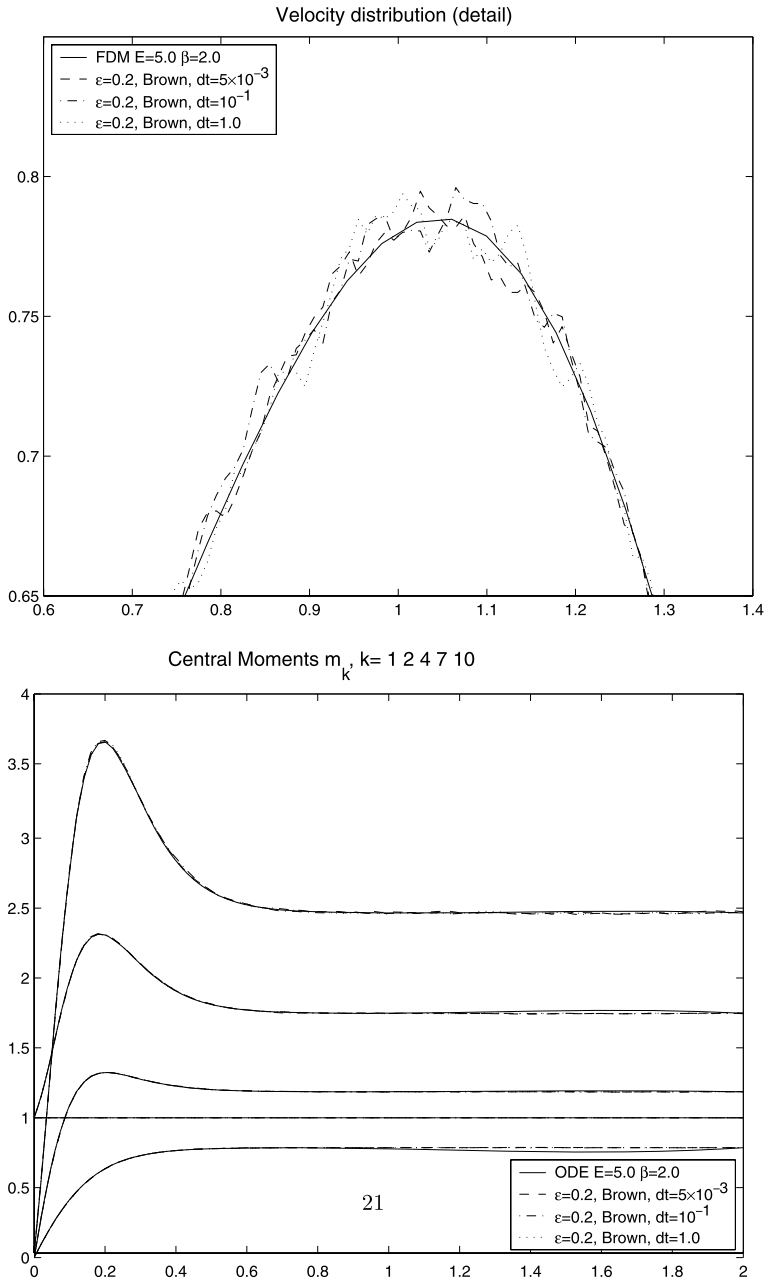


Fig. 5 The evolution between jumps is computed using a simple forward Euler method. The results here show that the time step is not critical

