A DSMC method for the Landau-Fokker-Planck equation

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Abstract. A simple and fast algorithm for simulation of collisional processes based on the Landau equation is presented. The simulation scheme is suitable for three-dimensional problems, where the work requirements for deterministic methods may be prohibitively large when the number of particles grows. The algorithm is verified for Maxwell particles and thereafter applied to a particles with Coulomb interaction. A series of numerical experiments related to various spatially homogeneous problems is presented. In order to study the accuracy of the method and the optimal choice of its parameters, comparisons with results obtained by fully conservative finite difference schemes are performed. The DSMC scheme is in turn used to verify the accuracy of the standard approximations with isotropic Rosenbluth potentials in two-dimensional finite difference computations.

Keywords: Kinetic theory, DSMC, Landau equation
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INTRODUCTION

It is well known that very efficient Monte Carlo methods exist for simulation of rarefied gases with short-range intermolecular forces [1, 2]. The starting point for this work was a paper by Bobylev and Nanbu [3] on how to use DSMC methods for long range forces, corresponding to infinite total scattering cross sections. We want to apply this theoretical work to specific problems and construct an algorithm for simulation of collisional processes based on the Landau-Fokker-Planck equation. We assume that a standard splitting scheme is used, and limit the discussion below to just the simulation of collisions for the spatially homogeneous case.

ALGORITHM DESCRIPTION

The spatially homogeneous Boltzmann equation for a distribution function $f(\mathbf{v},t)$ reads

$$\frac{\partial f}{\partial t} = \int_{\mathbb{R}^3\times S^2} g(|\mathbf{u}|,\mu)\left[f(\mathbf{v}',t)f(\mathbf{w}',t) - f(\mathbf{v},t)f(\mathbf{w},t)\right] d\mathbf{w}\, d\boldsymbol{\omega}, \tag{1}$$

where $\mathbf{v}$ and $\mathbf{w}$ are velocities of two particles before a collision, with center of mass velocity $\mathbf{U} = (\mathbf{v}+\mathbf{w})/2$ and relative velocity $\mathbf{u} = \mathbf{v}-\mathbf{w}$. The corresponding post-collision velocities are denoted $\mathbf{v}'$ and $\mathbf{w}'$, giving the relative velocity $\mathbf{u}' = \mathbf{v}'-\mathbf{w}' = |\mathbf{u}|\boldsymbol{\omega}$ after the collision. The scattering angle is $\theta = \arccos\mu \in [0,\pi]$, with $\mu = \mathbf{u}\cdot\boldsymbol{\omega}/|\mathbf{u}|$. In the Boltzmann equation we have $g(|\mathbf{u}|,\mu) = |\mathbf{u}|\sigma(|\mathbf{u}|,\theta)$, where $\sigma(|\mathbf{u}|,\theta)$ is the differential collision cross section.

We always assume that

$$\sigma_{\rm tot}(|\mathbf{u}|) = 2\pi\int_0^\pi \sigma(|\mathbf{u}|,\theta)\sin\theta\, d\theta = \infty, \tag{2}$$

i.e. the total scattering cross section is infinite (corresponding to long range potentials). This allows us to use the the simulation technique described in [3].

Below, we explain this method for a particular case when the scattering is concentrated at small angles (grazing collisions). The Boltzmann equation (1) reduces to the Landau-Fokker-Planck equation

$$\frac{\partial f}{\partial t} = \frac{1}{8}\frac{\partial}{\partial v_i}\int_{\mathbb{R}^3} |\mathbf{u}|\sigma_{\rm tr}(|\mathbf{u}|)\left(|\mathbf{u}|^2\delta_{ij} - u_i u_j\right)\left(\frac{\partial}{\partial v_j} - \frac{\partial}{\partial w_j}\right) f(\mathbf{v},t) f(\mathbf{w},t)\, d\mathbf{w}. \tag{3}$$

where

$$\sigma_{\rm tr}(|\mathbf{u}|) = 2\pi\int_0^\pi \sigma(|\mathbf{u}|,\theta)(1-\cos\theta)\sin\theta\, d\theta. \tag{4}$$

