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# Positive, conservative, equilibrium state preserving and implicit difference schemes for the isotropic Fokker-Planck-Landau equation

Christophe Buet <sup>\*</sup>      Kim-Claire Le Thanh <sup>†</sup>

## Abstract

The aim of this paper is to describe the discretization of the Fokker-Planck-Landau (FPL) collision term in the isotropic case, which models the self-collision for the electrons when they are totally isotropized by heavy particles background such as ions. The discussion focuses on schemes, which could preserve positivity, mass, energy and Maxwellian equilibrium on non uniform grid. The Chang and Cooper method is widely used by plasma's physicists for the FPL equation (and for Fokker-Planck type equations). We present a new variant that is both positive and conservative contrary to the existing one's. In the category of others difference schemes we propose a simple scheme on non-uniform grid, which is both positive, conservative and equilibrium state preserving in opposition to what exists. The case of Coulombian potential is emphasized. We address also the problem of the time discretization. In particular we show how to recast some implicit methods to get band diagonal system and to solve it by direct method with a linear cost. Numerical tests are performed.

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## 1 Introduction

The Fokker-Planck-Landau equation (FPLE) is commonly used in plasma physics when studying kinetic effects between charged particles under Coulomb interaction.

In particular, the isotropic Fokker-Planck-Landau operator is generally used in the modeling of inertial controlled fusion. More precisely, it is used to describe the electronic energy transport phenomena in laser produced plasma. In some conditions, it is well known that the fluid theory, for which the hydrodynamic equations are closed using the law for the thermal fluxes proposed by Spitzer-Harm [25] is not valid [15]. A more accurate solution is to use a model based on the expansion of the FPL operator in spherical harmonics [26] and to retain the two first terms (P1 model), and the isotropic FPL operator is the leading order term [15, 17]. Within this inertial controlled fusion context P1 model is sufficient to describe physical phenomena and 3-D FPL equation unnecessarily complicates the issue.

The most popular difference scheme for Fokker-Planck type equations is the Chang and Cooper method [6]. This method was originally devoted to linear Fokker-Planck equations and it was shown in [6] that in this case this method is positive and preserves the equilibrium states. On the contrary a paper of Larsen *et al.* [19] shows that this method applied for non-linear Fokker-Planck equations could produce non-positive solutions. It is also used for the isotropic Landau equation by Langdon [18], in the SPARK code by Epperlein [15] and by Kingham and Bell [17] in the code IMPACT. At our knowledge, in this non-linear case, there is no rigorous proof of the positivity and the energy conservation.

There exists also conservative or entropic schemes for this equation [1, 2, 3, 4, 10, 22, 23] based on the symmetrized weak form or on the "Log" weak symmetric form of the Landau equation. Unfortunately on non-uniform grid in energy these methods suffer from some limitations. Some of them could not be positive [3, 10], some others [1, 2, 22, 23] are not equilibrium state preserving. And the one's using Logarithm of the distribution function [3, 10] do not handle correctly highly peaked distribution functions.

Spectral methods were also developed by Pareschi *et al.* [21] and Filbet *et al.* [16] for the 3-D FPL equation and could be applied to the isotropic FPL equation. But these schemes approximate energy only with spectral accuracy, that means they are not conservative. Moreover discrete Maxwellians are not preserved and positivity is not ensured. Another disadvantage is that such method is not suitable to describe peaked functions.

It would be interesting to enlighten the situation about positive, conservative and equilibrium states preserving velocity difference schemes for the isotropic Landau equation. Conservation property is important. Especially conservation of the energy to avoid inopportune cooling or heating of the plasma. Preservation of equilibrium states, Maxwellian in this case, is important since it is the long time behavior for coupling with fluid limit or to have the right heat flux at equilibrium. But positivity is also important since it is true at the continuous level and for obvious physical reasons. Thus it would be in time discretization to ensure stability. It is quite surprising that this point is not analyzed in papers devoted to algorithms for the FPL equation [1, 2, 10, 15, 20, 22, 23].

In the first part of this paper we focus our attention on the Chang and Cooper method. Contrary to the existing works, we start from the weak symmetrized form of the isotropic Landau operator, so that the conservation of energy is obvious. We construct two variants of the Chang and Cooper method, a new one, called  $\mathcal{S}_1$ , and an other one, called  $\mathcal{S}_2$ , that is described by Langdon *et al.* [8, 18] in the Coulombian case but constructed directly from the Rosenbluth form of the operator. These two schemes only differ in the boundary condition. These two variants conserve the energy but we show that the second one,  $\mathcal{S}_2$ , is not positive. As we will also see, due to bad boundary conditions, the Chang and Cooper version used by Epperlein [15] or by Kingham and Bell [17], although positive, is not conservative in energy. In other hand we show that the Chang and Cooper method is not the only way to obtain positive, conservative and equilibrium preserving states even on non-uniform meshes. We propose a new scheme that shares the same properties with the Chang and Cooper method. This "equilibrium scheme", called  $\mathcal{S}_3$ , is based on the work of Larsen *et al.* [19] for Fokker-Planck equations. In the case of uniform meshes this scheme is nothing but the conservative positive and entropy scheme developed by Berezin *et al.* [1] and studied in detail by one of the authors [3, 4].

Time discretization is also a crucial point in the numerical simulation of the Fokker-Planck-Landau equation. Implicit schemes are attractive: they make the code robust and able to use large time steps well exceeding the characteristic collision time. The explicit method cannot be eliminate, since for practical computations, the number of discretization points will lie between 20 and 150 approximately. Despite its parabolic time step restriction, it could be cheaper for coarse grids. We study several implicit schemes. We begin with the well known fixed point method, described in particular in [15], that is conservative in mass and positive. However, this scheme is not conservative in energy. Then, we recall the contracted implicit method developed by Lemou and Mieussens [20]. Their scheme is conservative in mass and energy, the positivity is lacking but it is cheap. The last method studied is the Newton method. The mass and energy conservation is ensured. For the "contracted implicit" method and the Newton method, we show that by rewriting the problem, in the particular case of coulombian potentials, the linear systems involved can be solved by direct method in only  $\mathcal{O}(N)$  operations ( $N$  is the number of unknowns). This strategy can be applied to Maxwellian potential for the isotropic FPL equation but also for the 3-D equation. The key point, for the Coulombian potentials, is to remember that drift and diffusion coefficients satisfy Poisson equation, which can be solved efficiently at a linear cost by direct method (see also [7]). In fact, such a strategy works as soon as the discrete operator can be evaluated using recurrences relations, and then at a linear cost. We show, on numerical examples, the gain in these implicit methods compared to the explicit time discretization in terms of CPU times.

This paper is organized as follow: in the first part, we recall the continuous FPL equation

in the homogeneous and isotropic case and its properties. In a second part we present the Chang and Cooper type schemes and an equilibrium scheme. We show all the properties of these schemes: energy and equilibrium states conservation, positivity. We also indicate the simplifications occurring in the case of a uniform mesh, or in the Coulombian case. The third part is devoted to the time discretization: explicit and implicit schemes. In the fourth part we present some numerical tests in the Coulombian case.

## 2 The isotropic Fokker-Planck-Landau equation

Let us recall the homogeneous non-linear Fokker-Planck-Landau equation (FPL equation) in the isotropic case where the distribution function  $f(\vec{x}, \vec{v}, t)$  depends only on the modulus of the velocity  $v = \|\vec{v}\|$  and on the time  $t$ , in other words  $f(\vec{x}, \vec{v}, t) = f(v, t)$ . We consider  $f$  as a function of  $\varepsilon = v^2$  where  $\varepsilon$  is the energy variable. In this case, Fokker-Planck-Landau equation can be written:

$$\frac{\partial f(\varepsilon, t)}{\partial t} = Q(f)(\varepsilon) = \frac{1}{\sqrt{\varepsilon}} \frac{\partial}{\partial \varepsilon} \int_0^\infty g(\varepsilon, \varepsilon') \left( f(\varepsilon') \frac{\partial f(\varepsilon)}{\partial \varepsilon} - f(\varepsilon) \frac{\partial f(\varepsilon')}{\partial \varepsilon'} \right) d\varepsilon', \quad (2.1)$$

where  $g(\varepsilon, \varepsilon')$  is positive, symmetric and increasing ( $g(\varepsilon, \varepsilon') = \min(\varepsilon^{\frac{3}{2}}, \varepsilon'^{\frac{3}{2}})$  for Coulombian interactions and  $g(\varepsilon, \varepsilon') = \varepsilon^{\frac{3}{2}} \varepsilon'^{\frac{3}{2}}$  for Maxwellian interactions) and  $Q(f)$  is the so-called FPL collision operator. This operator can be written in the following weak form (let  $\phi(\varepsilon)$  be any test function)

$$\int_0^\infty \frac{\partial f(\varepsilon, t)}{\partial t} \phi(\varepsilon) \sqrt{\varepsilon} d\varepsilon = -\frac{1}{2} \int_0^\infty \int_0^\infty \left( \frac{\partial \phi(\varepsilon)}{\partial \varepsilon} - \frac{\partial \phi(\varepsilon')}{\partial \varepsilon'} \right) g(\varepsilon, \varepsilon') (f(\varepsilon') \frac{\partial f(\varepsilon)}{\partial \varepsilon} - f(\varepsilon) \frac{\partial f(\varepsilon')}{\partial \varepsilon'}) d\varepsilon' d\varepsilon. \quad (2.2)$$