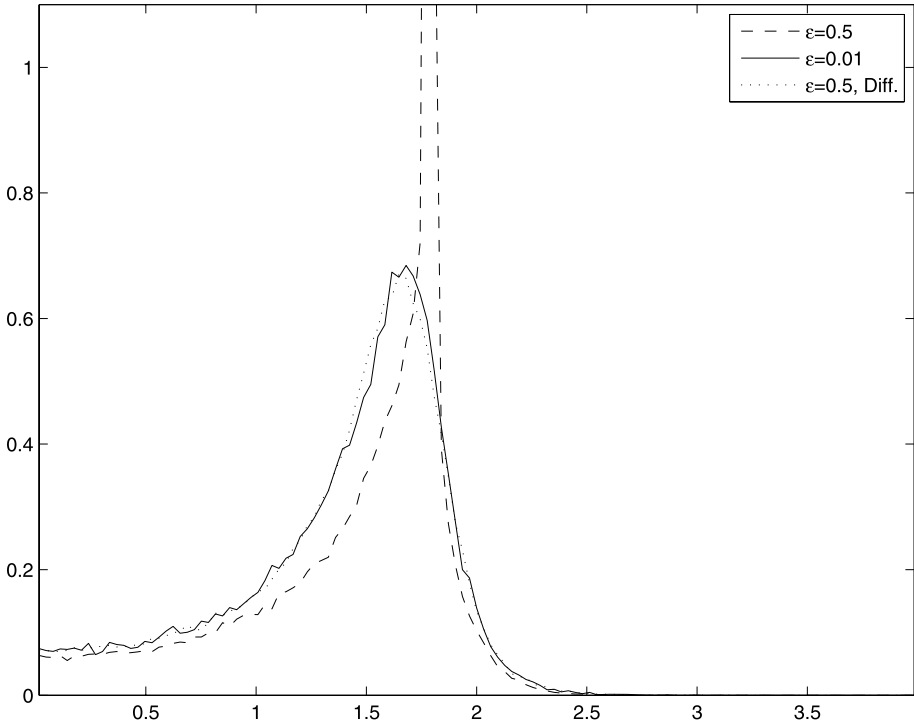


Fig. 6 Simulation of the Boltzmann equation: the distribution of the first velocity component v_x , i.e. an approximation of $\int_{\mathbb{R}^2} f(v, t) dv_y dv_z$ at $t = 0.06$

system:

$$\begin{aligned} \dot{m}_k &= Ekm_{k-1} - Ekm_1m_k - A_k m_k + \sum_{j=1}^{k-1} B_{kj}m_{k-j}m_j, \\ A_k &= \int_{-\pi}^{\pi} (1 - \cos^k \theta - \sin^k \theta)b(\theta) d\theta, \\ B_{kj} &= \binom{k}{j} \int_{-\pi}^{\pi} \cos^{k-j} \theta \sin^j \theta b(\theta) d\theta, \\ m_k(0) &= \frac{1}{2}(1 + (-1)^k). \end{aligned} \tag{26}$$

In the numerical calculations we have used $b(\theta) = |\theta|^{-1-\alpha}$ for different values of $\beta = \alpha + 1 \in]1, 3[$, and different values of the force parameter $E \in [2, 5]$. We have also varied n , the number of particles, and the time step used in solving the SDE, (21).

The first series of results, presented in Figs. 1, 2 (an enlargement), and Fig. 3 (for a stronger singularity) shows how the results depend on the level of truncation, and compares this with the result from using a much truncated model but with a Brownian correction. The parameters used were $E = 3.0$, $\beta = 2.0$, $n = 2000$, and $\epsilon = 0.2, 0.02, 0.002$. The time dt used in the Euler method for approximating the SDE was here taken to be $0.0001 \times dt_0$,

