# Fast Algorithms for Numerical, Conservative, and Entropy Approximations of the Fokker–Planck–Landau Equation<sup>1</sup>

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We present fast numerical algorithms to solve the nonlinear Fokker–Planck–Landau equation in 3D velocity space. The discretization of the collision operator preserves the properties required by the physical nature of the Fokker–Planck–Landau equation, such as the conservation of mass, momentum, and energy, the decay of the entropy, and the fact that the steady states are Maxwellians. At the end of this paper, we give numerical results illustrating the efficiency of these fast algorithms in terms of accuracy and CPU time. © 1997 Academic Press

# 1. INTRODUCTION: THE FOKKER-PLANCK-LANDAU EQUATION

The Fokker–Planck–Landau (FPL) equation is used for the description of binary collisions between charged particles, for which the interaction potential is the long-range Coulomb interaction.

We restrict ourselves to a single-species plasma since the methods can easily be extended to the multispecies case (see Remark 3.3). The present algorithms are based on the discretization of the FPL operator given in [5] the main features of which are summaried in Section 2.

We denote by f(x, v, t) the distribution function, a solution of the scaled FPL equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = Q(f, f), \qquad (1.1)$$

where Q(f, f) is the FPL collision operator:

$$Q(f,f) = \nabla_v \cdot \left( \int_{\mathbb{R}^3} \Phi(v - v_*) ((\nabla_v f) f_* - (\nabla_{v_*} f) f) \, dv_* \right)$$

$$(1.2)$$

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with

$$f = f(x, v, t), \quad f_* = f(x, v_*, t),$$
$$\nabla_v f = \nabla_v f(x, v, t), \quad \nabla_{v_*} f = \nabla_v f(x, v_*, t)$$

and  $\Phi(v)$  is the 3  $\times$  3 matrix:

$$\Phi(v) = |v|^{\gamma+2} S(v), \quad S(v) = I_3 - \frac{v \otimes v}{|v|^2}.$$
(1.3)

S(v) is the orthogonal projector onto the plane orthogonal to v;  $\gamma$  is a real parameter which leads to the usual classification in hard potentials ( $\gamma > 0$ ), Maxwellian molecules ( $\gamma = 0$ ), or soft potentials ( $\gamma < 0$ ). This latter case involves the Coulombian case itself (i.e.,  $\gamma = -3$ ). The present numerical analysis is concerned with the physically interesting case (the Coulombian one) and the Maxwellian case ( $\gamma = 0$ ) which enable us to compare the numerical results with exact solutions [6].

As is well known in the physics literature and is mathematically established by the work of Arsene'v and Buryac [13] and Desvillettes [14], the FPL collision operator is the limit of the Boltzmann operator for a sequence of a scattering cross section which converges in a convenient sense to a delta function at zero scattering-angle. In the case of a Coulomb interaction, Degond and Lucquin-Desreux obtained the FPL collision operator as the leading term of the cutoff Boltzmann operator when the parameter of the cutoff tends to zero [16]. Concerning the existence of solutions, Arsene'v and Peskov have established the existence of weak-solutions for a short time in the case of the spatially homogeneous FPL equation for the Coulomb potential.

The algebraic structure of the FPL operator is similar to that of the Boltzmann operator. This leads to wellknown physical properties such as the decay of the entropy, the conservation of mass, momentum, and energy, and the characterization of the equilibrium states by Maxwellians. Indeed, these properties can easily be shown on the weak form of the FPL operator,

$$\int_{\mathbb{R}^3} Q(f,f)(v)\psi(v) \, dv$$
  
=  $-\frac{1}{2} \int \int_{\mathbb{R}^3 \times \mathbb{R}^3} ff_* (\nabla_v \psi - \nabla_{v_*} \psi)^T \Phi(v - v_*) (\nabla_v (\ln f)$   
 $- \nabla_{v_*} (\ln f)) \, dv \, dv_*$  (1.4)

for any smooth test function  $\psi$ . From this duality relation, it is an easy matter to check that the only functions  $\psi$  such that for all f,  $\int Q(f, f)\psi dv = 0$ , are linear combinations of 1, v, and  $|v|^2$  (conservation of mass, momentum, and energy).

Furthermore, letting  $\psi = \ln(f)$  in (1.4) leads to the entropy inequality (H-theorem):

$$\int_{\mathbb{R}^3} Q(f, f)(v) \ln(f(v)) \, dv \le 0.$$
 (1.5)

The equilibrium distribution functions, i.e., the functions f such that Q(f, f) = 0 are Maxwellians,

$$M_{\mathcal{N},u,T}(v) = \frac{\mathcal{N}}{(2\pi v_{\rm th}^2)^{3/2}} \exp\left(\frac{-|v-u|^2}{2v_{\rm th}^2}\right), \qquad (1.6)$$

where  $\mathcal{N}$  is the density of particles and  $v_{\rm th}$  is the thermal velocity of the gas which depends on its temperature T through the relation:  $v_{\rm th} = \sqrt{kT/m}$ , where k is the Boltzmann constant and m is the mass of the particle.

In this paper, we are concerned with numerical approximations of the spatially homogeneous FPL equation in the whole 3D velocity space. The starting point of this work is the discretization of the FPL operator given in [5]. Alternate methods are finite difference schemes that have been investigated in [9] in the isotropic case and in [12, 8, 10] for the cylindrically symmetric problems. We also refer to Larroche [17] for a mass conserving finite volume scheme. Recently, conservative and entropic discretizations of axisymmetric FPL operators are investigated in [18]. In [4, 5] a numerical discretization in three-dimensional velocity space that satisfies discrete analogues of the above-mentioned properties is presented and is summarized in the next section. A bibliography on previous works on such methods can be found in [4, 5].

The discretization [4, 5] in three-dimensional velocity space satisfies all properties required by the physical nature of the problem. Unfortunately a direct numerical implementation of this method is very expensive. Its cost is of order  $N^2$  when N is the number of the discrete velocity points. Our first approach for reducing this cost is the use of the sublattices method following the works by Buet [1–3] on the Boltzmann equation. This leads to a cost  $N^2/$   $a^3$ , where *a* is the sublattice mesh size. The second strategy is an adaptation of multigrid methods to the FPL equation. It leads to a cost of the order of *N* ln *N*.