Note that the right hand side of (2.2) can be equivalently written in the so-called "Log" weak form

$$-\frac{1}{2} \int_0^\infty \int_0^\infty \left( \frac{\partial \phi(\varepsilon)}{\partial \varepsilon} - \frac{\partial \phi(\varepsilon')}{\partial \varepsilon'} \right) g(\varepsilon, \varepsilon') f(\varepsilon') f(\varepsilon) \left( \frac{\partial \log f(\varepsilon)}{\partial \varepsilon} - \frac{\partial \log f(\varepsilon')}{\partial \varepsilon'} \right) d\varepsilon' d\varepsilon, \quad (2.3)$$

or in (2.1), the collision operator can be written in the following diffusive form

$$Q(f)(\varepsilon) = \frac{1}{\sqrt{\varepsilon}} \frac{\partial}{\partial \varepsilon} (E(f)f(\varepsilon) + D(f) \frac{\partial f}{\partial \varepsilon}), \quad (2.4)$$

where the drift coefficient  $E$  and the diffusion coefficient  $D$  are given by

$$D(f) = \int_0^\infty g(\varepsilon, \varepsilon') f(\varepsilon') d\varepsilon' \text{ and } E(f) = - \int_0^\infty g(\varepsilon, \varepsilon') \frac{\partial f(\varepsilon')}{\partial \varepsilon'} d\varepsilon'. \quad (2.5)$$

### 2.1 General properties

Let us recall the most important properties of the problem (2.1).

This operator satisfies the conservation of mass (respectively energy) by choosing  $\phi(\varepsilon) = 1$  (respectively  $\phi(\varepsilon) = \varepsilon$ ) in (2.2)

$$\rho = \int_0^\infty f(\varepsilon, t) \sqrt{\varepsilon} d\varepsilon \text{ and } \rho \mathbf{E} = \int_0^\infty f(\varepsilon, t) \varepsilon^{\frac{3}{2}} d\varepsilon. \quad (2.6)$$

Note that the conservation properties are a consequence of the symmetry property (between  $\varepsilon$  and  $\varepsilon'$ ) of the collision operator. Let us also mention that the temperature  $\mathbf{T}$  of the plasma is defined as  $\frac{3}{2}\rho\mathbf{T} = \rho\mathbf{E}$ .

Any function of the type  $\psi(\varepsilon) = \alpha \exp(-\beta\varepsilon)$  where  $\alpha$  and  $\beta$  are arbitrary constants ( $\beta > 0$ ) is a stationary solution of equation (2.1). And we have the famous H-Theorem: for any solution  $f$  the entropy defined by

$$H(f) = \int_0^\infty f(\varepsilon) \log(f(\varepsilon)) \sqrt{\varepsilon} d\varepsilon, \quad (2.7)$$

satisfies

$$\frac{dH(f)}{dt} \leq 0 \quad \text{with} \quad \frac{dH(f)}{dt} = 0 \iff f(\varepsilon) = \alpha \exp(-\beta\varepsilon), \quad (2.8)$$

with  $\alpha$  and  $\beta$  such that  $f$  and  $M = \alpha \exp(-\beta\varepsilon)$  have the same mass and density.

For more details concerning the Landau equation we refer to [9, 12, 13, 14].

## 2.2 Coulombian interactions

In the Coulombian case,  $g(\varepsilon, \varepsilon') = \min(\varepsilon^{\frac{3}{2}}, \varepsilon'^{\frac{3}{2}})$  thus the drift and diffusion coefficients  $E(f)$  and  $D(f)$  are given by

$$E(f) = \frac{3}{2} \int_0^\varepsilon \sqrt{\varepsilon'} f(\varepsilon') d\varepsilon' \quad \text{and} \quad D(f) = \frac{3}{2} \int_0^\varepsilon \sqrt{\varepsilon'} \left( \int_{\varepsilon'}^\infty f(\varepsilon'') d\varepsilon'' \right) d\varepsilon'. \quad (2.9)$$

Deriving once  $E(f)$  and twice  $D(f)$  we have

$$f(\varepsilon) = \frac{2}{3} \frac{1}{\sqrt{\varepsilon}} \frac{\partial E(f)}{\partial \varepsilon} = -\frac{2}{3} \frac{\partial}{\partial \varepsilon} \frac{1}{\sqrt{\varepsilon}} \frac{\partial D(f)}{\partial \varepsilon}. \quad (2.10)$$

These relations are nothing else than the Poisson equations satisfy by the Rosenbluth potentials.

## 3 Semi-discretized problems

In this section we focus on the discretization in the energy variable. For numerical simulations, we reduce the integration domain in FPL equation to a bounded domain in the variable  $\varepsilon$  where  $\varepsilon \in [0, \mathcal{E}]$ . Thus we consider the approximate problem of (2.2) defined by

$$\int_0^\mathcal{E} \frac{\partial f(\varepsilon, t)}{\partial t} \phi(\varepsilon) \sqrt{\varepsilon} d\varepsilon = -\frac{1}{2} \int_0^\mathcal{E} \int_0^\mathcal{E} \left( \frac{\partial \phi(\varepsilon)}{\partial \varepsilon} - \frac{\partial \phi(\varepsilon')}{\partial \varepsilon'} \right) g(\varepsilon, \varepsilon') (f(\varepsilon') \frac{\partial f(\varepsilon)}{\partial \varepsilon} - f(\varepsilon) \frac{\partial f(\varepsilon')}{\partial \varepsilon'}) d\varepsilon' d\varepsilon. \quad (3.1)$$

Let us introduce  $\{\varepsilon_i\}_{1 \leq i \leq N}$  an increasing sequence such that  $\varepsilon_1 = 0$ ,  $\varepsilon_N = \mathcal{E}$  and  $\Delta\varepsilon_{i+\frac{1}{2}} = \varepsilon_{i+1} - \varepsilon_i$ .

We suppose that  $\{\Delta\varepsilon_{i+\frac{1}{2}}\}_{1 \leq i \leq N-1}$  is constant or increasing sequence. By convention we set  $\varepsilon_{\frac{1}{2}} = 0$ . Any function  $f(\varepsilon, t)$  is approximated on the grid by values  $\{f_i\}_{1 \leq i \leq N}$  supposed be approximations of  $\{f(\varepsilon_i)\}_{1 \leq i \leq N}$ . We also introduce the notations  $(\Delta\phi)_{i+\frac{1}{2}} = \phi_{i+1} - \phi_i$  and

$$(\mathbb{D}\phi)_{i+\frac{1}{2}} = \frac{(\Delta\phi)_{i+\frac{1}{2}}}{(\Delta\varepsilon)_{i+\frac{1}{2}}} \quad \text{as an approximation of the partial derivative } \partial_\varepsilon \phi(\varepsilon_{i+\frac{1}{2}}).$$

First, we consider the discretization of the expression  $\int_0^\mathcal{E} \frac{\partial f}{\partial t} \phi(\varepsilon) \sqrt{\varepsilon} d\varepsilon$  for any function  $\phi$ . By using the standard quadrature formula with respect to the measure  $\sqrt{\varepsilon} d\varepsilon$ , we approximate it by

$$\int_0^\mathcal{E} \frac{\partial f}{\partial t} \phi \sqrt{\varepsilon} d\varepsilon \simeq \sum_{i=1}^N (\phi_i \frac{df_i}{dt} \int_{\varepsilon_{i-\frac{1}{2}}}^{\varepsilon_{i+\frac{1}{2}}} \sqrt{\varepsilon} d\varepsilon) \stackrel{\text{def}}{=} \sum_{i=1}^N c_i \phi_i \frac{df_i}{dt}. \quad (3.2)$$

Thus the weights  $c_i$  are defined by  $c_1 = \frac{2}{3} \varepsilon_{\frac{3}{2}}$ ,  $c_i = \frac{2}{3} (\varepsilon_{i+\frac{1}{2}}^{\frac{3}{2}} - \varepsilon_{i-\frac{1}{2}}^{\frac{3}{2}})$  for  $i = 2, \dots, N$ .

