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Direct simulation Monte Carlo schemes for Coulomb interactions in plasmas

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Abstract

We consider the development of Monte Carlo schemes for molecules with Coulomb interactions. We generalize the classic algorithms of Bird and Nanbu-Babovsky for rarefied gas dynamics to the Coulomb case thanks to the approximation introduced by Bobylev and Nanbu [1]. Thus, instead of considering the original Boltzmann collision operator, the schemes are constructed through the use of an approximated Boltzmann operator. With the above choice larger time steps are possible in simulations; moreover the expensive acceptance-rejection procedure for collisions is avoided and every particle collides. Error analysis and comparisons with the original Bobylev-Nanbu (BN) scheme are performed. The numerical results show agreement with the theoretical convergence rate of the approximated Boltzmann operator and the better performance of Bird-type schemes with respect to the original scheme.

Keywords: `Coulomb interactions, plasma physics, Boltzmann equation, Landau equation, Monte Carlo methods.`

AMS Subject Classification: `65M99, 65L06, 82D05`

1. Introduction

When a gas is far from the thermodynamical equilibrium, the description of the system through the fluid equation is not satisfactory and its fundamentals properties depend upon the interactions of the particles. Collisional phenomena can be distinguished for long-range interactions and

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short-range interactions. Short-range interactions are typically of rarefied gases and they are described through the Boltzmann equation [2], while long-range interactions are normally encountered in plasmas and modeled through the Landau-Fokker-Planck equation [3]. Nowadays, numerical simulations of plasmas are receiving a great deal of attention both in research and in industry thanks to the numerous applications directly connected to these phenomena. In addition, there exist many practical situations in which the so-called Coulomb collisions are fundamental for correctly describing the plasma dynamics as for instance in magnetic fusion devices.

However, while the literature on Monte Carlo schemes for short-range forces is wide ([4], [5], [6], [7], [8], [9]) and many efficient methods have been developed for treating these problems, on the other hand, how to construct efficient Monte Carlo numerical methods for long-range interactions like the Coulomb potential field it is still not clear. The present work is a contribution in this direction. We observe that recently, some important results have been achieved by Nanbu and Bobylev in [10] and [1] on this subject. They proposed a new Monte Carlo numerical method which permits to efficiently simulate Coulomb collisions. The performance of this scheme has been studied in details by Caflisch et al in [11] and [12], in comparisons with the classical scheme for simulating Coulomb collisions by Takizuka and Abe [13]. Monte Carlo methods for plasmas have also been developed by Wang et al [14] while an interesting hybrid method has been realized and numerically tested by Caflisch et al [15] for accelerating the simulation of Coulomb collisions.

In the case of Coulomb interactions each particle interacts simultaneously with a large number of other particles, thus multiple collisional phenomena are involved adding difficulties to the numerical description. However, these multiple interactions can be seen as a number of simultaneous binary collisions, each of which gives a small contribution to the relaxation process through a small angle scattering between particles. [3].

The Landau-Fokker-Planck equation is a valid substitute to the Boltzmann operator when describing this type of systems. More precisely, the Landau-Fokker-Planck equation can be derived as an asymptotic form of the Boltzmann equation in the case of a Coulomb potential field, in which the large angle deflection of a charged particle in a multiple Coulomb interaction is considered as a series of consecutive weak binary collisions [1,16]. However, the classic Boltzmann collision integral is still able to describe the interactions, but the typical time between two consecutive collisions prohibits construction of efficient explicit schemes, since the resulting time step will be in these cases too small and an excessive use of the computational resources is needed. Moreover due to the small effect of a single interaction

such detailed modeling is unnecessary.

In the present work, starting from an approximation derived by Bobylev and Nanbu [1] for the Boltzmann collision operator, we derive a general class of direct Monte Carlo methods in the same spirit of Monte Carlo schemes for rarefied gas dynamic. Moreover, keeping separated the discretization of the time derivative and the approximation of the collision operator, we perform a series of numerical convergence tests for the approximated collision operator in order to show that the effective convergence rate coincides with the one hypothesized in [1].

The rest of the paper is organized as follow. In Section 2, we introduce the Boltzmann and Fokker-Planck equations and their properties. In Section 3, we derive the approximated Boltzmann operator and the limiting case in which, for small angle scattering, it converges to an approximated operator for the Landau-Fokker-Planck equation. Section 4 concerns the construction of direct simulation Monte Carlo methods. Several test problems which show the capabilities of the methods, the differences and analogies with the original Bobylev-Nanbu (BN) scheme, and the convergence rates are presented in Section 5. Some final considerations are discussed in Section 6.

2. The Boltzmann and the Landau-Fokker-Planck equations

Consider the Boltzmann equation

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

with the initial condition

$$f(x,v,t=0) = f_0(x,v), \tag{2}$$

where $f = f(x,v,t)$ is a non negative function describing the time evolution of the distribution of particles which move with velocity $v \in \mathbb{R}^3$ at the position $x \in \Omega \subset \mathbb{R}^3$ at time $t > 0$. The vector $a(v)$ represents the acceleration due to the force acting on particles such as gravity, electric field or magnetic field. The bilinear operator $Q(f,f)$ describes the binary collisions between particles and is given by

$$Q(f,f) = \int_{\mathbb{R}^3} \int_{S^2} B\left(|q|, \frac{q \cdot n}{|q|}\right) [f(v') f(v'_*) - f(v) f(v_*)] dn dv_* \tag{3}$$

where S^2 is the unit sphere in $\mathbb{R}^3$, $q = v - v_*$, $n \in S^2$ the unit normal. The post collisional velocity are computed by

$$v' = \frac{1}{2}(v + v_* + |q|n), \;\; v'_* = \frac{1}{2}(v + v_* - |q|n) \tag{4}$$