The simulation technique is based on the following first order time-explicit formula:

$$f(\mathbf{v},t+\Delta t) = \frac{1}{\rho}\int_{\mathbb{R}^3\times S^2} G(|\mathbf{u}|,\mu,\rho\Delta t) f(\mathbf{v}',t) f(\mathbf{w}',t)\, d\mathbf{w}\, d\boldsymbol{\omega}, \qquad \rho = \int_{\mathbb{R}^3} f(\mathbf{v},t)\, d\mathbf{v} \tag{5}$$

with time step Δt and kernel

$$G(|\mathbf{u}|,\mu,\tau) = \frac{1}{4\pi}\sum_{k=0}^{\infty}(2k+1)\,P_k(\mu)e^{-\frac{1}{2}k(k+1)|\mathbf{u}|\sigma_{\mathrm{tr}}(|\mathbf{u}|)\tau}, \tag{6}$$

where $P_k(\mu)$ are Legendre polynomials. As discussed in [3], there are many ways to to do a numerical simulation of (5), and in this paper we choose the simplest possible algorithm.

Let ε be a small positive number, and

$$\tau = \varepsilon|\mathbf{u}|\sigma_{\mathrm{tr}}(|\mathbf{u}|), \qquad \mu(\tau) = \begin{cases} 1-2\tau & 0 \leqslant \tau \leqslant 1 \\ -1 & \text{otherwise.} \end{cases} \tag{7}$$

The simulation algorithm can be summarized as:

- For N particles, generate a set of velocity vectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$.
- Repeat:
  - Advance time $t \to t+\Delta t$, $\Delta t = 4\varepsilon/N$.
  - Choose any pair $i \neq j$, $i,j = 1,\ldots,N$, randomly.
  - Compute the center of mass velocity $\mathbf{U} = (\mathbf{v}_i+\mathbf{v}_j)/2$ and relative velocity $\mathbf{u} = \mathbf{v}_i - \mathbf{v}_j$.
  - Find $\theta = \arccos\mu(\tau)$ in (7) and pick φ uniformly distributed in $[0, 2\pi]$. Then $\boldsymbol{\omega} = (\theta,\varphi) \in S^2$ is the new relative velocity $\mathbf{u}' = |\mathbf{u}|\boldsymbol{\omega}$.
  - Compute the new velocities $\mathbf{v}_i' = \mathbf{U} + \mathbf{u}'/2$ and $\mathbf{v}_j' = \mathbf{U} - \mathbf{u}'/2$.

It is clear that the algorithm satisfies all physical conservation laws.

TEST FOR MAXWELL PARTICLES

To verify the algorithm, we compare results from numerical simulations with exact analytical solutions for the moments of $f(\mathbf{v},t)$ for the Maxwellian case $|\mathbf{u}|\sigma_{\mathrm{tr}}(|\mathbf{u}|) = \text{const}$ in (3).

Figure 1 shows numerically computed moments $M_n(t) = \frac{1}{N}\sum_{i=1}^{N}|\mathbf{v}_i|^{2n}$ together with the analytical expressions $m_n(t) = \int_{\mathbb{R}^3}|\mathbf{v}|^{2n} f(|\mathbf{v}|,t)\, d\mathbf{v}$ for $n = 2,3,4$. The initial velocities are in this case uniformly distributed on the unit sphere, i.e., $|\mathbf{v}_i| = 1$. For the lowest order moments, we get good results already with a rather small amount of particles and few simulations.

In Fig. 2, we have the numerically computed relaxation of the pressure tensor elements $P_{\alpha\alpha}(t) = \frac{1}{N}\sum_{i=1}^{N} v_\alpha^2$, $\alpha = x,y$ compared with the steady state value $p_{\alpha\alpha}(\infty) = \langle|\mathbf{v}|^2\rangle/3$. The heat flux vector element $Q_x(t) = \frac{1}{2N}\sum_{i=1}^{N}|\mathbf{v}|^2 v_x$ is also shown. The initial distribution function $f_0(\mathbf{v})$ was here chosen as a combination of two three-dimensional Gaussian peaks along the x-axis

$$f_0(\mathbf{v}) = \alpha M_{-3,2}(\mathbf{v}) + (1-\alpha)M_{1,1}(\mathbf{v}), \tag{8}$$

where $M_{u,T}(\mathbf{v})$ is the Maxwellian velocity distribution centered at $(u,0,0)$ with temperature T.