Below, we present various strategies to construct schemes that have properties of conservation and if possible positivity and entropy decaying. These schemes differ intrinsically in the way we discretize the right-hand side of (3.1):

$$(r.h.s.) = -\frac{1}{2} \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} \left( \int_{\varepsilon_i}^{\varepsilon_{i+1}} \int_{\varepsilon_j}^{\varepsilon_{j+1}} \left( \frac{\partial \phi(\varepsilon)}{\partial \varepsilon} - \frac{\partial \phi(\varepsilon')}{\partial \varepsilon'} \right) g(\varepsilon, \varepsilon') (f(\varepsilon') \frac{\partial f(\varepsilon)}{\partial \varepsilon} - f(\varepsilon) \frac{\partial f(\varepsilon')}{\partial \varepsilon'}) d\varepsilon d\varepsilon' \right). \quad (3.3)$$

We must also introduce the Maxwellian associated to a distribution function  $f$ . For a distribution function  $f$  we define  $\bar{\rho}$  and  $\bar{\rho \mathbf{E}}$  the discretized analogous of the density and the energy (2.6) as  $\bar{\rho} = \sum_{i=1}^N c_i f_i$  and  $\bar{\rho \mathbf{E}} = \sum_{i=1}^N \varepsilon_i c_i f_i$ . The temperature is still defined by  $\frac{3}{2} \bar{\rho} \bar{\mathbf{T}} = \bar{\rho \mathbf{E}}$ . For a distribution function  $f$ , we denote by  $M = \alpha \exp(-\beta \varepsilon)$  the Maxwellian which has the same mass and energy as  $f$ .

It's easy to check that  $\tilde{T} = \frac{\sum_{i=1}^N \varepsilon_i c_i M_i}{\sum_{i=1}^N c_i M_i} = \frac{\sum_{i=1}^N \varepsilon_i c_i \exp(-\beta \varepsilon_i)}{\sum_{i=1}^N c_i \exp(-\beta \varepsilon_i)}$ , is a strictly monotone (decreasing) function of  $\beta$  with  $\lim_{\beta \rightarrow 0} \tilde{T} = T_{\max} = \frac{\sum_{i=1}^N \varepsilon_i c_i}{\sum_{i=1}^N c_i}$  and  $\lim_{\beta \rightarrow +\infty} \tilde{T} = T_{\min} = 0$ . Thus for any distribution function  $f$  such that  $0 \leq \bar{\mathbf{T}} \leq T_{\max}$  there is a unique  $\beta \geq 0$  such that  $\tilde{T} = \bar{\mathbf{T}}$  and consequently  $M$  is unique. Note that  $\beta \simeq \frac{1}{\bar{\mathbf{T}}}$ . For the rest of this work we consider only distribution functions such that  $0 \leq \bar{\mathbf{T}} \leq T_{\max}$ , that is, we exclude distribution function for which  $M$  is an increasing function of  $\varepsilon$  ( $\beta \leq 0$ ) (that means we exclude distribution function such that  $T_{\max} \leq \bar{\mathbf{T}} \leq \frac{2}{3} \mathcal{E}$ ).

To check the positivity of the schemes we need the following well-known result:

**Lemma 1.** *Consider the Cauchy problem for the ordinary differential equation*

$$\frac{df}{dt} = Lf \quad \text{and} \quad f(t=0) = f^0,$$

with  $f = \{f_i\}_{1 \leq i \leq N}$  and with the square matrix  $L = L(f, t)$  such that  $L_{ij} \geq 0$  for  $i \neq j$ ,  $L_{ii} \leq 0$ .

If there exists a constant  $C$  such that  $\forall i, j |L_{ij}(f, t)| \leq C$ , and if the initial data is non-negative i.e.  $f^0 \geq 0$ , then as long as the solution exists it is non-negative.

### 3.1 Chang and Cooper type schemes

One of the most popular method used for Fokker-Planck equations is due to Chang and Cooper [6]. Originally this method was proposed for the linear Fokker-Planck equation and

the construction is entirely devoted to the preservation of equilibrium states. The authors also show that in the linear case (and only in this case) the method provides non-negative solutions. At contrary others authors, see [19], have shown that for the non-linear Fokker-Planck equation this method can produce non-positive solutions. Let us recall the spirit of the Chang and Cooper method on the simple Fokker-Planck equation,

$$\frac{\partial f}{\partial t} = \frac{\partial F}{\partial v} = \frac{\partial}{\partial v}(vf + \sigma \frac{\partial f}{\partial v}) = \sigma \frac{\partial}{\partial v}(M \frac{\partial}{\partial v}(\frac{f}{M})),$$

where  $v \in \mathbb{R}$  and the equilibrium state  $M$  is a Maxwellian:  $M = M(v) = \exp(-|v|^2/2\sigma)$ . On a uniform grid of velocity space step  $\Delta v$  and  $v_i = i\Delta v$ , the Chang and Cooper method consists in discretizing the diffusion as usual and the drift in such a way that for  $f = M$  the fluxes  $F$  are all equal to zero. One takes at cell interface  $v_{i+\frac{1}{2}} = (i + \frac{1}{2})\Delta v$

$$F_{i+\frac{1}{2}} = \frac{\sigma}{\Delta v}(f_{i+1} - f_i) + v_{i+\frac{1}{2}} \left( (1 - \delta_{i+\frac{1}{2}})f_{i+1} + \delta_{i+\frac{1}{2}}f_i \right),$$

and forcing the fluxes to be zero for equilibrium leads to  $\delta_{i+\frac{1}{2}} = \frac{\sigma}{v_{i+\frac{1}{2}}\Delta v} - \left( \exp\left(\frac{v_{i+\frac{1}{2}}\Delta v}{\sigma}\right) - 1 \right)^{-1}$ .

The scheme writes as  $\frac{df_i}{dt} = \frac{1}{\Delta v}(F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}})$ .

This method is also one of the most used for FPL equation. And this is a non-linear problem. None of the main work in this area [15, 17, 18] contains the proof of the positivity of the Chang and Cooper method or the proof of the energy conservation. Moreover it is not clear that equilibrium states are preserved by this method for the FPL equation since, in this case, the coefficients of Chang and Cooper [6] are defined in an implicit manner for the FPL equation. In this section we propose a variant of this method which intrinsically contains the conservation of the energy, preserves discrete Maxwellian and is positive. We recall also the variants developed by Langdon *et al.* [8, 18] which is non positive and the one's developed by Epperlein in [15] and used by other people (see [17] for example) which is in fact non conservative in energy. For these two variants the problem comes from the boundary condition used at one end of the domain of computation  $\varepsilon = \mathcal{E}$ .

### 3.1.1 A new variant: scheme $\mathcal{S}_1$

Using for each integrals of (3.3) a midpoint quadrature formula, we approximate it by

$$(r.h.s.) = -\frac{1}{2} \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} ((\mathbb{D}\phi)_{i+\frac{1}{2}} - (\mathbb{D}\phi)_{j+\frac{1}{2}}) g_{i+\frac{1}{2}, j+\frac{1}{2}} (f_{j+\frac{1}{2}}(\mathbb{D}f)_{i+\frac{1}{2}} - f_{i+\frac{1}{2}}(\mathbb{D}f)_{j+\frac{1}{2}}) \Delta\varepsilon_{i+\frac{1}{2}} \Delta\varepsilon_{j+\frac{1}{2}}, \quad (3.4)$$

with  $g_{i+\frac{1}{2}, j+\frac{1}{2}} = g(\varepsilon_{i+\frac{1}{2}}, \varepsilon_{j+\frac{1}{2}})$ . Hence, the weak formulation of the semi-discretized model reads

$$\sum_{i=1}^N c_i \frac{\partial f_i}{\partial t} \phi_i = - \sum_{i=1}^{N-1} (\mathbb{D}\phi)_{i+\frac{1}{2}} \Delta\varepsilon_{i+\frac{1}{2}} \sum_{j=1}^{N-1} g_{i+\frac{1}{2}, j+\frac{1}{2}} (f_{j+\frac{1}{2}}(\mathbb{D}f)_{i+\frac{1}{2}} - f_{i+\frac{1}{2}}(\mathbb{D}f)_{j+\frac{1}{2}}) \Delta\varepsilon_{j+\frac{1}{2}}. \quad (3.5)$$