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The collision kernel $B(|q|, q \cdot n/|q|)$, which characterizes the detail of the interaction, is defined as

$$B(|q|, \cos\theta) = |q|\sigma(|q|, \theta), \ (0 \leq \theta \leq \pi) \tag{5}$$

Here $\cos\theta = q \cdot n/|q|$ and $\sigma(q, \theta)$ is the collision cross section at the scattering angle θ, that correspond to the number of particles scattered per unit time, per unit of incident flux and per unit of solid angle. We introduce also the total scattering cross section and the momentum scattering cross section that will be used in the remainder of the paper

$$\sigma_{tot}(|q|) = 2\pi \int_0^\pi \sigma(|q|, \theta) \sin\theta d\theta \tag{6}$$

$$\sigma_m(|q|) = 2\pi \int_0^\pi \sigma(|q|, \theta) \sin\theta (1 - \cos\theta) d\theta \tag{7}$$

In the case of hard sphere molecules the cross section and the collision kernel takes the form

$$\sigma(q, \theta) = \frac{d^2}{4}, \ B(|q|, \theta) = \frac{d^2}{4}|v - v_*| \tag{8}$$

while in the variable hard sphere case we have

$$\sigma(q, \theta) = C_\alpha |v - v_*|^{\alpha - 1}, \ B(|q|, \theta) = C_\alpha |v - v_*|^\alpha \tag{9}$$

with C_α and α positive constants. The case $\alpha = 0$ is referred as Maxwellian gas while for $\alpha = 1$ we recover the hard sphere model. In the case of Coulomb interactions the Rutherford formula holds

$$\sigma(|q|, \theta) = \frac{b_0^2}{4\sin^4(\theta/2)} \tag{10}$$

where $b_0 = e^2/(4\pi\epsilon_0 m_r |v - v_*|^2)$, with e the charge of the particle, ϵ_0 the vacuum permittivity and m_r the reduced mass, which corresponds to $m/2$, if the particles are of the same species, with m equal to the mass. Observe that the above formula implies that the scattering cross section tends to infinity as the angle θ tends to zero. In order to obtain finite and meaningful values for the total and the momentum cross section it is necessary to introduce a cut-off value for the impact parameter. The cut-off value is justified by the shielding effect phenomena, leading to the following values for the total cross section and the momentum cross section

$$\sigma_{tot}(|q|) = \pi\lambda_d^2 \tag{11}$$

$$\sigma_m(|q|) = 4\pi b_0^2 \log \Lambda \tag{12}$$

with $\lambda_d = (\frac{\epsilon_0 kT}{ne^2})^{1/2}$ the Debye length and $\Lambda = \frac{1}{\sin(\theta^{min}/2)}$.

In the case of grazing collisions it is possible to derive from the Boltzmann operator the Landau-Fokker-Planck operator (see [16] for details)

$$Q^L(f,f) = \frac{1}{8}\frac{\partial}{\partial v_i}\int_{\mathbb{R}^3} |q|\sigma_m(|q|)((|q|^2)\delta_{ij} - q_i q_j) \times \left(\frac{\partial}{\partial v_j} - \frac{\partial}{\partial v_{*j}}\right) f(v) f(v_*) dv_* \tag{13}$$

In the next section we will see how it is possible to construct numerical schemes starting from the Boltzmann equation which approximate the Landau operator (13).

3. The approximated Boltzmann equation

From now on, we will focus on the space homogeneous equation without force fields. Once the collision term is solved, the solution of the full Boltzmann equation can be recovered by computing the transport and the force term through a time splitting.

Although the divergence of the collision integral has been solved with the cut-off of the scattering cross section, the simulation of the Boltzmann equation for Coulomb interactions still represent a significant challenge, due to the too high computational cost which is necessary to directly simulate the equations with time explicit schemes. In fact rewriting Eq. (1) in the space homogenous case pointing out the gain and loss term

$$\frac{\partial f}{\partial t} = Q^+(f,f) - f(v)L[f](v), \;\; L[f](v) = \sigma_{tot}(|q|)\int_{\mathbb{R}^3} |q| f(v_*) dv_* \tag{14}$$

$$Q^+(f,f) = \int_{\mathbb{R}^3}\int_{S^2} B\left(|q|, \frac{q\cdot n}{|q|}\right) f(v') f(v'_*) dn dv_* \tag{15}$$

it is easy to observe that the large value of the total collision cross section forces the time step to be small, thus too many steps become necessary to compute the final solution, yielding this scheme useless. In fact discretizing the time derivative we obtain

$$f(v, t+\Delta t) = \Delta t Q^+(f,f) + f(v,t)\left(1 - \Delta t \sigma_{tot}(|q|)\int_{\mathbb{R}^3} |q| f(v_*) dv_*\right) \tag{16}$$

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now if we want to preserve a probabilistic interpretation we need the coefficients to be positive, thus Δt has to be extremely small if $\sigma_{tot}(|q|)$ is very large.

Recently an approximated Boltzmann operator has been developed by Bobylev and Nanbu ([1]), which permits use of larger time steps during the simulation even in the case of Coulomb collisions. Here we try to generalize this approach in order to construct Direct Monte Carlo schemes for small particles interactions.