The outline of the paper is as follows: In Section 2, we review the basis of the conservative discretizations introduced in [5]. Section 3 is devoted to a symmetrized version of the method [5] while Section 4 is concerned with the fast algorithms that are themselves the sublattices and the multigrid algorithms. In Section 5, we give numerical results.

## 2. A CLASS OF ENTROPY-DECREASING SCHEMES

By a standard splitting algorithm, we may restrict ourselves to the space-homogeneous FPL equation

$$\frac{\partial f}{\partial t} = Q(f, f), \quad f|_{t=0} = f_0(v), \tag{2.1}$$

where Q(f, f) is given by (1.2) and  $f_0$  is the initial data. We introduce a regular discretization of  $\mathbb{R}^3$ ,  $v_i = i\Delta v$ ,  $i = (i^1, i^2, i^3) \in \mathbb{Z}^3$ , and denote by  $\overline{f}_i$  an approximation of  $f(v_i)$ . Let D be a finite-difference operator that approximates the usual gradient operator  $\nabla$  at least up to the first order, and let  $D^*$  be its formal adjoint. For any "test sequence,"  $\overline{\psi} = (\overline{\psi}_i)_{i \in \mathbb{Z}^3}$ ,  $D\overline{\psi}$  is a sequence  $(D\overline{\psi})_{i \in \mathbb{Z}^3}$  of vectors of  $\mathbb{R}^3$ ,

$$(D\psi)_i = ((D^1\overline{\psi})_i, (D^2\overline{\psi})_i, (D^3\overline{\psi})_i) \in \mathbb{R}^3, \qquad (2.2)$$

where the components  $(D^s\overline{\psi})_i$ , s = 1, 2, 3, approximates the partial derivatives  $(\partial \psi / \partial x_s)(v_i)$ . Such an operator is of the form

$$(D\overline{\psi})_i = \sum_{k \in \mathbb{Z}^3} a_k \psi_{i+k}, \qquad (2.3)$$

where the vectors  $a_k = (a_{k,1}, a_{k,2}, a_{k,3}) \in \mathbb{R}^3$  satisfy

$$\sum_{k\in\mathbb{Z}^3} a_k = 0, \quad \sum_{k\in\mathbb{Z}^3} a_{k,s} k_r \Delta v = \delta_{sr}, \quad (2.4)$$

 $k_r$ , being the *r*th component of *k*. Conditions (2.4) state that *D* coincides with the exact gradient for constant or linear functions, or equivalently, that *D* is an approximation of  $\nabla$  at least up to the first order. The formal adjoint *D*\* or *D* is given by

$$(D^*\overline{\psi})_i = \sum_{k\in\mathbb{Z}^3} a_k^*\psi_{i+k}$$
(2.5)

with

$$a_k^* = a_{-k} \quad \forall k \in \mathbb{Z}^3. \tag{2.6}$$

Note that  $D^*$  is an approximation of  $-\nabla$ .

The approximation  $\overline{Q}(\overline{f},\overline{f})_i$  of  $Q(f,f)(v_i)$  is defined for any test sequence  $\psi$  by

$$\sum_{i\in\mathbb{Z}^{3}}\overline{Q}(\bar{f},\bar{f})_{i}\psi_{i} = -\frac{1}{2}\sum_{(i,j)\in\mathbb{Z}^{3}\times\mathbb{Z}^{3}}\bar{f}_{i}\bar{f}_{j}\left((D\overline{\psi})_{i}-(D\overline{\psi})_{j}\right)^{T}$$

$$\Phi(v_{i}-v_{j})\left((D(\ln\bar{f}))_{i}-(D(\ln\bar{f}))_{j}\right)\Delta v^{3}.$$
(2.7)

The scheme defined by (2.7) decays the entropy:

$$\sum_{i\in\mathbb{Z}^3}\overline{Q}(\bar{f},\bar{f})_i(\ln(\bar{f})_i\leq 0.$$
(2.8)

A collisional invariant is defined as a sequence  $\overline{\psi}_i$  such that

$$\sum_{i\in\mathbb{Z}^3}\overline{Q}(\bar{f},\bar{f})_i\overline{\psi}_i=0\quad\forall(\bar{f}_i)_{i\in\mathbb{Z}^3},$$
(2.9)

or equivalently from (2.7) such that

$$(D\overline{\psi})_i - (D\overline{\psi})_j \in \operatorname{Ker}(\Phi(v_i - v_j)) \quad \forall i, j \in \mathbb{Z}^3.$$
 (2.10)

A discrete equilibrium distribution function (i.e., a function  $\overline{f}_i$  such that  $\overline{Q}(\overline{f}, \overline{f})_i = 0$ ) is clearly, from (2.7), such that  $(\ln \overline{f})_i$  is a collisional invariant (i.e., satisfies (2.10)). It is proved in [5] that (2.10) is equivalent to the existence of a real number  $\lambda$ , *independent of i and j*:

$$(D\overline{\psi})_i - (D\overline{\psi})_j = \lambda(i-j)\,\Delta v \quad \forall i, j \in \mathbb{Z}^3.$$
(2.11)

However, nothing more can be said unless specifying the discrete differential operator D. This is shown on two simplest cases (we refer to [5] for details).

*Case* 1, the right (resp. left) uncentered operator  $D = D_+$  (resp  $D = D_-$ ) defined by

$$(D_{+}^{s}\overline{\psi})_{i} = \frac{\overline{\psi}_{i+e_{s}} - \overline{\psi}_{i}}{\Delta v}, \quad s = 1, 2, 3,$$

$$\left(\text{resp.} (D_{-}^{s}\overline{\psi})_{i} = \frac{\overline{\psi}_{i} - \overline{\psi}_{i-e_{s}}}{\Delta v}, \quad s = 1, 2, 3\right),$$
(2.12)

where  $e_s$  is the *s*th vector of the canonical basis of  $\mathbb{R}^3$ .

Case 2, the centered operator  $D = D_c$  defined by

$$(D_c^s \overline{\psi})_i = \frac{\overline{\psi}_{i+e_s} - \overline{\psi}_{i-e_s}}{2\Delta v}, \quad s = 1, 2, 3.$$
 (2.13)

The operators  $D_+$  and  $D_-$  are clearly first order, while  $D_c$  is second order. For these two cases, we have the following results.