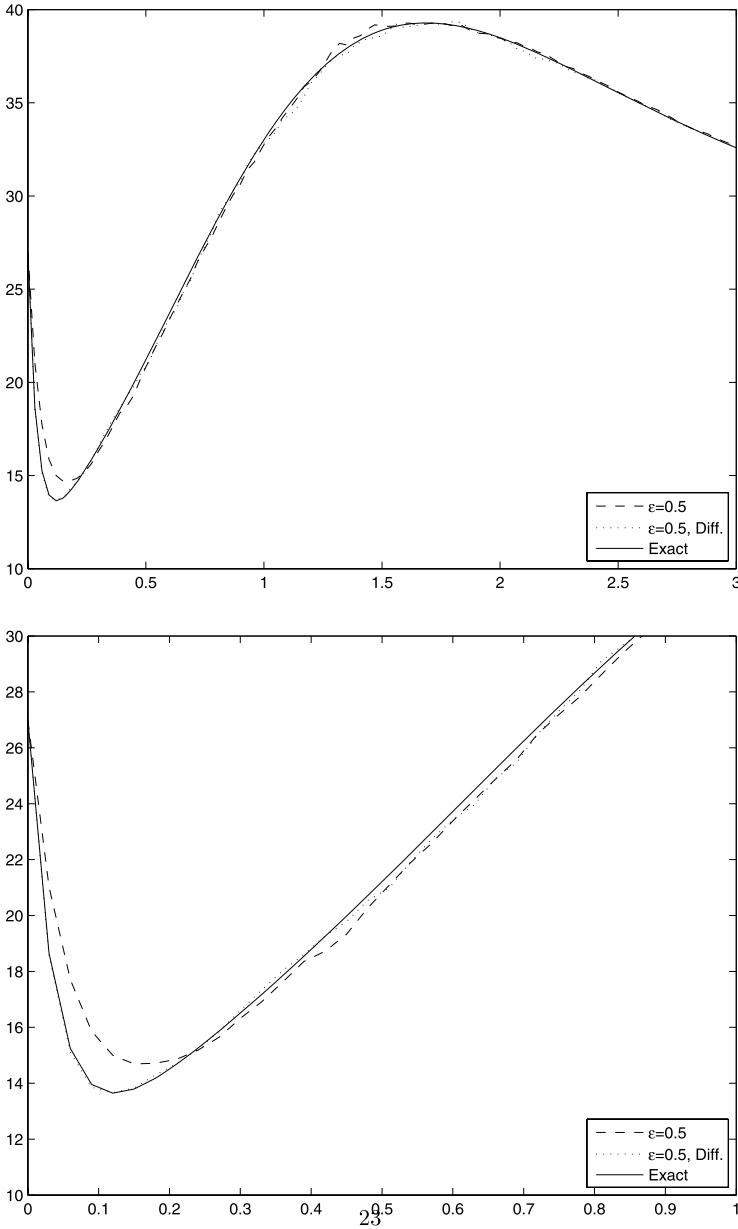


Fig. 7 Evolution of the moment $M_{6,0,0}$ with truncation at $\epsilon = 0.5$, with and without the diffusion correction. The moments for the Boltzmann equation are given as a reference. The enlargement shows that although the reference curve and the curve with the diffusion correction almost coincide, they are not identical

where dt_0 corresponds to a displacement of order ϵ from the Brownian motion. This is excessively small, and we will see below that it is far from necessary to get an accurate result. The calculation was then repeated 200 times to reduce noise. We see that $\epsilon = 0.2$ together with a Brownian approximation compares very well with a simulation using $\epsilon = 0.002$ with