Rewrite equation (1) in the homogenous case in the following form

$$\frac{\partial f}{\partial t} = \int_{\mathbb{R}^3} JF(U,q)dv_* \tag{17}$$

where $U = (v + v_*)/2$ denotes the center of mass velocity, and

$$F(U,q) \equiv f(U + q/2)f(U - q/2) = f(v)f(v_*) \tag{18}$$

while the operator J is defined as

$$JF(U,|q|\omega) = \int_{S^2} B(|q|, \omega \cdot n)[F(U,|q|n) - F(U,|q|\omega)]dn \tag{19}$$

with $\omega = q/|q|$. If we approximate the operator J in equation (17) by

$$J = \frac{1}{\tau}(\exp(\tau J) - \widehat{I}) \tag{20}$$

where $\widehat{I}$ is the identity operator and τ are assumed to be small, the equation reads

$$\frac{\partial f}{\partial t} = \frac{1}{\tau}\int_{\mathbb{R}^3}(\exp(\tau J) - \widehat{I})F(U,q)dv_* = \frac{1}{\tau}(P_\tau(f,f) - \varrho f) \tag{21}$$

with

$$P_\tau(f,f) = \int_{\mathbb{R}^3} \exp(\tau J)f(v)f(v_*)dv_* \tag{22}$$

The operator $\exp(\tau J)$ can be written as

$$\exp(\tau J)\psi(\omega) = \int_{S^2} B_\tau(\omega \cdot n, |q|)\psi(n)dn \tag{23}$$

where $\psi(\omega)$ is an arbitrary function and

$$B_\tau(\omega \cdot n, |q|) = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \exp(-\lambda_l(|q|)\tau)P_l(\omega \cdot n) \tag{24}$$

is the Green function, with $P_l(\omega \cdot n)$ the Legendre polynomial and $\lambda_l(|q|)$ equal to

$$\lambda_l(|q|) = 2\pi \int_{-1}^{1} B(\mu, |q|)(1 - P_l(\mu))d\mu \tag{25}$$

where $\mu = \omega \cdot n,\ -1 \leq \mu \leq 1$ Using the above expression we obtain

$$P_\tau(f, f) = \int_{\mathbb{R}^3 \times S^2} B_\tau(|q|, \frac{q \cdot n}{|q|}) f(v') f(v'_*) dn dv_* \tag{26}$$

Note that

$$\int_{S^2} B_\tau(\omega \cdot n, |q|) = 1 \tag{27}$$

3.1. *A first order approximation for the Landau-Fokker-Planck equation*

Assume now that the scattering cross section $\sigma(|q|, \theta)$ is concentrated at small angle near $\theta \approx 0$, thus $B_\tau(|q|, \mu)$ is concentrated near $\mu = 1$. In that situation it is possible to derive the following formal approximation

(28)
$$\lambda_l(u) \simeq 2\pi \int_{-1}^{1} B_\tau(|q|, \mu)(1 - P_l(1) + (1-\mu)P'_l(1))d\mu = \pi l(l+1) \int_{-1}^{1} B_\tau(|q|, \mu)(1-\mu)d\mu$$

where $P'_l(1) = l(l+1)/2$. The approximate Green function reads

(29)
$$B_\tau(\mu, |q|) \simeq B^L_\tau(\mu, |q|) = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} P_l(\mu) \exp\left(-\frac{l(l+1)}{2}|q|\sigma_m(|q|)\tau\right)$$

The superscript L in equation (29) means that equation (21) with the above kernel approximates the Landau-Fokker-Planck equation. For a formal proof we refer to the paper of Nanbu and Bobylev ([1]).

Consider now the case of a Coulomb potential field in a single component gas or plasma. This choice, with the cut-off of the scattering angle introduced in the previous section, leads to the following approximated equation of order $0(\tau)$

$$\frac{\partial f}{\partial t} = \frac{1}{\tau}\left(\int_{\mathbb{R}^3 \times S^2} D\left(\frac{q \cdot n}{|q|}, \frac{\tau}{2\varrho\tau_1}\right) f(v', t) f(v'_*, t) dn dv_* - \varrho f(v, t)\right) \tag{30}$$

where

$$\frac{1}{\tau_1} = 4\pi \left(\frac{e^2}{4\pi\epsilon_0 m_r}\right)^2 \frac{\varrho \ln \Lambda}{|q|^3} \tag{31}$$

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and

$$D(\mu,\tau_0)=\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\mu)\exp(-l(l+1)\tau_0). \tag{32}$$

4. DSMC schemes for Coulomb Interactions

Note that is not necessary to work with the collisional kernel $D(\mu,\tau_0)$ computed above, instead a simpler function $D^*(\mu,\tau_0)$ can be used, preserving the same accuracy $0(\tau)$, if the following condition remain satisfied

$$D^*(\mu,\tau_0)\geq 0,\ 2\pi\int_{-1}^{1}D^*(\mu,\tau_0)d\mu=1 \tag{33}$$

$$\lim_{\tau_0\to 0}D^*(\mu,\tau_0)=\frac{1}{2\pi}\delta(1-\mu) \tag{34}$$

$$\lim_{\tau_0\to 0}\frac{2\pi}{\tau_0}\int_{-1}^{1}[D^*(\mu,\tau_0)-D(\mu,\tau_0)]P_l(\mu)d\mu=0. \tag{35}$$

One possible substitution is represented by

$$D^*(\mu,\tau_0)=\frac{A}{4\pi\sinh A}\exp(\mu A) \tag{36}$$

where $A=A(\tau)$ satisfy

$$\coth A-\frac{1}{A}=\exp^{-\frac{\tau}{\varrho\tau_1}} \tag{37}$$

It is now clear that it is possible to apply slightly modified versions of the standard direct Monte Carlo algorithms for Maxwell molecules to the equation

$$\frac{\partial f}{\partial t}=\frac{1}{\tau}(P_\tau^*(f,f)-\varrho f) \tag{38}$$

with

$$P_\tau^*(f,f)=\int_{\mathbb{R}^3\times S^2}D^*\left(\frac{q\cdot n}{|q|},\frac{\tau}{2\varrho\tau_1}\right)f(v',t)f(v'_*,t)dndv_* \tag{39}$$