To simplify we note  $K_{i+\frac{1}{2}} = \sum_{j=1}^{N-1} g_{i+\frac{1}{2}, j+\frac{1}{2}} (f_{j+\frac{1}{2}}(\mathbb{D}f)_{i+\frac{1}{2}} - f_{i+\frac{1}{2}}(\mathbb{D}f)_{j+\frac{1}{2}}) \Delta\varepsilon_{j+\frac{1}{2}}$  the numerical flux. By identifying the terms involving  $\phi_i$  in (3.5), we obtain the system of ordinary



differential equation

$$\frac{df_i}{dt} = Q_i^{S_1} \quad 1 \leq i \leq N, \quad (3.6)$$

with  $Q_1^{S_1} = K_{\frac{3}{2}}/c_1$ ,  $Q_i^{S_1} = (K_{i+\frac{1}{2}} - K_{i-\frac{1}{2}})/c_i$  for  $2 \leq i \leq N-1$  and  $Q_N^{S_1} = -K_{N-\frac{1}{2}}/c_N$ . We can rewrite the numerical flux

$$K_{i+\frac{1}{2}} = E_{i+\frac{1}{2}} f_{i+\frac{1}{2}} + D_{i+\frac{1}{2}} \frac{f_{i+1} - f_i}{\Delta \varepsilon_{i+\frac{1}{2}}} \quad 1 \leq i \leq N-1, \quad (3.7)$$

and the drift and diffusion coefficients are given by

$$E_{i+\frac{1}{2}} = - \sum_{j=1}^{N-1} g_{i+\frac{1}{2}, j+\frac{1}{2}} (\mathbb{D}f)_{j+\frac{1}{2}} \Delta \varepsilon_{j+\frac{1}{2}} \quad \text{and} \quad D_{i+\frac{1}{2}} = \sum_{j=1}^{N-1} g_{i+\frac{1}{2}, j+\frac{1}{2}} f_{j+\frac{1}{2}} \Delta \varepsilon_{j+\frac{1}{2}}. \quad (3.8)$$

By integrating by parts the drift term reads

$$E_{i+\frac{1}{2}} = \sum_{j=1}^{N-1} (g_{i+\frac{1}{2}, j+\frac{1}{2}} - g_{i+\frac{1}{2}, j-\frac{1}{2}}) f_j - g_{i+\frac{1}{2}, N-\frac{1}{2}} f_N. \quad (3.9)$$

**Remark 1.** We assume that  $\{g_{i+\frac{1}{2}, j+\frac{1}{2}}\}_{1 \leq i \leq N, 1 \leq j \leq N}$  is an increasing sequence. Then, even if the  $f_i$ 's are positive,  $E_{i+\frac{1}{2}}$  can be negative if  $f_N \neq 0$ . In other hand, since the  $f_{i+\frac{1}{2}}$ 's are positive,  $D_{i+\frac{1}{2}}$  remains positive.

We turn now to the discretization of  $f_{i+\frac{1}{2}}$ . We suppose that  $f_{i+\frac{1}{2}}$  is an approximation of  $f(\varepsilon_{i+\frac{1}{2}})$  given by the following definition [6]

**Definition 1.** The Chang and Cooper average  $f_{i+\frac{1}{2}}$  of quantities  $f_i$  and  $f_{i+1}$  is defined by

$$f_{i+\frac{1}{2}} = \delta_{i+\frac{1}{2}} f_i + (1 - \delta_{i+\frac{1}{2}}) f_{i+1} \quad 1 \leq i \leq N-1, \quad (3.10)$$

with

$$\delta_{i+\frac{1}{2}} = \frac{1}{\alpha_{i+\frac{1}{2}}} - \frac{1}{\exp(\alpha_{i+\frac{1}{2}}) - 1} \quad 1 \leq i \leq N-1, \quad (3.11)$$

and  $\alpha_{i+\frac{1}{2}} = \frac{E_{i+\frac{1}{2}}}{D_{i+\frac{1}{2}}} \Delta \varepsilon_{i+\frac{1}{2}}$ .

To be comfortable we denote  $h(\alpha) = \frac{1}{\alpha} - \frac{1}{\exp(\alpha) - 1}$  (thus  $\delta_{i+\frac{1}{2}} = h(\alpha_{i+\frac{1}{2}})$ ). This smooth function is decreasing and bounded such that  $h(-\infty) = 1$ ,  $h(0) = 1/2$  and  $h(+\infty) = 0$ . Moreover, his derivative is negative and bounded too ( $h'(\pm\infty) = 0$ ). Note that whatever the value of  $\alpha_{i+\frac{1}{2}}$  (positive or negative) if  $\delta_{i+\frac{1}{2}}$  exists we get  $0 \leq \delta_{i+\frac{1}{2}} \leq 1$ . Therefore, since the  $f_i$ 's are positive the  $f_{i+\frac{1}{2}}$ 's remain positive. Now we clarify the expression of  $\delta_{i+\frac{1}{2}}$ . We recall that  $f$  is the N-dimensional column vector with components  $\{f_i\}_{1 \leq i \leq N}$ . Thus, assuming that  $\delta$  is the (N-1)-dimensional column vector with components  $\{\delta_{i+\frac{1}{2}}\}_{1 \leq i \leq N-1}$ , we can write  $\delta_{i+\frac{1}{2}}$  as a function of  $f$  and introducing  $\mathcal{H} = \{\mathcal{H}_{i+\frac{1}{2}} = h(\alpha_{i+\frac{1}{2}})\}_{1 \leq i \leq N-1}$ , the system to be solved for  $\delta$  is

$$\delta(f) = \mathcal{H}(\delta(f), f), \quad (3.12)$$

where  $f$  is a distribution function that has density  $\bar{\rho}$  and energy  $\overline{\rho\mathbf{E}}$  and  $\mathcal{H}$  is a (N-1)-dimensional vector valued function. Using a Newton's method requires  $\mathcal{O}(N^3)$  operations. But we will see that for Coulombian potentials this cost can be reduced to  $\mathcal{O}(N)$  operations (see also [7]). Note that this is also true for Maxwellian potentials [5].

**Proposition 1.** *The flux  $K_{i+\frac{1}{2}}$  satisfies the following relation*

$$K_{i+\frac{1}{2}} = A_{i+\frac{1}{2}}f_{i+1} - B_{i+\frac{1}{2}}f_i \quad 1 \leq i \leq N-1, \quad (3.13)$$

where

$$A_{i+\frac{1}{2}} = v(\alpha_{i+\frac{1}{2}}) \frac{D_{i+\frac{1}{2}}}{\Delta\varepsilon_{i+\frac{1}{2}}}, \quad \text{and} \quad B_{i+\frac{1}{2}} = u(\alpha_{i+\frac{1}{2}}) \frac{D_{i+\frac{1}{2}}}{\Delta\varepsilon_{i+\frac{1}{2}}}, \quad (3.14)$$

and with  $u(x) = \frac{x}{\exp(x) - 1}$  and  $v(x) = \frac{x \exp(x)}{\exp(x) - 1}$ .

*Proof.* The proof is the same as in Chang and Cooper's paper [6] but in the non-linear case. By substituting the Chang and Cooper average  $f_{i+\frac{1}{2}}$  in the right-hand side of the relation (3.7) we get

$$K_{i+\frac{1}{2}} = E_{i+\frac{1}{2}}((1 - \delta_{i+\frac{1}{2}})f_{i+1} + \delta_{i+\frac{1}{2}}f_i) + D_{i+\frac{1}{2}} \frac{f_{i+1} - f_i}{\Delta\varepsilon_{i+\frac{1}{2}}} \quad 1 \leq i \leq N-1.$$

As  $\alpha_{i+\frac{1}{2}} = \frac{E_{i+\frac{1}{2}}}{D_{i+\frac{1}{2}}} \Delta\varepsilon_{i+\frac{1}{2}}$ , we can write  $E_{i+\frac{1}{2}} = \frac{\alpha_{i+\frac{1}{2}} D_{i+\frac{1}{2}}}{\Delta\varepsilon_{i+\frac{1}{2}}}$ . Thus, if we develop  $\delta_{i+\frac{1}{2}}$  we have

$$K_{i+\frac{1}{2}} = \frac{\alpha_{i+\frac{1}{2}} \exp(\alpha_{i+\frac{1}{2}})}{\exp(\alpha_{i+\frac{1}{2}}) - 1} \frac{D_{i+\frac{1}{2}}}{\Delta\varepsilon_{i+\frac{1}{2}}} f_{i+1} - \frac{\alpha_{i+\frac{1}{2}}}{\exp(\alpha_{i+\frac{1}{2}}) - 1} \frac{D_{i+\frac{1}{2}}}{\Delta\varepsilon_{i+\frac{1}{2}}} f_i.$$

And now, we can write  $K_{i+\frac{1}{2}} = A_{i+\frac{1}{2}}f_{i+1} - B_{i+\frac{1}{2}}f_i$ . □

### 3.1.2 Properties

We summarize the conservation properties of the scheme  $\mathcal{S}_1$  in the following proposition:

**Proposition 2.** *The scheme  $\mathcal{S}_1$  conserves the mass and the energy and has the Maxwellians  $M = \exp(-\beta\varepsilon)$  as equilibrium states.*