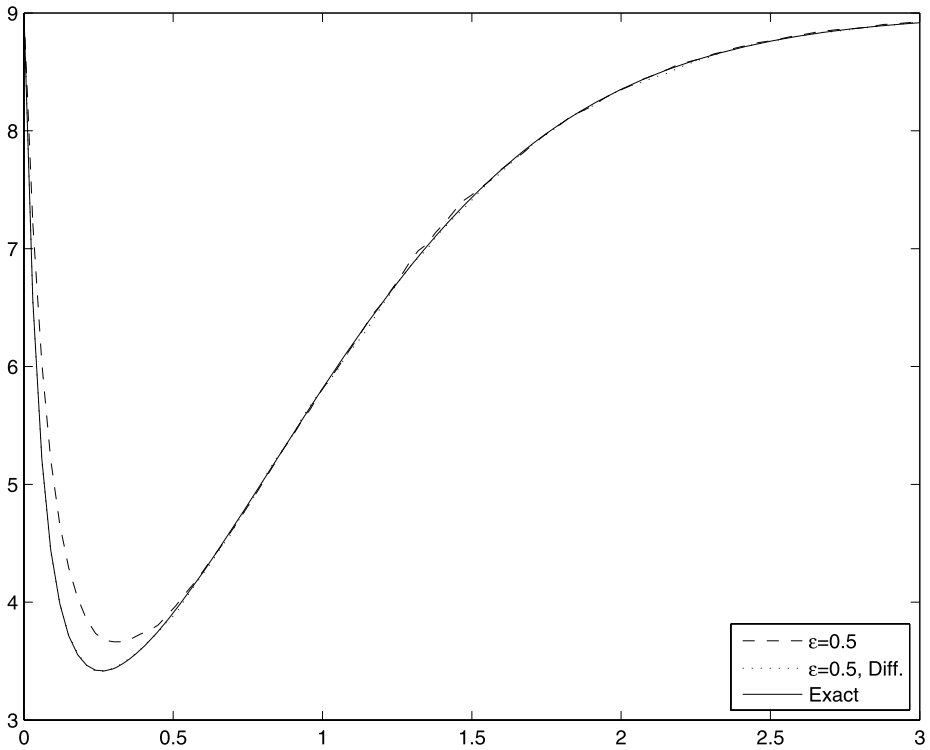


Fig. 8 Evolution of the moment $M_{4,0,0}$ with truncation at $\epsilon = 0.5$, with and without the diffusion correction. The moments for the Boltzmann equation are given as a reference

no approximation. The estimates in [32] give a convergence rate of $\epsilon^{3-\beta}$ without the Brownian correction, and a rate of $\epsilon^{4-\beta}$ with the Brownian term added. Hence it is not surprising to see that, when the singularity in the crosssection $b(\theta)$ is stronger, the influence of the truncation and of the Brownian approximation is much more important.

Figure 4 shows results for different values of n , the number of particles used in the simulation. There are at least two reasons for using a large value of n , when simulating kinetic equations: first, the Boltzmann equation itself assumes a limit of infinitely many particles, and secondly, a large value of n reduces the noise when computing moments or other functions. In this series we have taken $n \times$ number of simulated trajectories $\simeq const$, and very large in order to obtain a noiseless result. The calculations show that in fact it is not necessary to use a very large number of particles to find a good agreement, $n = 50$ is quite enough, both to get a reasonable agreement of the distribution functions and of the evolution of moments. However, with a small number of particles, it is necessary to repeat the calculations many times to avoid excessive noise in the result.

The last example for the Kac model, Fig. 5, shows some simulations that illustrate the influence of the time-step in the Euler method for solving the SDE (21). The reference time step is so large that the mean step is of the order ϵ , and the figure shows that both for computing the distribution function and the evolution of moments, it is not necessary to decrease the step size much below the reference value to get a good result.

The simulation is carried out in very much the same way for velocities in \mathbb{R}^3 , the main difference being the in which the diffusion is added. To compute the matrices R_j , we have