The only difference is the way the angle is sampled. In most of the DSMC methods (Hard sphere or Variable Hard Sphere scattering models) the angle

is sampled uniformly over the sphere, while here is sampled accordingly to $D^*(\mu, \tau_0)$. Let us discretize the time and denote $f^n(v)$ the approximation of $f(v, n\Delta t)$, the forward Euler scheme can be used to solve Eq. (38)

$$f^{n+1} = \left(1 - \frac{\varrho \Delta t}{\tau}\right) f^n + \frac{\varrho \Delta t}{\tau} P_\tau^*(f, f) \tag{40}$$

This equation has the following probabilistic interpretation: a particle with velocity v_i will not collide with probability $(1 - \varrho\Delta t/\tau)$ and it will collide with probability $\varrho\Delta t/\tau$ accordingly to the collision law described by $P_\tau^*(f, f)$. Observe that the probabilistic interpretation holds till $\varrho\Delta t \leq \tau$, otherwise the coefficient in front of f^n becomes negative. Note that taking the limit of the above relation, $\varrho\Delta t = \tau$, leads to the scheme of Nanbu and Bobylev. The possibility to take different values of $\Delta t \leq \tau/\varrho$ permits reduction of the statistical fluctuations and reduction of the error due to the time discretization at no additional cost since, in contrast to the Variable Hard sphere case, here no acceptance-rejection procedure is present.

Hence a Monte Carlo algorithm for the solution of the approximated space homogeneous Landau-Fokker-Planck equations reads as follows

Algorithm 1 (Nanbu-Babovsky (NB) for Coulomb Interactions).

1. *Given N samples v_k^0 with $k = 1, 2, .., N$ computed from the initial distribution function $f(v, t = 0)$*
2. *DO $n = 1$ to n_{TOT} with $n_{TOT} = t_{final}/\Delta t$*
   Given $\{v_k^n, k = 1, ..., N\}$
   (a) *Set $N_c = round(\varrho N \Delta t/2\tau)$, where the round is statistical*
   (b) *Select N_c pairs (i, j) uniformly among all possible pairs*
   (c) *Perform the collision between i and j particles according to the following collision law*
      i. *Compute the cumulative scattering angle $\cos\theta$ as*

$$\cos\theta = \frac{1}{A} \ln(\exp^{-A} + 2U \sinh A) \tag{41}$$

where U is a random number and $A = A(\tau)$ is computed through the solution of the non linear equation

$$\coth A - \frac{1}{A} = \exp^{-\frac{\tau}{\varrho\tau_1}} \tag{42}$$

      ii. *With the above value of $\cos\theta$ perform the collision between i and j and compute the post collisional velocity according to*

$$v_i' = v_i - \frac{1}{2}(q(1 - \cos\theta) + h \sin\theta) \tag{43}$$

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$$v_j' = v_j + \frac{1}{2}(q(1-\cos\theta) + h\sin\theta) \tag{44}$$

where $q = v_i - v_j$*, while* h *is defined as*

$$h_x = q_\perp \cos\epsilon$$

$$h_y = -(q_y q_x \cos\epsilon + q q_z \sin\epsilon)/q_\perp$$

$$h_z = -(q_z q_x \cos\epsilon - q q_y \sin\epsilon)/q_\perp$$

where $q_\perp = (q_y^2 + q_z^2)^{1/2}$ *and* $\epsilon = 2\pi U_1$ *with* U_1 *a random number*

iii. set $v_i^{n+1} = v_i^{'}$ *and* $v_j^{n+1} = v_j^{'}$

(d) Set $v_i^{n+1} = v_i$ *for the particles that have not been selected*

END DO

We noticed the structure of the approximate operator analyzed in the previous section is similar to the structure of the classical Boltzmann collision integral. Thus it is possible to construct, in the same spirit of Maxwell molecules for rarefied gas dynamic, a Monte Carlo scheme based on the classical Bird method.

From the inspection of the approximated Landau operator, it follows that the average number of significant collisions in a time step Δt is given by

$$N_c = \frac{N}{2}\frac{\varrho \Delta t}{\tau} \tag{48}$$

which means that the average time between two collisions is given by

$$\frac{\Delta t}{N_c} = \frac{2\tau}{\varrho N} \tag{49}$$

The Bird method, in the case of Maxwell molecules, can be seen as a NB scheme in which the smallest possible time step $\Delta t_1 = \Delta t/N_c$ is used, in fact only one pair collide each Δt_1

$$f^{n+1} = \left(1 - \frac{\varrho \Delta t_1}{\tau}\right) f^n + \frac{\varrho \Delta t_1}{\tau} P_\tau^*(f,f) = \left(1 - \frac{2}{N}\right) f^n + \frac{2}{N} P_\tau^*(f,f) \tag{50}$$

Hence the Bird algorithm for the approximated Landau-Fokker-Planck equation reads

Algorithm 2 (Bird for Coulomb Interactions).