LEMMA 2.1 (Uncentered case). (i) The collisional invariants (i.e., the sequences  $\overline{\psi}_i$  such that (2.11) holds) are linear combinations of 1,  $v_i$ , and  $|v_i|^2$ .

(ii) The equilibrium distribution functions are the discrete Maxwellians.

(iii) Conservation of mass, momentum, and energy hold.

LEMMA 2.2 (Centered case). (i) The collisional invariants are linear combinations of  $v_i$ ,  $|v_i|^2$ , and of the following eight sequences  $\overline{\chi}_{i_*}$ , labelled by  $i_* \in \{0, 1\}^3$ , defined by

$$(\overline{\chi}_{i_*})_i = \begin{cases} 1 & \text{if } i^k \equiv i_*^k (mod2) \ \forall k \in \{1, 2, 3\}, \\ 0 & \text{otherwise}, \end{cases}$$
(2.14)

where  $i^k$  denotes the kth component of  $i \in \mathbb{Z}^3$ .

(ii) The discrete equilibrium functions are exponentials of the above described collisional invariants.

(iii) Conservation of mass, momentum, and energy hold. But seven other independent spurious conservation laws hold associated with  $(\overline{\chi}_{i_*})_{i_* \in [0,1]^3}$ ,

$$\sum_{i\in\mathbb{Z}^{3}}\overline{Q}(\bar{f},\bar{f})_{i}(\bar{\chi}_{i_{*}})_{i}=0 \quad \forall i_{*}\in\{0,1\}^{3}.$$
 (2.15)

(Note that  $1 = \sum_{i_* \in \{0,1\}^3} \overline{\chi}_{i_*}$ , so that conservation of mass can be deduced from the eight conservation laws (2.15).)

The use of the centered discrete difference operator leads to nonphysical equilibrium states (i.e., non-Maxwellian functions). On the other hand, the use of the uncentered discrete operator destroys the symmetry of the problem and does not give satisfactory results. To overcome this problem, we introduce a symmetrization of the discrete FPL operator, based on the averaging of the uncentered discretizations in the various directions of coordinates.

# 3. SYMMETRIZATION OF THE UNCENTERED DISCRETE DIFFERENTIATION

By combing "upwind" and "downwind" uncentered differences in the various direction of coordinates, we define eight uncentered difference operators denoted by  $D_{\varepsilon}$ , for  $\varepsilon = (\varepsilon_1, \varepsilon_2, \varepsilon_3) \in \{-1, 1\}^3$  as

$$(D_{\varepsilon}f)_{i} = \frac{1}{\Delta v} \begin{pmatrix} \varepsilon_{1}(f_{i+\varepsilon_{1}e_{1}} - f_{i}) \\ \varepsilon_{2}(f_{i+\varepsilon_{2}e_{2}} - f_{i}) \\ \varepsilon_{3}(f_{i+\varepsilon_{3}e_{3}} - f_{i}) \end{pmatrix}.$$
 (3.1)

At variance, there is only one centered operator denoted by  $D_c$ :

$$(D_c f)_i = \frac{1}{2\Delta v} \begin{pmatrix} f_{i+e_1} - f_{i-e_1} \\ f_{i+e_2} - f_{i-e_2} \\ f_{i+e_3} - f_{i-e_3} \end{pmatrix}.$$
 (3.2)

We denote by  $Q^{\varepsilon}$  and  $Q^{c}$  the corresponding discretized FPL operator defined by the duality relation (2.7). In this section we introduce the symmetrization of the FPL operator  $Q^{us}$  obtained by taking the average of the operators  $Q^{\varepsilon}$  over all  $\varepsilon \in \{-1, 1\}^{3}$ :

$$Q^{us} = \frac{1}{8} \sum_{\varepsilon \in \{-1,1\}^3} Q^{\varepsilon}.$$
 (3.3)

We also introduce a new difference operator  $\Delta$  as

$$(\Delta f)_{i} = \frac{1}{(\Delta v)^{2}} \begin{pmatrix} f_{i+e_{1}} + f_{i-e_{1}} - 2f_{i} \\ f_{i+e_{2}} + f_{i-e_{2}} - 2f_{i} \\ f_{i+e_{3}} + f_{i-e_{3}} - 2f_{i} \end{pmatrix}$$
(3.4)

and denote by  $Q^{\Delta}$  the operator defined by the duality relation

$$\sum_{i\in\mathbb{Z}^{3}} Q_{i}^{\Delta}\psi_{i} = -\frac{1}{2} \sum_{(i,j)\in\mathbb{Z}^{3}\times\mathbb{Z}^{3}} \bar{f}_{i}\bar{f}_{j} \left((\Delta\overline{\psi})_{i} - (\Delta\overline{\psi})_{j}\right)^{\mathrm{T}}\Phi^{\Delta}(v_{i} - v_{j})$$

$$(\Delta(\ln \bar{f}))_{i} - (\Delta(\ln \bar{f}))_{j})\Delta v^{3},$$
(3.5)

where we have set

$$\Phi^{\Delta}(v) = |v|^{\gamma} \text{Diag}(|v|^2 - v_1^2, |v|^2 - v_2^2, |v|^2 - v_3^2) \quad (3.6)$$

and Diag(x, y, z) denotes the diagonal matrix whose diagonal elements are x, y, and z.

With these notations, a simple calculation yields the following result.

**PROPOSITION 3.1.** We have

$$\sum_{i\in\mathbb{Z}^3} Q_i^{us}\psi_i = \sum_{i\in\mathbb{Z}^3} Q_i^c\psi_i + \frac{\Delta v^2}{4} \sum_{i\in\mathbb{Z}^3} Q_i^{\Delta}\psi_i.$$
(3.7)

The operator  $Q^{us}$  is the sum of two contributions: the first one is the centered operator  $Q^c$  and the second one is a sort of viscosity term which serves to eliminate all spurious collisional invariants that may be generated by

the first contribution (see Lemma 2.2)). The numerical implementation of  $Q^{us}$  in the form (3.7) is clearly less expensive than the one in the form (3.3).