COULOMB PARTICLES

We now consider the practically important case of particles interacting with a Coulomb potential. The cross section is given by the Rutherford formula

$$\sigma(|\mathbf{u}|,\theta) = \text{const}\cdot|\mathbf{u}|^{-4}\sin^{-4}\frac{\theta}{2}. \tag{9}$$

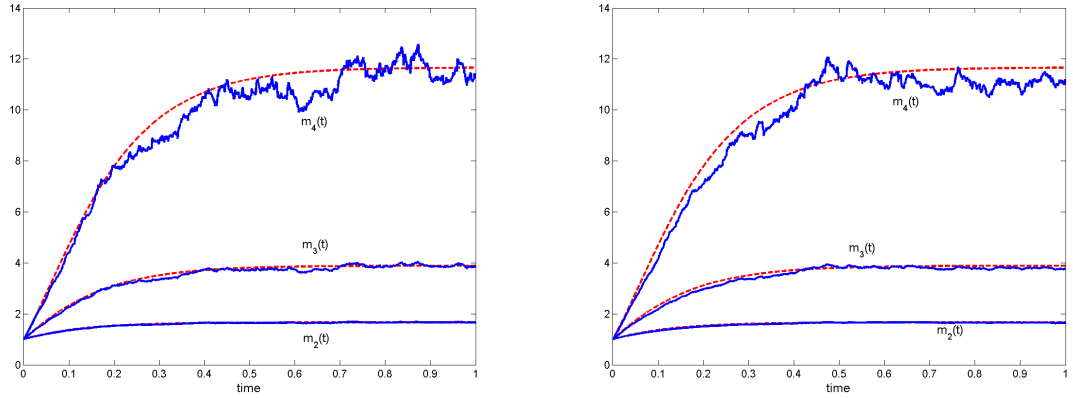

FIGURE 1. Low order moments computed with 20 (right) and 40 (left) simulations with identical initial distribution ($\varepsilon = 0.1$). The dashed curves are the corresponding analytical values. The number of particles is rather low, $N = 200$.

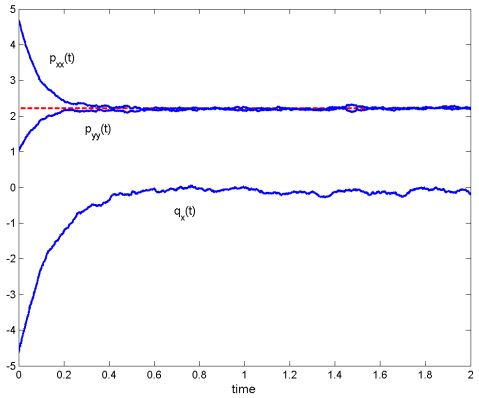

FIGURE 2. The time relaxation of components of the pressure tensor and the heat flux vector in an anisotropic case. $N = 200$ and 20 simulations were performed.

With angular cut-off at a small angle $\theta_{\min}$, we can approximate the momentum transfer cross section (4) by

$$\sigma_{\mathrm{tr}}(|\mathbf{u}|) \approx \mathrm{const} \cdot |\mathbf{u}|^{-4} \int_{\theta_{\min}}^{\pi} \frac{\cos\theta/2}{\sin\theta/2}\, d\theta = \mathrm{const} \cdot |\mathbf{u}|^{-4}. \tag{10}$$

Therefore, we have $\tau \sim \varepsilon |\mathbf{u}|^{-3}$ in this case.

In order to verify our method, we use the numerical results obtained by well-known completely conservative finite-difference schemes, see [4] and references therein. Such schemes give practically exact results for isotropic solutions with space-independent $f = f(|\mathbf{v}|,t)$, and we use these results for our tests. In particular, the left hand side plot of Fig. 3 shows a comparison of moments $m_{2,3,4}(t)$ for a mono-energetic initial distribution function with $|\mathbf{v}| = 1$ at $t = 0$.