1. *Given N samples v_k^0 with $k = 1, 2, .., N$ computed from the initial distribution function $f(v, t = 0)$*
2. *set time counter $t_c = 0$*
3. *set $\Delta t_c = 2\tau/\varrho N$*
4. *DO $n = 1$ to n_{TOT} with $n_{TOT} = t_{final}/\Delta t$*
   (a) *repeat*
      i. *Select a random pair (i, j) uniformly within all possible pairs*
      ii. *perform the collision accordingly to the collision law defined in the first algorithm and produce $v_i^{'}$ and $v_j^{'}$*
      iii. *Set $\tilde{v}_i = v_i^{'}$ and $\tilde{v}_j = v_j^{'}$*
      iv. *update the time counter $tc = tc - \Delta t_c$ until $t_c \geq (n + 1)\Delta t$*
   (b) *Set $v_i^{n+1} = \tilde{v}_i, i = 1, ..., N$*
   END DO

The main difference with respect to the previous algorithm is that multiple collisions between particles are allowed in Δt. Moreover in this case the stability condition can be violated and τ can be greater than $\varrho\Delta t$. Thus, as the number of samples increase to infinity, the Nanbu-Babovsky scheme converge in probability to the discretized approximated Boltzmann equation. On the other hand, the Bird scheme converges to the solution of the approximated Boltzmann equation increasing the number of samples, in fact Δt_1 approaches zero. Thus for $\tau \to 0$ the first converges to the solution of the discretized Landau-Fokker-Planck equation while the second converges to the exact solution of the Landau-Fokker-Planck equation.

Remark 4.1. Observe that τ, although in the schemes has a role similar to the Knudsen number in rarefied gas dynamics, has not a clear physical meaning. Mathematically the parameter in front of the collision operator is a measure of the goodness of the approximation. Once it is fixed it gives a model for the interactions between particles which approximates the Landau operator as τ goes to zero.

5. Numerical Tests

5.1. *Test case*

The behavior of the DSMC schemes is illustrated through a series of tests in which the relaxation of the velocity distribution function with anisotropic temperature T is considered. Thus the initial distribution is

taken to be ellipsoidal with $T_x \neq T_y = T_z$. The initial values for temperature and density are set to

$$T = 4 \times Ry, \ \varrho = 0.5 \tag{51}$$

where Ry is the Rydberg constant. The initial difference in the temperature is fixed to $\Delta T_0 = 0.8$. The approximate analytic solution of the Fokker-Planck equation, in the case of small temperature difference, for $\Delta T = T_x - T_y$ is given by [17]

$$\Delta T = \Delta T_0 \exp^{-\frac{8}{5\sqrt{2\pi}}\frac{t}{\tau_T}} \tag{52}$$

the relaxation time τ_T corresponds to

$$\frac{1}{\tau_T} = \frac{\varrho e^4 \log \Lambda}{\pi\sqrt{2}\epsilon_0^2 m^{1/2}(kT)^{3/2}} \tag{53}$$

where the Coulomb logarithm value is fixed to $\log \Lambda = 0.5$. The simulations are run for most of the relaxation process; because all the schemes reach the same final equilibrium state and start from the same initial data, our interest is to analyze the different behaviors of the methods when particles are both far from these two situations. Thus, fixing $t_f = 40$ with the values above reported we obtain $\Delta T_f / \Delta T_0 \simeq 0.2$ for the analytic solution, in the rest of the equilibrium process the schemes and the analytic solution become closer till they coincide. We remark that although analytic, the solution is still obtained through approximations and valid for ranges in which ΔT_0 is small. This is made more clear by the Figures at the end of the section, even for very small τ the schemes do not relax at the same rate of the approximate formula (52).

5.2. *Simulations*

Our aim is to perform comparisons between the Bird scheme and the Bobylev-Nanbu (BN) scheme. The curves which describe the behavior of the Nanbu-Babovsky (NB) scheme with different choices of the time step lie between this two extreme cases. In the sequel we will analyze

- the deterministic error;
- the statistical fluctuations of the two schemes.

The sources of errors for the methods are due to

- approximation of the Boltzmann operator;
- finite number of particles;

- discretization of the time derivative if present;
- conservative algorithm used for collisions.

In order to make a fair comparison of the methods and to stress the capacity to describe the relaxation phenomena we try to eliminate the common sources of errors. First we compute the deterministic error due to the substitution of the original collision operator with its approximation and to the discretization of the time derivative. To that aim we increase the number of samples and average the solution of M independent realizations removing statistical fluctuations

$$\overline{u}(t) = \frac{1}{M}\sum_{i=1}^{M} u_i(t) \tag{54}$$

where $\overline{u}(t)$ indicates the average solution at time t and

$$u_i(t) = \frac{T_i(t)_x - T_i(t)_y}{T(0)_x - T(0)_y} \tag{55}$$

with i the realization number. The number of samples used in the convergence analysis test for each realization is N=2×10^6 while the number of realizations is $M = 5$. Observe however that, using the Bird method together with a large number of particles for each realization, leads to a very accurate discretization of the time derivative (the effective time step is a function of 1/N), while with the Babovsky-Nanbu scheme the increase of the samples number does not affect the treatment of the time derivative. Note that since no acceptance-rejection procedure is necessary the two methods have approximately the same computational cost. Summarizing the first test tries to measure the deterministic error computing the numerical order of accuracy with respect to τ of the two methods. From the theoretical analysis we expect both methods to be first order in τ. Note however that for BN method the error is due to both the approximation of the operator and the to discretization of the time derivative. The order of accuracy r in τ is computed as

$$r(\tau) = \log_2 R(\tau),\ R(\tau) = \frac{|\overline{u}(4\tau) - \overline{u}(2\tau)|}{|\overline{u}(2\tau) - \overline{u}(\tau)|} \tag{56}$$

with R the error ratio. Our second purpose is to measure the stochastic fluctuations of the two methods. To this aim we compare the two variances defined as

$$\Sigma^2(\tau, N) = \frac{1}{M}\sum_{i=1}^{M}(u_i - \overline{u})^2 \tag{57}$$

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Fixing the parameter τ, i.e. the approximation of the Boltzmann operator, the variances of the two methods are compared for increasing number of samples starting from $N = 100$ to $N = 3200$. In this test the number of realizations is chosen equal to $M = 1500$. Thanks to multiple collisions we expect the Bird scheme to have slightly less fluctuations with respect to the BN scheme.