On the other hand, it is possible to reduce the computational cost of the viscosity term (3.5) by replacing the sum over  $(i, j) \in \mathbb{Z}^3 \times \mathbb{Z}^3$  in (3.5) by a sum over  $(i, j) \in \mathbb{Z}^3 \times \mathbb{Z}^3$  with  $|i - j| \leq \sqrt{2}$ . In the following proposition we show that this reduction does not affect the conservation properties and does not generate any spurious collisional invariant. We denote by  $Q^{usr}$  the FPL operator using this reduction procedure, i.e.,

$$\sum_{i\in\mathbb{Z}^3} Q_i^{\mu sr} \psi_i = \sum_{i\in\mathbb{Z}^3} Q_i^c \psi_i + \frac{\Delta v^2}{4} \sum_{i\in\mathbb{Z}^3} Q_i^{\Delta r} \psi_i$$
(3.8)

with

$$\sum_{i \in \mathbb{Z}^3} Q_i^{\Delta r} \psi_i = -\frac{1}{2} \sum_{\substack{i, j \in \mathbb{Z}^3 \times \mathbb{Z}^3 \\ |i-j| \le \sqrt{2}}} \bar{f}_i \bar{f}_j \times ((\Delta \overline{\psi})_i - (\Delta \overline{\psi})_j)^{\mathrm{T}} \Phi^{\Delta} (v_i - v_j)$$

$$((\Delta (\ln \bar{f}))_i - (\Delta (\ln \bar{f}))_j) \Delta v^3$$
(3.9)

and we have

PROPOSITION 3.2. For the discrete FPL operator defined by formulas (3.8) and (3.9), the collisional invariants are of the form

$$\psi_i = A|v_i|^2 + \langle B, v_i \rangle + C. \tag{3.10}$$

*Proof.* By Lemma 2.2 the collisional invariants for the centered difference operator have the form

$$\psi_{i} = A |v_{i}|^{2} + \langle B, v_{i} \rangle + \sum_{k \in \{0,1\}^{3}} C_{k}(\chi_{k})_{i}, \qquad (3.11)$$

where  $C_k = C_{k_1k_2k_3}$  are arbitrary coefficients and  $\chi_k$  is defined in Lemma 2.2. But the viscosity term (3.9) gives the following additional relations:

$$(\Delta \overline{\psi})_i - (\Delta \overline{\psi})_j \in \operatorname{Ker} \Phi^{\Delta}(i-j)$$
(3.12)

for all *i*, *j* such that  $|i - j| \le \sqrt{2}$  which implies

$$[|i-j|^2 - (i_k - j_k)^2][C_{\overline{i+e_k}} - C_{\overline{j+e_k}} - (C_{\overline{i}} - C_{\overline{j}})] = 0 \quad (3.13)$$

for all  $k \in \{1, 2, 3\}$  and for all *i*, *j* such that  $|i - j| \le \sqrt{2}$ . The notation  $\overline{i}$  denotes the class of *i* modulo 2, that is the vector whose components are the classes of *i*'s components modulo 2 ( $\overline{i} \in \{0, 1\}^3$ ). To simplify we suppose that i = (0, 0, 0) and denote by  $(e_1, e_2, e_3)$  the canonical basis of  $\mathbb{R}^3$ .

For each fixed  $k \in \{1, 2, 3\}$  we choose  $l \in \{1, 2, 3\}$  such and the associated finite difference operators as: that  $k \neq l$  and take  $j = e_l$ , we get by (3.13)

$$C_{e_k} - C_{\overline{e_l} + e_k} - (C_{000} - C_{e_l}) = 0$$
(3.14)

for all  $k \neq l$ . Now, taking  $j = e_k + e_l$  with  $k \neq l$  we obtain

$$C_{e_k} - C_{e_l} - (C_{000} - C_{\overline{e_k} + e_l}) = 0.$$
 (3.15)

Combining these last two relations, we get  $C_{e_{k}} = C_{000}$  for all  $k \in \{1, 2, 3\}$ . Inserting this in (3.15) we have also  $C_{\overline{e_k}+e_l} = C_{000}$  for all  $k, l \in \{1, 2, 3\}.$ 

Finally, by writing (3.13) for k = 1 and  $j = e_2 + e_3$ , we obtain  $C_{111} = C_{000}$  which concludes the proof thanks to relation  $1 = \sum_{k \in \{0,1\}^3} \chi_k$ .

Remark 3.3. Extension to the multispecies Fokker-Planck equation. We extend the above method to two species of particles denoted by indces a and b, respectively. The distribution functions of these two species satisfy the following system of homogeneous FPL equations:

$$\frac{\partial f_a}{\partial t} = Q_a(v_a), \quad \frac{\partial f_b}{\partial t} = Q_b(v_b), \tag{3.16}$$

where we have set (with  $\alpha = a$  or b and  $\beta = b$  or a, respectively):

$$Q_{\alpha}(v_{\alpha}) = \frac{1}{m_{\alpha}} \nabla_{v_{\alpha}} \cdot \int_{\mathbb{R}^{3}} \Phi(v_{\alpha} - v_{\beta})$$

$$\left(\frac{1}{m_{\alpha}} \nabla_{v_{\alpha}} f_{\alpha} f_{\beta} - \frac{1}{m_{\beta}} \nabla_{v_{\beta}} f_{\beta} f_{\alpha}\right) dv_{\beta}.$$
(3.17)

Let  $\psi_{\alpha} = \psi_{\alpha}(v_{\alpha})$  be two test functions (for  $\alpha = a$  and b). We have

$$\int_{\mathbb{R}^{3}} Q_{a}(v_{a})\psi_{a} dv_{a} + \int_{\mathbb{R}^{3}} Q_{b}(v_{b})\psi_{b} dv_{b}$$

$$= -\int_{\mathbb{R}^{3}\times\mathbb{R}^{3}} f_{a}f_{b} \times \left(\frac{1}{m_{a}}\nabla_{a}\psi_{a} - \frac{1}{m_{b}}\nabla_{b}\psi_{b}\right)^{\mathrm{T}} \quad (3.18)$$

$$\Phi(v_{a} - v_{b})\left(\frac{1}{m_{a}}\nabla_{a}\ln f_{a} - \frac{1}{m_{b}}\nabla_{b}\ln f_{b}\right).$$

We consider different mesh sizes for the two species and define two regular discretizations of  $\mathbb{R}^3$  according to:

$$v_i^a = i\Delta v_a, v_i^b = i\Delta v_b \quad \text{for } i \in \mathbb{Z}^3, \tag{3.19}$$

$$(D_{\alpha}\psi)i = \frac{1}{\Delta v_{\alpha}} \sum_{k \in \mathbb{Z}^3} a_k \psi_{i+k}.$$
 (3.20)

We also consider the operators  $D_{\alpha,\varepsilon}$  and  $D_{\alpha,c}$  defined by (3.1) and (3.2) with the mesh size  $\Delta v_{\alpha}$ . With these notations, it is an easy matter to see that we have

**PROPOSITION 3.4.** For the centered difference operators  $D_{\alpha,c}$ , we have the conservation of mass, momentum, and energy. However, for the uncentered difference operators  $D_{\alpha,\varepsilon}$  the conservation of energy holds if and only if  $\Delta v_a = \Delta v_b$ .