*Proof.* Mass and energy conservation properties come from (3.4) by taking  $\phi = 1, \varepsilon$ . Let us now check the second point which is not so clear as for linear Fokker-Planck equations. First we have  $M_{i+1} - M_i = -M_{i+1}(\exp(-\beta\Delta\varepsilon_{i+\frac{1}{2}}) - 1)$ . Assuming that  $M_{i+\frac{1}{2}}$  is computed by Chang and Cooper average formula (3.10) with

$$\delta_{i+\frac{1}{2}} = \frac{1}{\beta\Delta\varepsilon_{i+\frac{1}{2}}} - \frac{1}{\exp(\beta\Delta\varepsilon_{i+\frac{1}{2}}) - 1} \quad 1 \leq i \leq N-1, \quad (3.15)$$

we get

$$M_{i+\frac{1}{2}} = \left( \frac{1}{\beta\Delta\varepsilon_{i+\frac{1}{2}}} - \frac{1}{\exp(-\beta\Delta\varepsilon_{i+\frac{1}{2}}) - 1} \right) (M_i - M_{i+1}) + M_{i+1}.$$

Therefore

$$M_{i+\frac{1}{2}} = \left( \frac{1}{\beta \Delta \varepsilon_{i+\frac{1}{2}}} + \frac{M_{i+1}}{M_{i+1} - M_i} \right) (M_i - M_{i+1}) + M_{i+1} = -\frac{M_{i+1} - M_i}{\beta \Delta \varepsilon_{i+\frac{1}{2}}}. \quad (3.16)$$

Thanks to (3.16) the drift term reads for a Maxwellian

$$E_{i+\frac{1}{2}} = -\sum_{j=1}^{N-1} g_{i+\frac{1}{2}, j+\frac{1}{2}} (M_{j+1} - M_j) = \sum_{j=1}^{N-1} g_{i+\frac{1}{2}, j+\frac{1}{2}} M_{j+\frac{1}{2}} \beta \Delta \varepsilon_{j+\frac{1}{2}} = \beta D_{i+\frac{1}{2}}.$$

Thus the coefficients  $\delta_{i+\frac{1}{2}}$  defined by (3.15) are solution of the equation (3.12) when  $f = M$ . Furthermore, in that case the fluxes  $K_{i+\frac{1}{2}}$  vanish. So Maxwellians are equilibrium states of the scheme  $\mathcal{S}_1$ .  $\square$

Now we analyse the positivity of the scheme. For linear Fokker-Planck equations, Chang and Cooper [6] have shown that their scheme is non-negative. Afterwards, Larsen *et al.* [19] have pointed out that for non-linear Fokker-Planck equations, but with local drift and diffusion coefficients, the Chang and Cooper method can produce negative solution. Our case is a non-linear Fokker-Planck equation with non-local drift and diffusion coefficients. For this case we can show that the Chang and Cooper scheme  $\mathcal{S}_1$  is positive.

**Proposition 3.** *The solutions of (3.6) with non-negative initial conditions  $f_i(t = 0)$  are non-negative.*

We don't have existence result for (3.6). The problem is that we have very few information about the solutions of (3.12): existence can be obtain by Brouwer's fixed point theorem but we have nothing about uniqueness and regularity of the solutions as functions of  $f$ .

*Proof.* From the Proposition (1) we get  $K_{i+\frac{1}{2}} = A_{i+\frac{1}{2}} f_{i+1} - B_{i+\frac{1}{2}} f_i$  where  $A_{i+\frac{1}{2}}$  and  $B_{i+\frac{1}{2}}$  are given by (3.14). The function  $u(x) = \frac{x}{\exp(x) - 1}$  is positive, decreasing from  $-\infty$  to 0,

while  $v(x) = \frac{x \exp(x)}{\exp(x) - 1}$  is positive too, increasing from 0 to  $+\infty$ . To prove the positivity

we use Lemma 1. Thus all we need to do is showing that the  $A_{i+\frac{1}{2}}$ 's and  $B_{i+\frac{1}{2}}$ 's are positive and bounded. As a result (see Remark 1) we have  $D_{i+\frac{1}{2}} \geq 0$ . Moreover  $u$  and  $v$  are positive functions therefore  $A_{i+\frac{1}{2}}$  and  $B_{i+\frac{1}{2}}$  are positive too. Now we have to show that  $A_{i+\frac{1}{2}}$  and  $B_{i+\frac{1}{2}}$  are bounded. At first we assume that  $f$  is a distribution function that has density  $\bar{\rho}$  and energy  $\bar{\rho E}$  thus we get  $f_j \leq \frac{\bar{\rho}}{\max_i c_i}, \forall j; 1 \leq j \leq N - 1$ . So that we can bound the drift term as following

$$|E_{i+\frac{1}{2}}| = \left| \sum_{j=1}^{N-1} g_{i+\frac{1}{2}, j+\frac{1}{2}} (f_j - f_{j+1}) \right| \leq \frac{\bar{\rho}}{\max_i c_i} 2 \sum_{j=1}^{N-1} g_{i+\frac{1}{2}, j+\frac{1}{2}} \leq \frac{\bar{\rho}}{\max_i c_i} 2(N-1) g_{N-\frac{1}{2}, N-\frac{1}{2}}.$$

Consequently, there exists  $C > 0$  such that  $|E_{i+\frac{1}{2}}| < C$ . In the same way we get an upperbound for the diffusion coefficients

$$D_{i+\frac{1}{2}} \leq \frac{\bar{\rho}}{\max_i c_i} 2 \sum_{j=1}^{N-1} g_{i+\frac{1}{2}, j+\frac{1}{2}} \Delta \varepsilon_{j+\frac{1}{2}}.$$

To continue we distinguish two cases. First we suppose that  $|\alpha_{i+\frac{1}{2}}| \geq 1$ . Then we get

$$A_{i+\frac{1}{2}} = \frac{\exp(\alpha_{i+\frac{1}{2}})}{\exp(\alpha_{i+\frac{1}{2}}) - 1} E_{i+\frac{1}{2}} \quad \text{and} \quad B_{i+\frac{1}{2}} = \frac{1}{\exp(\alpha_{i+\frac{1}{2}}) - 1} E_{i+\frac{1}{2}}.$$

And even if  $|\alpha_{i+\frac{1}{2}}| \rightarrow \infty$ ,  $A_{i+\frac{1}{2}}$  and  $B_{i+\frac{1}{2}}$  remain bounded. Now we assume that  $|\alpha_{i+\frac{1}{2}}| \leq 1$  then  $u(\alpha_{i+\frac{1}{2}})$  and  $v(\alpha_{i+\frac{1}{2}})$  are bounded and  $A_{i+\frac{1}{2}}$  and  $B_{i+\frac{1}{2}}$  too since  $D_{i+\frac{1}{2}}$  is also bounded. Thus, thanks to Lemma 1 this ends the proof.  $\square$

It is easy to check that the above results about positivity, energy conservation and equilibrium states for  $\mathcal{S}_1$  don't depend on the definition of the coefficients  $c_i$ , see (3.2), or on our choice for the value of  $\varepsilon_1$ . If one takes the Chang and Cooper coefficients  $\delta_{i+\frac{1}{2}}$  at equilibrium, that is given by (3.15), or freeze the value given by the initial data, it is easy to see that if it is done in the expression of the fluxes given by (3.7) the scheme is still positive but no more conservative in energy and if it is done in (3.13) this is the converse. The algebra that permits to pass from the form (3.7) to the form (3.13) is valid if and only if the coefficients verify at all times the relation (3.12). This remark is still valid if one does not calculate exactly the Chang and Cooper coefficients by an iterative method.

We don't have any H-theorem but as we will see on numerical examples, the entropy is quite decaying with this scheme.

### 3.1.3 The case of physical interest: Coulombian potential

We write now the Rosenbluth coefficients in the case of Coulombian potentials

( $k_{i+\frac{1}{2},j+\frac{1}{2}} = \min(\varepsilon_{i+\frac{1}{2}}^{\frac{3}{2}}, \varepsilon_{j+\frac{1}{2}}^{\frac{3}{2}})$ ). To simplify we denote  $\Delta\varepsilon_i^{\frac{3}{2}} = \varepsilon_{i+\frac{1}{2}}^{\frac{3}{2}} - \varepsilon_{i-\frac{1}{2}}^{\frac{3}{2}}$ . From (3.8) the drift term reads

$$E_{i+\frac{1}{2}} = \sum_{j=1}^i \Delta\varepsilon_j^{\frac{3}{2}} f_j - f_N \varepsilon_{i+\frac{1}{2}}^{\frac{3}{2}} \quad 1 \leq i \leq N-1, \quad (3.17)$$

and for the diffusive term we have

$$D_{i+\frac{1}{2}} = \sum_{j=1}^i \Delta\varepsilon_{j+\frac{1}{2}} f_{j+\frac{1}{2}} \varepsilon_{j+\frac{1}{2}}^{\frac{3}{2}} + \varepsilon_{i+\frac{1}{2}}^{\frac{3}{2}} \sum_{j=i+1}^{N-1} \Delta\varepsilon_{j+\frac{1}{2}} f_{j+\frac{1}{2}} \quad 1 \leq i \leq N-1. \quad (3.18)$$

As  $D_{i+\frac{1}{2}}$  depends on the  $f$  midpoint values it is clear that (3.10) is non-linear in the  $f_{i+\frac{1}{2}}$ 's. We therefore have to solve a full matrix that arises from the implicit differencing of the  $f_{i+\frac{1}{2}}$ 's. A way to compute the Chang and Cooper average (3.10) is to consider the second equation of (2.9). Thus we have to solve an elliptic equation, namely  $-\frac{2}{3} \frac{\partial}{\partial \varepsilon} \frac{1}{\sqrt{\varepsilon}} \frac{\partial}{\partial \varepsilon} (D(f(\varepsilon))) = f(\varepsilon)$ .