5.3. *Results*

Here we report the solution of the tests described in the previous Section. In Figure 1 the solution for the relaxation of temperature in the different directions is showed for the Bird method, while in Figure 3 for the BN method. The behavior of the schemes has been analyzed using six different values for the parameter τ

$$\tau = 2 \ \tau = 1 \ \tau = 0.5 \ \tau = 0.25 \ \tau = 0.125 \ \tau = 0.0625 \tag{58}$$

Moreover the solution with $\tau = 0.03125$ with $N = 2 \times 10^6$ and $M = 10$ realizations has been computed as a reference solution. In both Figures the analytic and approximated solution is reported (blue line) showing a discrepancy with the computed solution even with the more accurate one. The time step used in the BN scheme is chosen in order to satisfy the relation $\varrho \Delta t/\tau = 1$. In Figures 2 and 4 the convergence rate r is plotted for respectively Bird and BN. Both the schemes approach the value 1 when $\tau \to 0$ as expected from the theory. Anyway it is possible to observe from Figure 5, in which the solution of the two methods for the same values of τ (respectively $\tau = 2$, $\tau = 1$, $\tau = 0.5$ and $\tau = 0.25$) has been compared, that the two algorithm furnish a different relaxation rate for large values of the approximation parameter of the collision operator, while for small values the two methods in practice coincide. This behavior can be explained observing that while $\tau \to 0$ also the time step $\Delta t \to 0$ thus the error introduced by the BN scheme in the discretization of the time derivative disappears.

In order to show the different performance in terms of statistical fluctuations we fixed the parameter $\tau = 1$ and perform several simulations increasing the number of samples N. In Figure 6 a comparison between the two variances, obtained with Bird and BN, has been plotted. The statistical fluctuations of the two method are approximately the same for all the initial choices of N; nevertheless it is possible to see how the Bird scheme oscillates slightly less then BN scheme for all the values. This behavior is mainly due to the presence of the time discretization error in the BN scheme. If, instead of choosing a large value for τ we keep it small, the variance of the two methods become practically the same. In fact, if we want a fine

approximation of the collision operator with the Bobylev-Nanbu method the time step has to be very small, which means we are neglecting the time discretization error.

6. Conclusion

In this work we have proposed a generalization of the Monte Carlo scheme proposed by Bobylev and Nanbu for the solution of plasma physics problems in which the predominant collisions are of Coulomb type. This result is achieved by extending the classic Nanbu and Bird algorithms for rarefied gas dynamic to the case of plasma physics. The new methods provide more accurate results for a fixed τ with respect to the original BN algorithm without increasing the computational cost. In the resulting algorithms not all particles collide at each time step and some particles collide more than once. From the physical point of view this result is counterintuitive, in fact, all other computational models in literature about Coulomb interactions are based on all particles colliding simultaneously. In the limit of small values of τ all methods become essentially equivalent.

In future we hope to extend the methods described in [18] for rarefied gas dynamics to Coulomb interactions and to generalize the hybrid techniques developed in [19,20] to plasma physics problems close to thermodynamic equilibrium. Another interesting research direction consists in developing a more accurate approximation in τ of the Landau operator. This would allow the use of larger time steps in the simulations.

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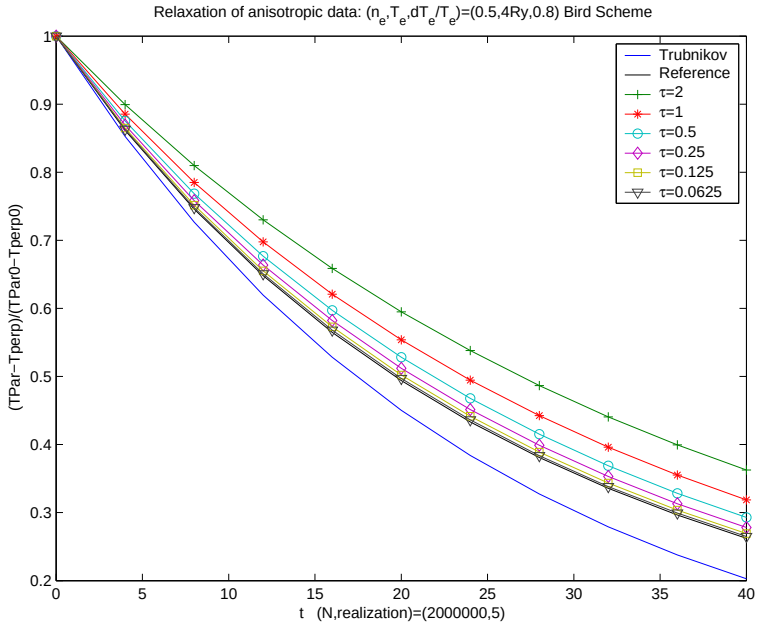

Fig. 1. Relaxation of the velocity distribution function with anisotropic initial data for different values of τ. Bird scheme.