#### 4. FAST ALGORITHMS

#### 4.1. Deterministic Schemes: Sublattices Methods

The computational complexity is of order  $N^2$  which is much too big for a practical use of the discrete FPL operators. To reduce this cost, a first strategy is to use sublattices as it was done for the Boltzmann collision operator [1]. We present a brief description of the method and show how to preserve the physical properties. We also show how to design the algorithm in order to avoid spurious collisional invariants. In this section we deal with the uncentered discrete difference operator although the following results remain valid if we use the symmetrized operator given by (3.3).

For  $a \in \mathbb{Z}$ ,  $a \ge 2$ , we define the discrete operator  $Q_i[a]$ by the duality relation

$$\sum_{i\in\mathbb{Z}^3} Q_i[a]\psi_i = -\frac{1}{2}\sum_{i\equiv j\,[a]}\bar{f}_i\bar{f}_j$$

$$((D\overline{\psi})_i - (D\overline{\psi})_j)^{\mathrm{T}} \Phi(v_i - v_j)((D(\ln \bar{f}\,))_i - (D(\ln \bar{f}\,))_j) \Delta v^3,$$
(4.1)

where the definition of  $i \equiv j [a]$  means that i - j is a multiple of a. The following result makes the collisional invariants for this discretization precise.

PROPOSITION 4.1. Let A and B real constants, and let  $C_i$  only depending on the class of i modulo a (i.e.,  $C_i$  =  $C_{\bar{i}}$  with  $\bar{i}$  the class of *i* modulo *a*); then

$$\overline{\psi}_i = A|v_i|^2 + \langle B, v_i \rangle + C_{\overline{i}}$$

are collisional invariants generated by the discrete operator  $Q_i[a]$  defined by (4.1).

*Proof.*  $\overline{\psi}$  is a collisional invariant for the operator  $Q_i[a]$ if and only if

$$(D\overline{\psi})_i - (D\overline{\psi})_i \in \operatorname{Ker} \Phi(i-j) \tag{4.2}$$

for all *i*, *j* such that  $i \equiv j[a]$ . Replacing  $\overline{\psi}_i$  successively by  $|v_i|^2$ ,  $v_i$ , and  $C_{\overline{i}}$ , we easily obtain the desired result.

Now we shall modify this method in order to preserve the Maxwellians as unique possible equilibrium states: Let a and b two mutually prime integers, i.e., such that  $a \land b = 1$ , where  $a \land b$  is the greatest common divisor of aand b. We consider the two corresponding operators  $Q_i[a]$ and  $Q_i[b]$  defined by the duality formula (4.1).

We set

$$Q_i[a, b] = \frac{1}{2}(Q_i[a] + Q_i[b])$$
 for all  $i \in \mathbb{Z}^3$ . (4.3)

We have the following result.

**PROPOSITION 4.2.** If we use the uncentered difference operator, then the collisional invariants of the discrete operator given by formula (4.3) are the linear combinations of mass, momentum, and energy.

*Proof.* A collisional invariant of the discrete operator  $Q_i[a, b]$  must be a collisional invariant for both  $Q_i[a]$  and  $Q_i[b]$ . Therefore, if  $\overline{\psi}$  is a collisional invariant generated by  $Q_i[a, b]$  then

$$(D\psi)_i - (D\psi)_i \in \operatorname{Ker} \Phi(i-j) \tag{4.4}$$

for all *i*, *j* such that  $i \equiv j[a]$  or  $i \equiv j[b]$ .

Therefore, for *i* and  $k \in \mathbb{Z}^3$ , we have

$$(D\overline{\psi})_{i+ak} - (D\overline{\psi})_i = \lambda(i,k)ak \tag{4.5}$$

$$(D\psi)_{i+bk} - (D\psi)_i = \mu(i,k)bk \tag{4.6}$$

with  $\lambda(i, k), \mu(i, k) \in \mathbb{R}$ .

Thus, from (4.5), we can write two relations,

$$(D\overline{\psi})_{i+ak} - (D\overline{\psi})_{i+al} = \lambda(i+la,k-l)a(k-l)$$
  
 $(D\overline{\psi})_{i+ak} - (D\overline{\psi})_{i+al} = \lambda(i,k)ak - \lambda(i,l)al,$ 

for all *i*, *k*,  $l \in \mathbb{Z}^3$  and easily obtain:  $\lambda(i, k) = \lambda(i, l)$  for all *i*, *k*,  $l \in \mathbb{Z}^3$ , which means that  $\lambda(i, k)$  is independent of *k*, and the same is true for  $\mu(i, k)$ . Let  $\lambda(i, k) = \lambda_i$ , and  $\mu(i, k) = \mu_i$ . Now by writing

$$(D\overline{\psi})_{i+abk} - (D\overline{\psi})_i = \lambda_i abk = \mu_i abk \quad \forall i, k \in \mathbb{Z}^3, \quad (4.7)$$

we obtain  $\lambda_i = \mu_i = \alpha_i$  for all  $i \in \mathbb{Z}^3$ . On the other hand, we have

$$2a\alpha_{i}k = (D\overline{\psi})_{i+2ak} - (D\overline{\psi})_{i}$$
$$= (D\overline{\psi})_{i+2ak} - (D\overline{\psi})_{i+ak} + (D\overline{\psi})_{i+ak} - (D\overline{\psi})_{i}$$
$$= a\alpha_{i+ak}k + a\alpha_{i}k$$

which gives

$$\alpha_{i+ak} = \alpha_i \quad \forall i, k \in \mathbb{Z}^3$$

and this is also true for  $b: \alpha_{i+bk} = \alpha_i \forall i, k \in \mathbb{Z}^3$ .