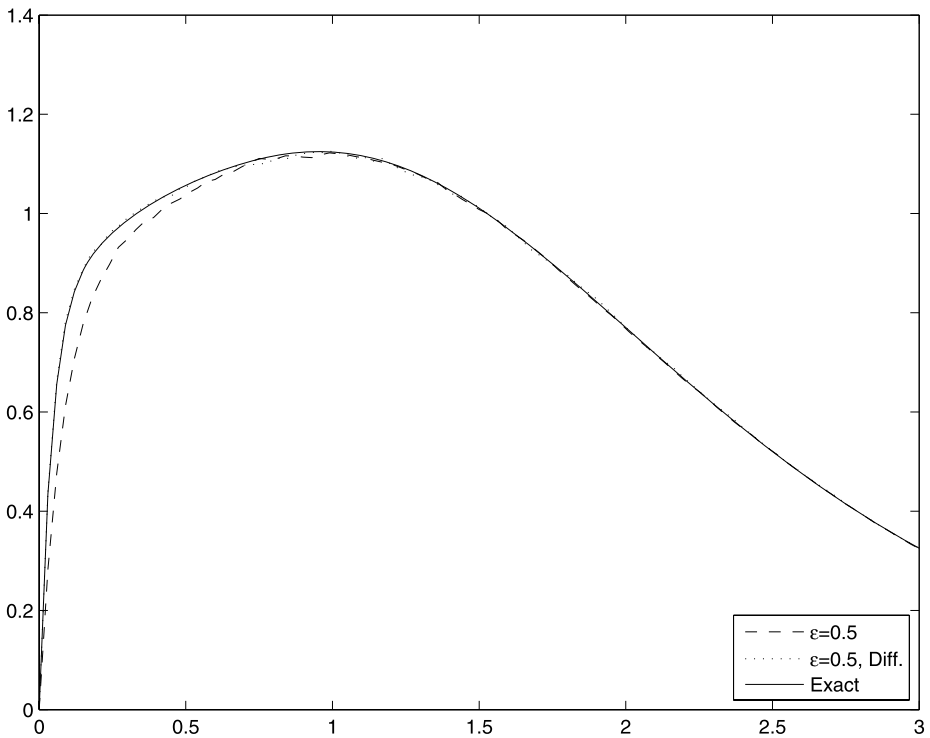


Fig. 9 Evolution of the moment $M_{2,0,2}$ with truncation at $\epsilon = 0.5$, with and without the diffusion correction. The moments for the Boltzmann equation are given as a reference

used routines from the Gnu Scientific Library [16] to evaluate the square root. This is rather time consuming, and the code spends a major part of the time doing this; still the method is faster than just using a smaller truncation, also before any attempts have been made to making the code efficient.

In this case we do not have an alternative method for computing the velocity distribution, but rather we compare the velocity distribution with a calculation with very small truncation. Because we are dealing with the case of Maxwellian interactions, there is a closed set of equations that describe the evolution of moments for the limiting Boltzmann equation also here.

All calculations were carried out with a constant force field $F = (1, 0, 0)$, and the number of particles was $n = 500$. The initial data was $\frac{1}{2}(\delta_{(1,0,0)} + \delta_{(-1,0,0)})$.

The first graph, Fig. 6 compares the approximations of

$$\int_{\mathbb{R}^2} f(v_x, v_y, v_z, t) dv_y dv_z,$$

with and without the diffusion correction, and a reference solution obtained by carrying out a simulation with a very small truncation of the crosssection.

We also compare the evolution of moments of the form

$$M_{j_x, j_y, j_z}(t) = \frac{1}{n} \sum_{k=1}^n v_{kx}^{j_x} v_{ky}^{j_y} v_{kz}^{j_z},$$

with the moments (computed as the solution of the closed ODE-system) for solutions to the limiting Boltzmann equation,

$$\int_{\mathbb{R}^3} f(v_x, v_y, v_z, t) v_{0x}^{j_x} v_{0y}^{j_y} v_{0z}^{j_z} dv_x dv_y dv_z.$$

We consider the solutions to the ode's to be exact. Hence Figs. 7, 8 and 9 show the evolution of $M_{6,0,0}(t)$, $M_{4,0,0}(t)$, and $M_{2,0,2}(t)$, respectively, for a strong truncation of the collision term $\varepsilon = 0.5$, with and without the diffusion correction, and compared with the moments for the limiting Boltzmann equation.

5 Conclusions

The paper presents a method to compute accurate solutions to non-cutoff Boltzmann equations in the non-cutoff case, by approximating the small jumps by a diffusion. We have presented numerical examples showing that it works well, and gives accurate results.

There are several open issues that merit being studied. From a numerical point of view, of course one would have to find good means of choosing n , the level of truncation, and an efficient method for solving (21).

Some results that aim at putting the method on a solid theoretical ground will be presented in [32].

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