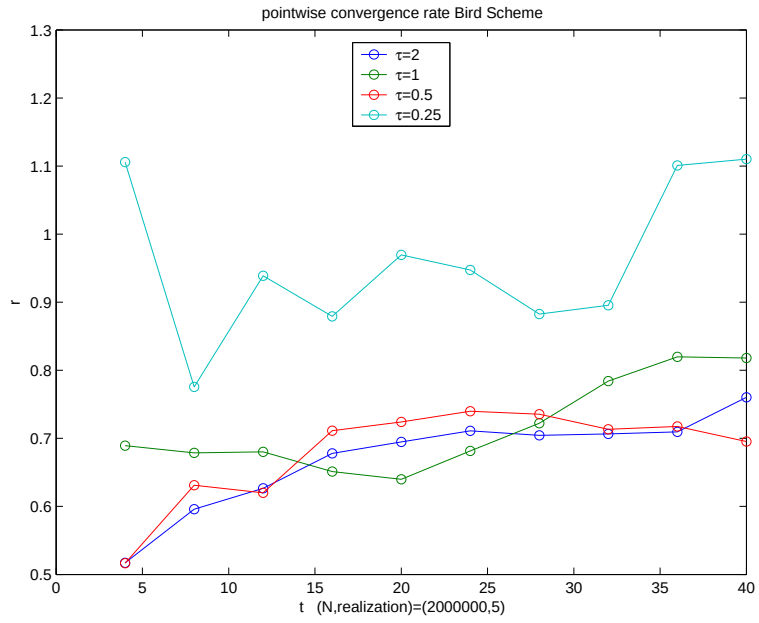

Fig. 2. Pointwise order of accuracy $r(\tau) = \log 2(R(\tau))$ for the Bird scheme for decreasing values of the parameter τ.

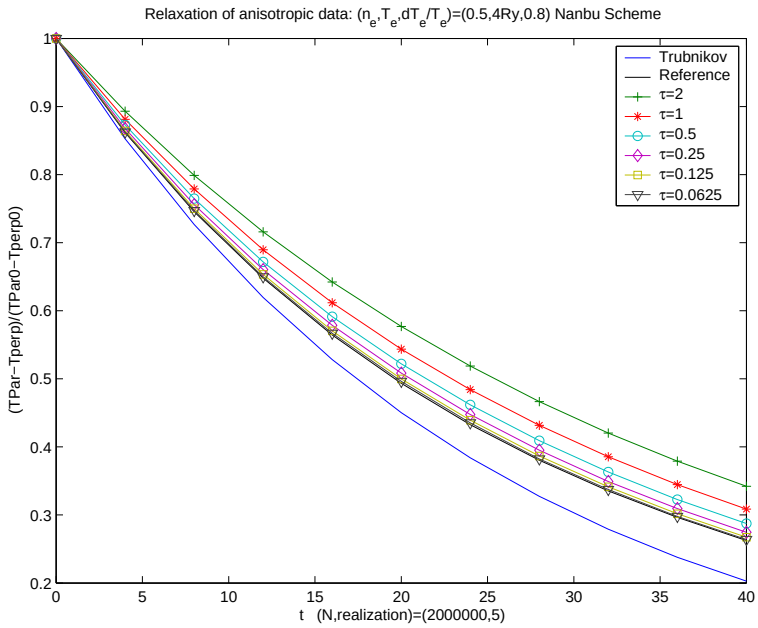

Fig. 3. Relaxation of the velocity distribution function with anisotropic initial data for different values of τ. Bobylev-Nanbu scheme.

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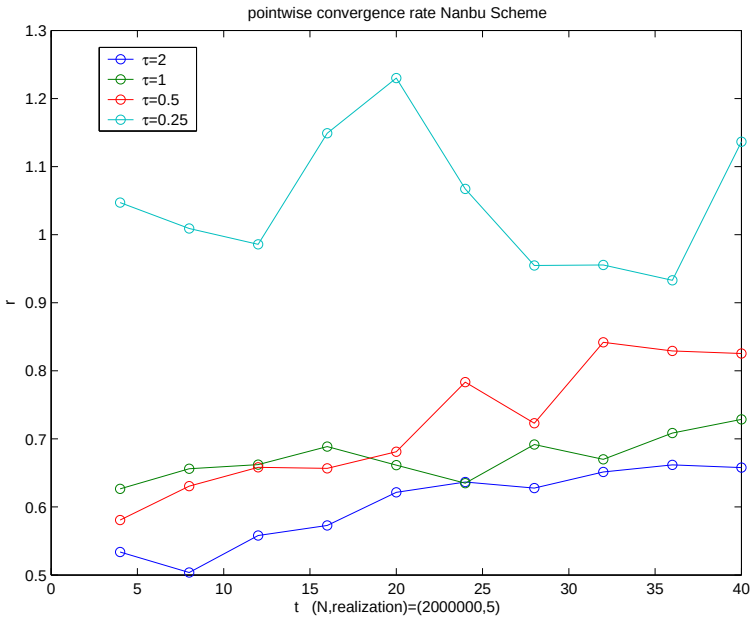

Fig. 4. Pointwise order of accuracy $r(\tau) = \log 2(R(\tau))$ for the Bobylev-Nanbu scheme for decreasing values of the parameter τ.