Now let *i* and *j* two arbitrary elements of  $\mathbb{Z}^3$ , since  $a \land b = 1$ , the Bezout identity gives the existence of two triples  $q, r \in \mathbb{Z}^3$  such that

$$i - j = aq + br. \tag{4.8}$$

Then we have

$$\alpha_j = \alpha_{j+aq} = \alpha_{j+aq+br} = \alpha_{i}$$

and, finally, we deduce that  $\alpha_i$  does not depend on *i* and then

$$(D\overline{\psi})_i - (D\overline{\psi})_j = \alpha(i-j) \tag{4.9}$$

for all  $i, j \in \mathbb{Z}^3$ . In the case of the uncentered difference operator D, this classically implies (see [5]) that  $\psi_i$  is a linear combination of the mass, the momentum, and the energy, and concludes the proof of Proposition 4.2.

## 4.2. Random Methods: Multigrid Algorithms

In this section we compute the discrete FPL collision operator by using a multigrid method with numerical integration of Monte-Carlo type. The computational complexity of this simulation is of order  $N \ln N$ , where N is the number of discrete velocity points. This approach takes its inspiration from the method of Greengard and Rokhlin [19]. In a subsequent work [7], a new method goes further in the adaptation of [19] to the FPL equation.

#### 4.2.1. Description of the Method

To simplify the notations, we set

$$H(v,w) = -\frac{1}{2}f(v)f(w)[\nabla_v \psi - \nabla_w \psi]^T$$
  

$$\Phi(v-w)[\nabla_v(\ln f) - \nabla_w(\ln f)].$$
(4.10)

We assume that the discrete velocity domain is a cube  $C_0$  of length 1 which contains  $N = (2^n)^3 = 8^n$  discrete points lying on a regular cubic lattice. The algorithm is the following:

• Step 0. We just write the FPL operator in a weak form:

$$\int_{C_0} Q(f, f)(v) \psi(v) \, dv = \int_{C_0 \times C_0} H(v, w) \, dv dw.$$
(4.11)

• Step 1. We split the cube  $C_0$  (the parent) into 8 regular boxes  $C_1^r$  (the children),  $r \in \{0, 1\}^3$ . Each box  $C_1^r$  is of length  $\frac{1}{2}$  and its center is

$$O_1^r = \left(\frac{1}{2^2} + \frac{r_1}{2}, \frac{1}{2^2} + \frac{r_2}{2}, \frac{1}{2^2} + \frac{r_3}{2}\right)$$
(4.12)

with  $r = (r_1, r_2, r_3) \in \{0, 1\}^3$ . we set  $I_1 = \{0, 1\}^3$ . Again, we do not do any numerical approximation; we only write

$$\int_{C_0} Q(f,f)(v)\psi(v) \, dv = \sum_{(r,r') \in I_1^2} \int_{C_1^r \times C_1^{r'}} H(v,w) \, dv dw.$$
(4.13)

• Step k ( $k \ge 2$ ). We denote by  $C_k^r$  the boxes of level k obtained after splitting each of those of level k - 1 (the parents) into eight regular boxes (the children). More precisely  $C_k^r$  is the box of length  $1/2^k$  and whose center is

$$O_k^r = \left(\frac{1}{2^{k+1}} + \frac{r_1}{2^k}, \frac{1}{2^{k+1}} + \frac{r_2}{2^k}, \frac{1}{2^{k+1}} + \frac{r_3}{2_k}\right)$$
(4.14)

with  $r = (r_1, r_2, r_3) \in I_k = \{0, 1, ..., 2^k - 1\}^3$ . If  $C_{k-1}^R$  is the father of  $C_k^r$  then it is easy to see that

$$O_{k-1}^{R} = \left(\frac{1}{2^{k}} + \frac{R_{1}}{2^{k-1}}, \frac{1}{2^{k}} + \frac{R_{2}}{2^{k-1}}, \frac{1}{2^{k}} + \frac{R_{3}}{2^{k-1}}\right)$$

with

$$R_{i} = \frac{r_{i}}{2} \qquad \text{if } r_{i} \text{ is even}$$

$$R_{i} = \frac{r_{i} - 1}{2} \qquad \text{if } r_{i} \text{ is odd.}$$

$$(4.15)$$

*Remark* 4.3. To obtain the children of  $C_k^r$ , we add to the center  $O_k^r$  the quantities

$$rac{1}{2^{k+1}}(arepsilon_1,arepsilon_2,arepsilon_3),$$

where

$$(\varepsilon_1, \varepsilon_2, \varepsilon_3) \in \{-1, 1\}^3$$

*Remark* 4.4. To obtain the nearest neighbours of  $C_k^r$ , we add to the center the quantities  $(1/2^k)(\varepsilon_1, \varepsilon_2, \varepsilon_3)$ , where  $(\varepsilon_1, \varepsilon_2, \varepsilon_3) \in \{-1, 0, 1\}^3$  (27 neighbours).

The box  $C_k^r$  will be said to be "well separated" from  $C_k^{r'}$  if and only if  $C_k^{r'}$  is a child of one of the nearest

neighbours of the parent of  $C_k^r$  and is not a nearest neighbour of  $C_k^r$ .

The notation *ws* means "well separated" and *nws* means "not well separated," i.e., neighbours.

To simplify the algorithm we only describe the method for level 2:

At level 2, we split each box  $C_1^r$  of level 1 into 8 boxes and write

$$\int_{C_0} Q(f,f)(v)\psi(v) \, dv = \sum_{\substack{(r,r') \in I_2^2 \\ r \, ws \, r'}} \int_{C_2^r \times C_2^{r'}} H(v,w) \, dv dw + \sum_{\substack{(r,r') \in I_2^2 \\ r \, mws \, r'}} \int_{C_2^r \times C_2^{r'}} H(v,w) \, dv dw.$$
(4.16)

If  $C_2^r$  is "well separated" from  $C_2^{r'}$ , then we replace the corresponding integral by a numerical approximation of Monte-Carlo type. In the second case we do not do any numerical approximation and pass to level 3. We repeat this process until step n, where we perform a Monte-Carlo approximation not only for the "well-separated" boxes but also for the nearest neighbours.

#### 4.2.2. Numerical Integration of Monte-Carlo Type

We assume that we are at a fixed level k and we want to approximate the expression

$$\int_{C_k^r \times C_k^{r'}} H(v, w) \, dv dw \tag{4.17}$$

when  $C_k^r$  and  $C_k^{r'}$  are "well separated."