The non-linear system which solution is  $f^\delta = \{f_{i+\frac{1}{2}}\}_{1 \leq i \leq N-1}$  is then replaced by a non-linear system in  $D(f)$  and the matrix involved is tri-diagonal (see [5, 7]). We can use a new expression for  $f_{i+\frac{1}{2}}$

$$f_{i+\frac{1}{2}} = -\frac{1}{\Delta\varepsilon_{i+\frac{1}{2}}} \left( \frac{D_{i+\frac{3}{2}} - D_{i+\frac{1}{2}}}{\Delta\varepsilon_{i+1}^{\frac{3}{2}}} - \frac{D_{i+\frac{1}{2}} - D_{i-\frac{1}{2}}}{\Delta\varepsilon_i^{\frac{3}{2}}} \right), \quad (3.19)$$

which can be solved, for a given distribution function by a Newton's method, with the cost of a tridiagonal system that is  $\mathcal{O}(N)$  operations at each iteration.

### 3.1.4 About other existing variants of the Chang and Cooper method for the isotropic FPL equation

We want to emphasize that the two known other Chang and Cooper method for the isotropic FPL equation are not conservative and positive at the same time. As we will see the first one conserves the energy but is not positive. The second one does not conserve the energy but is positive.

The first one, we call it the scheme  $\mathcal{S}_2$ , reduces to the Langdon's scheme in the case of a Coulombian potential. Another option consists in integrating the right-hand side of (3.5) up to  $\varepsilon_{N+1}$ , assuming that  $f_{N+1} = 0$  and constraining the flux at the last point  $\varepsilon_{N+\frac{1}{2}}$  to be identically equal to zero. This strategy was carried by Langdon [18] and Decoster and Langdon [8] in the case of Coulombian interactions. We extend their method to the general case. The derivation begins as for the  $\mathcal{S}_1$  scheme using the weak formulation (3.4) but with  $N + 1$  points. We denote by  $\tilde{E}_{i+\frac{1}{2}}, \tilde{D}_{i+\frac{1}{2}}, \tilde{K}_{i+\frac{1}{2}}, i = 1, \dots, N$  the drift coefficients, the diffusion coefficients and the fluxes using respectively (3.8) and (3.7) with  $N + 1$  points.

Imposing  $\frac{df_{N+1}}{dt} = \tilde{K}_{N+\frac{1}{2}} = 0$  with  $f_{N+1} = 0$  leads to

$$\tilde{E}_{N+\frac{1}{2}} f_{N+\frac{1}{2}} - \tilde{D}_{N+\frac{1}{2}} \frac{f_N}{\Delta\varepsilon_{N+\frac{1}{2}}} = 0. \quad (3.20)$$

Thanks to (3.20) the diffusion becomes

$$\tilde{D}_{i+\frac{1}{2}} = \sum_{j=1}^{N-1} g_{i+\frac{1}{2}, j+\frac{1}{2}} f_{j+\frac{1}{2}} \Delta\varepsilon_{j+\frac{1}{2}} + g_{i+\frac{1}{2}, N+\frac{1}{2}} \frac{\tilde{D}_{N+\frac{1}{2}}}{\tilde{E}_{N+\frac{1}{2}}} f_N. \quad (3.21)$$

We integrate by parts the drift term and get

$$\tilde{E}_{i+\frac{1}{2}} = \sum_{j=1}^N (g_{i+\frac{1}{2}, j+\frac{1}{2}} - g_{i+\frac{1}{2}, j-\frac{1}{2}}) f_j \Delta\varepsilon_{j+\frac{1}{2}}. \quad (3.22)$$

We assume that  $\{g_{i+\frac{1}{2}, j+\frac{1}{2}}\}_{1 \leq i \leq N, 1 \leq j \leq N}$  is an increasing sequence. Then, if the  $f_i$ 's are positive,  $\tilde{E}_{i+\frac{1}{2}}$  is positive too. In other hand, even if the  $f_{i+\frac{1}{2}}$ 's are positive  $\tilde{D}_{i+\frac{1}{2}}$  can be negative if  $f_N \neq 0$ .

The discretization of  $f_{i+\frac{1}{2}}$  is still given by the Chang and Cooper average (3.10) and (3.11)

with  $\tilde{\alpha}_{i+\frac{1}{2}} = \frac{\tilde{E}_{i+\frac{1}{2}}}{\tilde{D}_{i+\frac{1}{2}}} \Delta\varepsilon_{i+\frac{1}{2}}$ . As in the previous scheme, the  $(N-1)$ -dimensional vector  $\tilde{\delta}$  with

components  $\{\tilde{\delta}_{i+\frac{1}{2}}\}_{1 \leq i \leq N}$  is the root of a non-linear equation like (3.12). By construction this scheme conserves the energy and discrete Maxwellians (see [5] for more details).

Comparing formally the drift and diffusion functional discretized respectively by  $\mathcal{S}_1$  and  $\mathcal{S}_2$  we get for  $1 \leq i \leq N - 1$

$$\tilde{E}_{i+\frac{1}{2}} = E_{i+\frac{1}{2}} + f_N g_{i+\frac{1}{2}, N+\frac{1}{2}} \quad \text{and} \quad \tilde{D}_{i+\frac{1}{2}} = D_{i+\frac{1}{2}} + g_{i+\frac{1}{2}, N+\frac{1}{2}} \frac{\tilde{D}_{N+\frac{1}{2}}}{\tilde{E}_{N+\frac{1}{2}}} f_N. \quad (3.23)$$

In the case of the Coulombian potential one can check (see [5]) that leads to the relation

$$\frac{\tilde{D}_{N+\frac{1}{2}}}{\tilde{E}_{N+\frac{1}{2}}} = \frac{\tilde{D}_{N-\frac{1}{2}}}{\tilde{E}_{N-\frac{1}{2}}} \text{ and thus}$$

$$E_{i+\frac{1}{2}} = \tilde{E}_{i+\frac{1}{2}} - f_N \varepsilon_{i+\frac{1}{2}}^{\frac{3}{2}} \quad D_{i+\frac{1}{2}} = \tilde{D}_{i+\frac{1}{2}} - \frac{\tilde{D}_{N-\frac{1}{2}}}{\tilde{E}_{N-\frac{1}{2}}} \varepsilon_{i+\frac{1}{2}}^{\frac{3}{2}}. \quad (3.24)$$

This is the Langdon version of the Chang and Cooper method for the FPL equation derived originally only for Coulombian potential and using the Rosenbluth form of the equation. But using (3.24) one can see that  $\tilde{D}_{N-\frac{1}{2}}$  could become negative. To see that this scheme is not positive it suffices to consider the following initial data: let  $f$  a distribution function with fixed density  $\bar{\rho}$  and energy  $\bar{\rho}\bar{\mathbf{E}}$  and of the form  $f = a\delta_{\varepsilon_1} + b\delta_{\varepsilon_N}$ . Thus  $b = \bar{\rho}\bar{\mathbf{E}}/(c_N\varepsilon_N)$  and  $a = (\bar{\rho} - \bar{\rho}\bar{\mathbf{E}}/\varepsilon_N)/c_1$  and  $a$  and  $b$  are positive. With such an initial condition and for sufficiently fine grids it's easy to verify that  $\frac{df_{N-1}}{dt} < 0$  and consequently  $f_{N-1}$  gets negative too.

The second well known implementation of the Chang and Cooper method is the one proposed by Epperlein for Coulombian collisions [15] and used in the code SPARK or by Kingham and Bell in the recent code IMPACT [17]. These authors assume that the diffusion term and the distribution function vanish at  $\varepsilon_{N+\frac{1}{2}}$  and that the distribution function vanishes at  $\varepsilon_{N+1}$ . Thus the numerical flux is zero and consequently the density is conserved. But the Epperlein velocity discretization is nothing else than a miscellany of what we called scheme  $\mathcal{S}_1$  and scheme  $\mathcal{S}_2$ : the drift term is the one discretized by scheme  $\mathcal{S}_2$ , formula (3.22), and the diffusion term the one computed by  $\mathcal{S}_1$ , formula (3.18). So the discrete operator has no weak symmetrized form. Thus one can have a doubt concerning the energy conservation since the energy conservation's proof is based on the existence of a weak symmetrized form of the collision operator. Numerical tests confirm this fact. The proof of positivity of this scheme is like those of the  $\mathcal{S}_1$  scheme since the diffusion term is non-negative.