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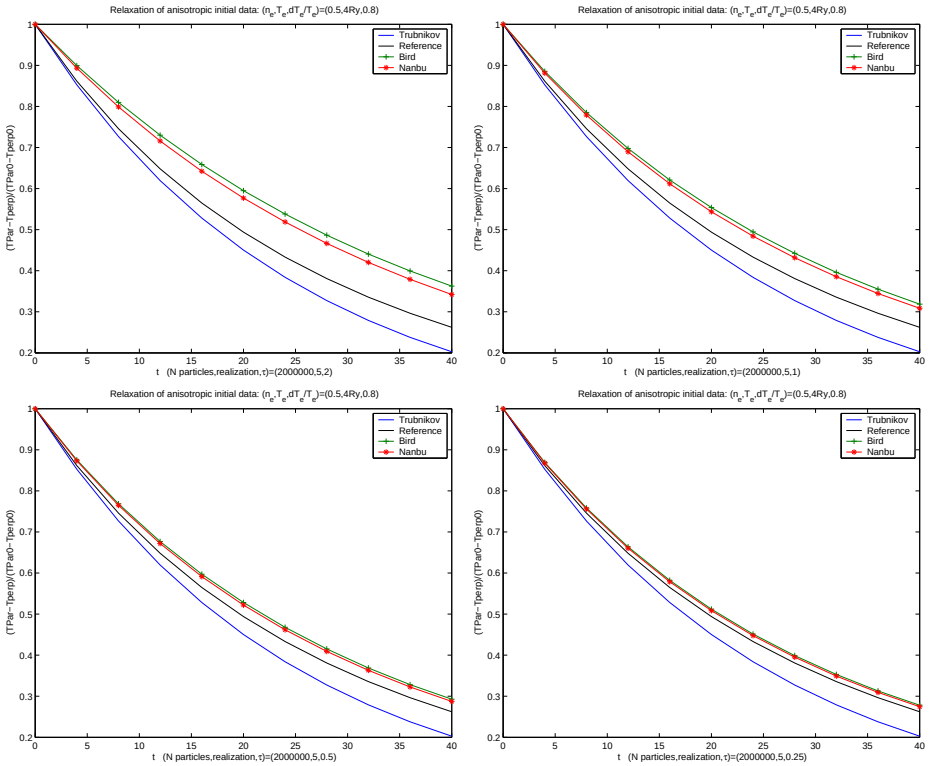

Fig. 5. Comparison of the Bird and Bobylev-Nanbu method for $\tau = 2$ top left, $\tau = 1$ top right, $\tau = 0.5$ bottom left, $\tau = 0.25$ bottom right. In each Figure the Trubnikov (blue line) and the reference solution (black line) are depicted.

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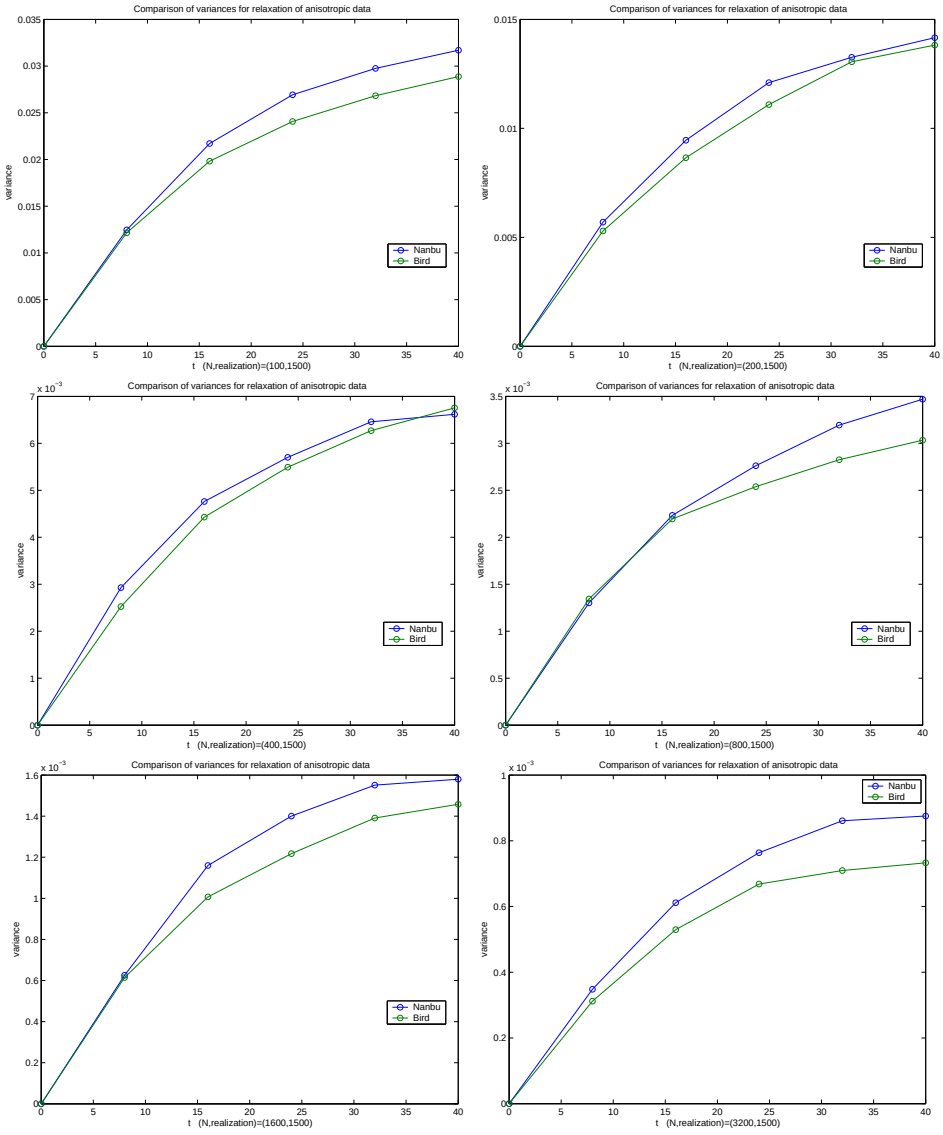

Fig. 6. Comparison of the Bird and Bobylev-Nanbu variance for $\tau = 1$ and $N = 100$ top left $N = 200$ top right $N = 400$ middle left $N = 800$ middle right $N = 1600$ bottom left $N = 3200$ bottom right with $M = 1500$ realizations.