A direct approximation requires  $8^{2(n-k)}$  evaluations. But this leads to an amount of work proportional to  $N^2$ . Therefore, in order to have a cost of order  $N \ln N$  we must use only  $n_k = 8^{n-k}$  evaluations to approximate (4.17) such that after  $n_k$  iterations all the pairs  $(i, j) \in C'_k \times C'_k$  were chosen. One way is the following.

Let  $\{1, 2, ..., n_k\}$  be a numbering of the  $n_k$  elements of  $C_k^r$  or  $C_k^r$  and let  $\pi$  be a randomly chosen permutation of  $\{1, 2, ..., n_k\}$ . In the first time step we approximate (5.21) by a Monte Carlo quadrature formula using pairs  $(l, \pi(l)) \in C_k^r \times C_k^r$ . In the second time step we use pairs  $(r, \pi^2(r))$ , etc. until covering the maximum number of possible pairs  $(l, l') \in C_k^r \times C_k^r$ , i.e., until the number of iterations reaches the order of  $\pi$  in the group  $\mathscr{I}_{n_k}$  of permutations of the set  $\{1, 2, ..., n_k\}$ . Therefore, for all the pairs  $(l, l') \in C_k^r \times C_k^r$  to be chosen, the permutation  $\pi$  must be of order  $n_k$ . If such a choice of  $\pi$  is possible then after  $n_k$  iterations in time the integral will be well approximated since all pairs  $(l, l') \in C_k^r \times C_k^r$  will have been chosen. For the next  $n_k$ 

time steps, we change randomly the permutation  $\pi$  and repeat the same process.

Finally, when  $C_k^r$  and  $C_k^{r'}$  are "well separated," the Monte-Carlo approximation of (4.17) is given by

$$H_{k}^{r,r'} \stackrel{def}{=} 8^{n-k} (\Delta v)^{6} \sum_{(i,\pi(i)) \in C_{k}^{r} \times C_{k}^{r'}} H(v_{i}, v_{\pi(i)}).$$
(4.18)

This way of choosing random collision pairs  $(v_i, v_{\pi(i)})$  was first suggested by Babovsky in [20] as an improvement of Nanbu's scheme of the Boltzmann equation. In this work, we can also find a similar (Monte Carlo) quadrature formula which is proved to be consistent with the corresponding integral. This method can be applied to prove the consistency with (4.18) of the integral:

$$\int_{C_k^r \times C_k^{r'}} H(v, w) \, dv \, dw$$

However, the use of the multigrid methodology introduces additional consistency errors that have not been analysed precisely. The method is probably more precise in the Coulomb case, where the collision cross section decays as the relative velocity increases than for other interactions forces with nondecreasing cross sections. Morever, rigorous proofs of those statements are beyond the scope of this paper and will be the subject of future works.

Finally, we point out that the conservation properties and the decrease of the entropy are still satisfied. Indeed the expression (4.10) of H(v, w) vanishes when we replace  $\psi$  by 1,  $v_i$ , or  $v_i^2$  and becomes negative when we replace  $\psi$ by ln f. On the other hand, a rigorous treatment of spurious collisional invariants is not clear and is not addressed here. It seems, however, that the multigrid method does not generate spurious collisional invariants (when we use the uncentered or the symmetrized uncentered difference operators), and the numerical tests confirm clearly this assertion.

## 5. NUMERICAL RESULTS

We present numerical tests of the above two methods (sublattices and multigrids) on two cases: the Maxwellian case ( $\gamma = 0$ ) and the Coulombian case ( $\gamma = -3$ ). In all these tests, we use a regular grid of size  $\Delta v$  in the velocity space which contains  $N = (2^n)^3$  points and *n* takes the value n = 4 (grid  $16 \times 16 \times 16$ ) or the value n = 5 (grid  $32 \times 32 \times 32$ ). The length of this grid is denoted by  $v_{\text{max}}$ and the number of points of one edge is  $2^n$ . The discrete velocity domain is then the set of points  $v_i = (i^1 \Delta v, i^2 \Delta v, i^3 \Delta v)$  with  $i = (i^1, i^2, i^3)$  ( $0 \le i^k \le 2^n - 1, k = 1, 2, 3$ ). We also consider the center of the domain  $v_0 = (v_{\text{max}}/2, v_{\text{max}}/2, v_{\text{max}}/2)$ . If *f* is the distribution function, we set:  $f_i = f(v_i)$ . Finally, we make precise that all the following numerical tests are performed within the uncentered and symmetrized FPL operator. In these tests, we consider the evolution in time of the following quantities:

• Discrete kinetic entropy,

$$H_d(t) = \sum_{i \in \mathbb{Z}^3} f_i(t) \log f_i(t) \,\Delta v^3. \tag{5.1}$$

• Discrete moment of order 4,

$$\mathcal{M}_d^{(4)}(t) = \sum_{i \in \mathbb{Z}^3} \left( |i| \Delta v \right)^4 f_i(t) \Delta v^3.$$
(5.2)

Discrete temperatures,

$$T_{x}(t) = \sum_{i \in \mathbb{Z}^{3}} (i^{1}\Delta v - u_{0}^{1})^{2} f_{i}(t) \Delta v^{3}$$
(5.3)

$$T_{y}(t) = \sum_{i \in \mathbb{Z}^{3}} (i^{2} \Delta v - u_{0}^{2})^{2} f_{i}(t) \Delta v^{3}$$
(5.4)

$$T_{z}(t) = \sum_{i \in \mathbb{Z}^{3}} (i^{3} \Delta v - u_{0}^{3})^{2} f_{i}(t) \Delta v^{3}$$
(5.5)

$$T(t) = \frac{1}{3} [T_x(t) + T_y(t) + T_z(t)], \qquad (5.6)$$

where  $i = (i^1, i^2, i^3), u_0 = (u_0^1, u_0^2, u_0^3) = (1/\mathcal{N}) \int_{\mathbb{R}^3} v f(v) dv$ , and  $\mathcal{N} = \int_{\mathbb{R}^3} f(v) dv$ .