For more details the reader can refer to [5]. We can remark that these three Chang and Cooper type schemes are equivalent when the integrating domain is not bounded. The only difference between these schemes lies in the manner to treat boundary conditions when the integrating domain is reduced to  $[0, \mathcal{E}]$ .

### 3.2 Equilibrium scheme (scheme $\mathcal{S}_3$ )

The Chang and Cooper method is not the only way to provide positive, conservative and equilibrium states preserving schemes for the FPL equation on non-uniform grid. The scheme we'll propose in this section share also these properties and is simpler and thus cheaper.

This scheme is based on the work of Larsen *et al.* [19]. Their work is for linear and non-linear Fokker-Planck equations. But they do not consider non-linearity as in the Landau equation, that is drift and diffusion coefficients are functionals of the distribution functions. One of the two main ideas exposed in their paper to preserve Maxwellian states is to remark that  $\varepsilon$ -derivative that appears in the flux can be rewritten as  $\frac{\partial}{\partial \varepsilon} = -\beta y \frac{\partial}{\partial y}$  where  $y = \exp(-\beta\varepsilon)$ . Thus it becomes easy to preserve Maxwellians in the weak form of the Fokker-Planck equation.

Following these authors, in the case of the FPL equation, we set

$$\overline{\Delta\varepsilon}_{i+\frac{1}{2}} = -\frac{(\Delta M)_{i+\frac{1}{2}}}{\beta M_{i+1}} = \frac{\exp(\beta\Delta\varepsilon_{i+\frac{1}{2}}) - 1}{\beta} \simeq \Delta\varepsilon_{i+\frac{1}{2}}. \quad (3.25)$$

Thus we consider the following approximation of the weak symmetrized form of the problem

$$\sum_{i=1}^N c_i \frac{\partial f_i}{\partial t} \phi_i = -\frac{1}{2} \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} \left( \frac{\Delta\phi_{i+\frac{1}{2}}}{\Delta\varepsilon_{i+\frac{1}{2}}} - \frac{\Delta\phi_{j+\frac{1}{2}}}{\Delta\varepsilon_{j+\frac{1}{2}}} \right) g_{i+\frac{1}{2},j+\frac{1}{2}} \left( f_{j+\frac{1}{2}} \frac{\Delta f_{i+\frac{1}{2}}}{\Delta\varepsilon_{i+\frac{1}{2}}} - f_{i+\frac{1}{2}} \frac{\Delta f_{j+\frac{1}{2}}}{\Delta\varepsilon_{j+\frac{1}{2}}} \right) \overline{\Delta\varepsilon}_{j+\frac{1}{2}} \overline{\Delta\varepsilon}_{i+\frac{1}{2}}, \quad (3.26)$$

with the approximations  $f_{i+\frac{1}{2}}$  taken decentred and defined by  $f_{i+\frac{1}{2}} = f_{i+1}$ .

As in the previous section we obtain the system of ordinary equation for the approximation of the FPL equation

$$\frac{df_i}{dt} = Q_i^{\mathcal{S}_3} \quad 1 \leq i \leq N, \quad (3.27)$$

where  $Q_1^{\mathcal{S}_3} = K_{\frac{3}{2}}/c_1$ ,  $Q_i^{\mathcal{S}_3} = (K_{i+\frac{1}{2}} - K_{i-\frac{1}{2}})/c_i$  for  $2 \leq i \leq N-1$  and  $Q_N^{\mathcal{S}_3} = -K_{N-\frac{1}{2}}/c_N$  with the numerical flux

$$K_{i+\frac{1}{2}} = \frac{\overline{\Delta\varepsilon}_{i+\frac{1}{2}}}{\Delta\varepsilon_{i+\frac{1}{2}}} \sum_{j=1}^{N-1} g_{i+\frac{1}{2},j+\frac{1}{2}} \left( f_{j+1} \frac{\Delta f_{i+\frac{1}{2}}}{\Delta\varepsilon_{i+\frac{1}{2}}} - f_{i+1} \frac{\Delta f_{j+\frac{1}{2}}}{\Delta\varepsilon_{j+\frac{1}{2}}} \right) \overline{\Delta\varepsilon}_{j+\frac{1}{2}} \quad 1 \leq i \leq N-1.$$

By factorizing the terms  $f_i$  and  $f_{i+1}$  in the last sum, the numerical flux reads

$$K_{i+\frac{1}{2}} = A_{i+\frac{1}{2}} f_{i+1} - B_{i+\frac{1}{2}} f_i, \quad (3.28)$$

with

$$\begin{cases} A_{i+\frac{1}{2}} = \frac{\overline{\Delta\varepsilon}_{i+\frac{1}{2}}}{\Delta\varepsilon_{i+\frac{1}{2}}} \left( \frac{1}{\overline{\Delta\varepsilon}_{i+\frac{1}{2}}} \sum_{j=1}^{N-1} g_{i+\frac{1}{2},j+\frac{1}{2}} f_{j+1} \overline{\Delta\varepsilon}_{j+\frac{1}{2}} + \sum_{j=1}^{N-1} (g_{i+\frac{1}{2},j+\frac{1}{2}} - g_{i+\frac{1}{2},j-\frac{1}{2}}) f_j - f_N g_{i+\frac{1}{2},N-\frac{1}{2}} \right), \\ B_{i+\frac{1}{2}} = \frac{1}{\Delta\varepsilon_{i+\frac{1}{2}}} \sum_{j=1}^{N-1} g_{i+\frac{1}{2},j+\frac{1}{2}} f_{j+1} \overline{\Delta\varepsilon}_{j+\frac{1}{2}}. \end{cases} \quad (3.29)$$

The fluxes can be also written using drift and diffusion coefficients

$$K_{i+\frac{1}{2}} = \overline{E}_{i+\frac{1}{2}} f_{i+1} + \overline{D}_{i+\frac{1}{2}} \frac{f_{i+1} - f_i}{\Delta\varepsilon_{i+\frac{1}{2}}}, \quad (3.30)$$

where the drift coefficients  $\frac{\Delta\varepsilon_{i+\frac{1}{2}}}{\Delta\varepsilon_{i+\frac{1}{2}}} \overline{E}_{i+\frac{1}{2}}$  are defined by (3.9) and the diffusion coefficients  $\overline{D}_{i+\frac{1}{2}}$

are defined by (3.8) with  $f_{i+\frac{1}{2}} = f_{i+1}$  and  $\overline{\Delta\varepsilon}_{i+\frac{1}{2}}$  in place of  $\Delta\varepsilon_{i+\frac{1}{2}}$ .

We can summarize the properties of this scheme in the following proposition

**Proposition 4.** *If  $g_{i+\frac{1}{2},j+\frac{1}{2}}$  is an increasing sequence and  $\Delta\varepsilon_{i+\frac{1}{2}} \leq \Delta\varepsilon_{N-\frac{1}{2}}$  the scheme  $\mathcal{S}_3$  is conservative in mass and energy. Moreover it is positive and preserves the equilibrium state when is reached.*

*Proof.* Mass and energy conservation are easily checked by setting  $\phi = 1$  and  $\phi = \varepsilon$  in the weak symmetrized form of the discrete FPL equation (3.26).

Using the definition (3.25) of  $\overline{\Delta\varepsilon}_{i+\frac{1}{2}}$  and the definition of the  $f_{i+\frac{1}{2}}$ 's it's easy to see that for  $f = M$  we have

$$f_{j+\frac{1}{2}} \frac{\Delta f_{i+\frac{1}{2}}}{\overline{\Delta\varepsilon}_{i+\frac{1}{2}}} - f_{i+\frac{1}{2}} \frac{\Delta f_{j+\frac{1}{2}}}{\overline{\Delta\varepsilon}_{j+\frac{1}{2}}} = -\beta(M_{j+1}M_{i+1} - M_{i+1}M_{j+1}) = 0$$

thus the scheme preserves the Maxwellians states.