A comparison of second order moments for anisotropic solutions with initial data

$$f(|\mathbf{v}|,\mu,t=0) = \frac{1}{2\pi}\delta(|\mathbf{v}|-1)\delta(\mu), \qquad \mu = \cos(\theta) \tag{11}$$

is shown in the right hand side plot of Fig. 3. We compare the so-called parallel ($T_{||} = T_z$) and perpendicular ($T_\perp = T_x + T_y$) temperatures $T_\alpha(t) = \frac{1}{N}\sum_{i=1}^{N} v_\alpha^2$, $\alpha = x,y,z$, with coordinate axes such that $\theta \in [0,\pi]$ in (11) is the angle with the z-axis. In this case, the DSMC results help to estimate the accuracy of the standard approximation (isotropic Rosenbluth potentials) often used for finite difference methods. [4]. Typical particle velocity distributions for this problem are shown in Fig. 4.

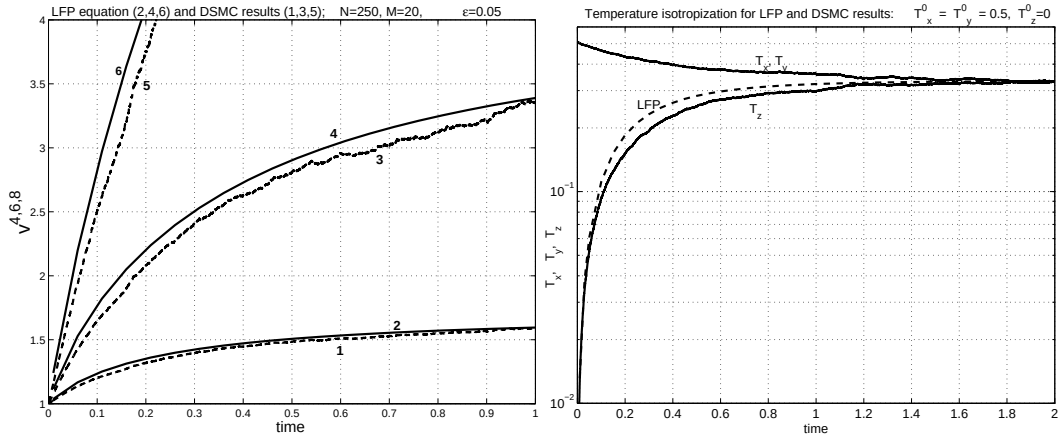

FIGURE 3. Left: Monte Carlo results are dashed curves and the results from the finite difference computations are solid curves. Right: Monte Carlo results are solid curves and the dashed curve is T_z from the finite difference computation.

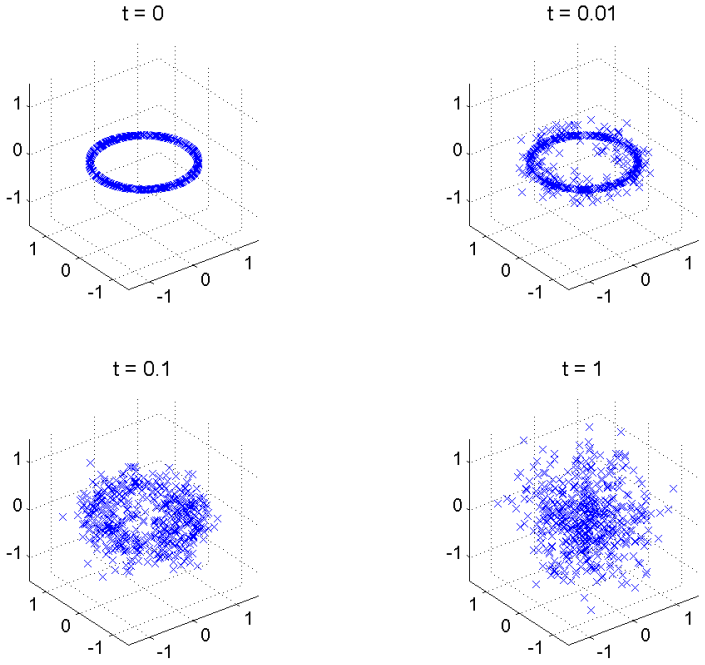

FIGURE 4. The velocities of the particles in a Coulomb simulation.

CONCLUSIONS

Thus, in this paper, we have proposed and verified a very simple and fast algorithm for solving three-dimensional problems for the Landau-Fokker-Planck equation. An additional advantage of the method is that it can be easily generalized to multi-component plasma and combined with existing particle methods for Vlasov-Maxwell equations to account also for the collisionless step in the splitting scheme.

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