• Quadratic error: if  $f^{\text{exact}}$  is an exact solution in the Maxwellian case [6], and f is the approximate solution by sublattices or multigrids schemes corresponding to the initial data  $f_0(v) = f^{\text{exact}}(0, v)$ , then we define the quadratic error as

$$EQ(t) = \sum_{i \in \mathbb{Z}^3} |f_i(t) - f_i^{\text{exact}}(t)|^2 (\Delta v)^3.$$
(5.7)

The numerical tests are performed with:  $v_{\text{max}} = 6$ , n = 4, or 5 (i.e.,  $N = 16^3$ , or  $32^3$ ). The two methods (sublattices and multigrid) are tested on two different types of initial datas:

*Test* 1. The Maxwellian case: the initial data is chosen in the class of known exact isotropic solutions [6]. Our numerical results are compared with the simplest element of this class of exact solutions,

$$f^{\text{exact}}(v,t) = M_{\mathcal{N}_{v_0,T}}(v)(1+c_2Q_2[(v-v_0)/v_{th}]\exp(-8\mathcal{N}t)),$$





FIG. 1. Kinetic entropy for Maxwellian case.

where:

$$Q_2(v) = \frac{1}{120} \left( v^4 - 10v^2 + 15 \right) \tag{5.9}$$

Sublattices method

is a Sonine polynomial. We recall that  $v_0 = (3., 3., 3.)$  is the center of the domain and choose  $v_{\rm th} = 0.6$ ,  $\mathcal{N} = 5$ . We note that, in this case, the temperatures in various directions  $T_x$ ,  $T_y$ , and  $T_z$  are equal because of the isotropy of the solution and of the isotropy properties of the FPL operator. The evolutions of the entropy and the order 4 moment are compared with their exact evolution in time (Figs. 1 and 3). The evolution of the entropy induced by the multigrid scheme is a little more accurate than the one induced by the sublattice algorithm. To reach the same accuracy, it is necessary to decrease the sublattice size, and then to increase the computational cost. On the other hand, oscillations arise in the time evolution of the moment of order 4 for the multigrid scheme, while the evolution is smooth for the sublattices algorithm. Notice, however, that the relative variations of the moment of order 4 and, thus, of these oscillations, are small. The quadratic error between the distribution function obtained by the numerical schemes and the exact solution of the FPL equation is plotted (Fig. 6) and shows the efficiency of the randommultigrid method in terms of accuracy.

*Test* 2. The Coulombian case: the initial data is now chosen to be bi-Maxwellian i.e., a sum of two Maxwellian functions,

$$f_0(v) = \frac{1}{2} \left( M_{\mathcal{N}, v_{01}, T}(v) + M_{\mathcal{N}, v_{02}, T}(v) \right), \tag{5.10}$$

where  $M_{\mathcal{N},u,T}$  is given by (1.6), and

$$v_{01} = (2., 3., 3.), \quad v_{02} = (4., 3., 3.).$$

We finally choose  $v_{th} = 0.45$ ,  $\mathcal{N} = 5$ .

The evolutions in time of the entropy and of the temperatures are now compared with the results of exact schemes 2.7 which have a quadratic complexity. The curves of Figs. 2, 5 show that the multigrid algorithm is a little more accurate than the sublattices method. The curves of Fig. 5 give the relaxations in time of the temperatures in various directions of velocity coordinates to their final values and confirm the accuracy of these algorithms. These temperatures are constant if we choose an isotropic initial distribution (as in Test 1 for the Maxwellian case). In the result given by Fig. 4, however, we again observe oscillations of the sublattices method gives smoother results. As in Test 1, we note that these oscillations have small relative values.

The curves given in Fig. 7 illustrate the fact that two sublattice sizes are necessary to avoid non-Maxwellian steady states as it is shown in Proposition 4.2. Indeed, a simple use of only one sublattice size (a = 5 for  $32 \times 32 \times 32$  grid) leads to a final distribution function which is far from the realistic equilibrium state. This is shown

#### Sublattices method

#### Multigrid method



FIG. 2. Kinetic entropy for Coulombian case.



Multigrid method



FIG. 3. Moment of order 4 for Maxwellian case.

by plotting the relaxation of the value of the distribution function at the center of the grid (Fig. 7). A difference between the two relaxations given by the use of one (a = 5) or two (a = 5, b = 6) sublattice sizes is observed (Fig. 7). These simulations were carried on a *DEC AlphaServer* 2100 4/275 OSF/1 monoprocessor, and the CPU times per iteration in time for the two algorithms are listed on the following table (in units of seconds (s) or minutes (min)):





FIG. 4. Moment of order 4 for Coulombian case.

Sublattices method

Sublattices method

Multigrid method



FIG. 5. Températures Tx, Ty, and T for Coulombian case.

Sublattice sizes	$16 \times 16 \times 16$		$32 \times 32 \times 32$	
	2,3	3,4	5,6	7,8
Sublattices	3 s	1.3 s	30 s	14 s
Multigrids	0.4 s		8 s	
Quadratic schemes	53 s		60 min	

## 6. CONCLUSIONS

We have implemented two methods to decrease the computational time required for the evaluation of the discrete FPL operator 2.7. The first one is a sublattices method,

#### Sublattices method

#### Multigrid method







**FIG. 7.** Coulombian case: Relaxations and Equilibrium states using one and two sublattice sizes. The numerical equilibrium state obtained by using two sublattices sizes coincides with the realistic (the Maxwellian) final distribution.

while the second one is a multigrid method with random evaluations. We have noticed that both algorithms are conservative and decrease the kinetic entropy. Their computational cost is highly reduced, compared with the original quadratic scheme (divided by a factor of order 40 for a  $16 \times 16 \times 16$  grid and by a factor of order 200 for a 32  $\times$  32  $\times$  32 grid). The sublattices algorithm does not give satisfactory results when the sublattice sizes are too big (for instance, 9, 10 for a grid  $32 \times 32 \times 32$ ), since the number of collisional invariants to be suppressed is large. The numerical tests show that the multigrid algorithm is a little bit more accurate than the sublattice scheme and the CPU times are better. On the other hand, the sublattices method (which is deterministic) provides smoother results in some circumstances. To remove these oscillations, a deterministic version of the multigrid method is proposed in a forthcoming paper [7]. This alternative approach mainly consists on replacing the Monte Carlo integrations by multipole expansions in the spirit of the work by Greengard and Rokhlin [19] and allows us to control the error by the simple choice of the order of these multipole expansions.

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