Let us now check the positivity. The fluxes are given by (3.28) and (3.29). Now, to use Lemma 1 we have just to check that  $A_{i+\frac{1}{2}}$  and  $B_{i+\frac{1}{2}}$  are positive and bounded. As  $g_{i+\frac{1}{2},j+\frac{1}{2}}$  is positive,  $B_{i+\frac{1}{2}}$  is obviously positive. We can write

$$\begin{aligned} A_{i+\frac{1}{2}} &= \frac{\overline{\Delta\varepsilon}_{i+\frac{1}{2}}}{\Delta\varepsilon_{i+\frac{1}{2}}} \left( \frac{1}{\overline{\Delta\varepsilon}_{i+\frac{1}{2}}} \sum_{j=1}^{N-2} g_{i+\frac{1}{2},j+\frac{1}{2}} \widetilde{f}_{j+1} \overline{\Delta\varepsilon}_{j+\frac{1}{2}} + \sum_{j=1}^{N-1} (g_{i+\frac{1}{2},j+\frac{1}{2}} - g_{i+\frac{1}{2},j-\frac{1}{2}}) f_j \right. \\ &\quad \left. + f_N g_{i+\frac{1}{2},N-\frac{1}{2}} \left( \frac{\overline{\Delta\varepsilon}_{N-\frac{1}{2}}}{\overline{\Delta\varepsilon}_{i+\frac{1}{2}}} - 1 \right) \right). \end{aligned}$$

Assuming that  $g_{i+\frac{1}{2},j+\frac{1}{2}}$  is an increasing sequence and that  $\Delta\varepsilon_{i+\frac{1}{2}} \leq \Delta\varepsilon_{N-\frac{1}{2}}$  leads to the positivity of  $A_{i+\frac{1}{2}}$ . Now,  $\overline{\Delta\varepsilon}_{i+\frac{1}{2}}/\Delta\varepsilon_{i+\frac{1}{2}} \in [0, 1]$  therefore  $A_{i+\frac{1}{2}}$ ,  $B_{i+\frac{1}{2}}$  are bounded since, due to mass conservation, we have  $f_i \leq \frac{\overline{\rho}}{\min_j c_j}$ . According to Lemma (1),  $f_i$  cannot vanish in finite time. That completes the proof.  $\square$

One could replace the exact equilibrium  $M_i$  in the definition of the scheme by an approximate equilibrium state  $\widetilde{M}_i$  with same mass and energy and the resulting scheme is still conservative, positive but the equilibrium state is now  $\widetilde{M}_i$ . This could be useful since this scheme requires the knowledge of the equilibrium state and normally this can be done only by solving a non-linear equation with an iterative method.

If we stand  $f_{i+\frac{1}{2}} = f_i$  instead of  $f_{i+\frac{1}{2}} = f_{i+1}$  in the numerical flux and if we take  $\overline{\Delta\varepsilon}_{i+\frac{1}{2}} = \frac{(\Delta M)_{i+\frac{1}{2}}}{\beta M_i}$ , the Maxwellians are also preserved but we can show that  $\mathcal{S}_3$  is positive if and only if the energy grid is uniform.

On a uniform grid all the terms  $\overline{\Delta\varepsilon}_{i+\frac{1}{2}}$  are equal and up to a multiplicative constant the flux reduces to

$$K_{i+\frac{1}{2}} = \sum_{j=1}^{N-1} g_{i+\frac{1}{2},j+\frac{1}{2}} (f_{i+1} f_j - f_i f_{j+1}).$$

The scheme is then nothing else than the scheme provided by Berezin and Pekker [1] which is also an entropic scheme as shown in [4].

For Maxwellian ( $g(\varepsilon, \varepsilon') = \varepsilon^{\frac{3}{2}} \varepsilon'^{\frac{3}{2}}$ ) or Coulombian ( $g(\varepsilon, \varepsilon') = \min(\varepsilon^{\frac{3}{2}}, \varepsilon'^{\frac{3}{2}})$ ) potentials the evaluation of all the coefficients  $A_{i+\frac{1}{2}}$  and  $B_{i+\frac{1}{2}}$  can be achieved in only  $\mathcal{O}(N)$  operations as explained in [3, 4].

When applied to Coulombian potentials it can be easily checked that the  $\overline{D}_{i+\frac{1}{2}}$  satisfies a relation of the type (3.19).



The second idea of Larsen *et al.* in [19] to preserve equilibrium states in the discretization of Fokker-Planck equations and which could be applied to the isotropic FPL equation is to write  $\frac{\partial f}{\partial \varepsilon} = M \frac{\partial}{\partial \varepsilon} \left( \frac{f}{M} \right) - \beta f$  in the weak formulation (2.2). Proceeding as above leads to a scheme which is indeed conservative in mass and energy and preserves the Maxwellians. But at this time, we cannot show the positivity. Nevertheless it could be possible to derive a positive scheme since there are sufficiently degrees of freedom in the discretization, namely the factor  $f_{i+\frac{1}{2}}$  and  $M_{i+\frac{1}{2}}$ .

## 4 Time discretizations

Time discretization is also a key point in the numerical simulation of the FPL equation. As we have seen above,  $\mathcal{S}_1$  and  $\mathcal{S}_3$  can be evaluate in  $\mathcal{O}(N)$  operations in the Coulombian case (this is true for all known schemes dealing with the FPL equation for Coulombian potential). Thus the only problem could arise with the time discretization. For ICF applications the scheme must be able to take into account time steps in the range from  $.01\tau$  to  $10\tau$ , where  $\tau = \sqrt{\frac{\pi}{3}} \frac{1}{\rho} \left( \frac{\rho \mathbf{E}}{\rho} \right)^{\frac{3}{2}}$  is the collision time. Moreover the number of discretization points  $N$  will be between 20 and 150. Despite the parabolic stability condition inherent to such an equation it is not clear that implicit time discretization could be cheaper than explicit time discretization. Thus we explore all the ways. Contrary to "Log" schemes for the isotropic FPL equation, [3, 11], we can exhibit a good stability condition (positivity) for explicit schemes. It will be possible to measure the gain obtained using implicit discretization for example. We recall the more natural way to obtain an implicit solution, the fixed point method using an M-matrix. One must converge to ensure energy conservation but at each iteration one has to invert a tridiagonal band matrix which is very cheaper. We examine also two other methods, the classical and widely used Newton's method and the "contracted implicit" method (non-iterative method) developed by Lemou and Mieussens [20]. For these two methods we show that by recasting them properly gives band diagonal system which can be solved by direct method like LU in  $\mathcal{O}(N)$  operations. The key point to achieve that is to remember that drift and diffusion coefficients satisfy (2.10) in continuous and it is anything else only to remember that for 3-D FPL equation Rosenbluth potentials satisfy Poisson equation. After that the game is to minimize the size of the band to have the minimum lower cost as possible.

### 4.1 Explicit time discretization

Let us introduce explicit scheme in time such as the well known Euler forward scheme

$$f^{n+1} - f^n = \Delta t Q(f^n), \quad (4.1)$$

where  $\Delta t$  is the time step,  $f^n$  is the approximation of  $f(\varepsilon, t^n)$  and  $t^{n+1} = t^n + \Delta t$  and  $Q$  is the discrete operator defined by (3.6) for  $\mathcal{S}_1$  or by (3.27) for  $\mathcal{S}_3$ . We exhibit a condition such that the scheme remains positive. For the schemes  $\mathcal{S}_1$  and  $\mathcal{S}_3$  we get from relation (3.13) and (3.28)

$$f_i^{n+1} = f_i^n (1 - \Delta t P_i^n) + \Delta t G_i^n,$$

where  $P_i^n = \frac{1}{c_i} (A_{i-\frac{1}{2}}^n + B_{i+\frac{1}{2}}^n)$  and  $G_i^n = \frac{1}{c_i} (A_{i+\frac{1}{2}}^n f_{i+1}^n + B_{i-\frac{1}{2}}^n f_{i-1}^n)$ . Above we saw, for  $\mathcal{S}_1$  and  $\mathcal{S}_3$ , that if  $f_i \geq 0$  for all  $i \in [1, N]$  then  $A_{i+\frac{1}{2}}$  and  $B_{i+\frac{1}{2}}$  are non-negative and bounded for

all  $i$ . Consequently  $G_i^n$  and  $P_i^n$  are positive and bounded too. Now, if  $\Delta t \leq \max_i (P_i^n)^{-1}$  then  $f_i^{n+1}$  is positive. For a given time step we define the  $CFL$  number as  $CFL = \Delta t \max_i P_i^n$ . Such time stability condition can't be obtained using "Log" schemes, that is, schemes based on the "Log" form of the equation (see [3]). As proved in [4], our time restriction could be bounded below by using mass, energy and the  $L^\infty$  norm of the distribution function, but from a practical point of view it is unnecessary.

## 4.2 Implicit time discretization

The implicit scheme consists in solving

$$f^{n+1} - f^n = \Delta t Q(f^{n+1}), \quad (4.2)$$

where  $f^n$  is supposed being the approximation of  $f(\varepsilon, t^n)$ .

### 4.2.1 A positive fixed point method

The first discretization uses a Picard fixed point method based on a semi-implicit algorithm, namely

$$\frac{f_i^k - f_i^n}{\Delta t} = \frac{1}{c_i} \left( A_{i+\frac{1}{2}}^{k-1} f_{i+1}^k - (A_{i-\frac{1}{2}}^{k-1} + B_{i+\frac{1}{2}}^{k-1}) f_i^k + B_{i-\frac{1}{2}}^{k-1} f_{i-1}^k \right),$$

which can be written in the compact form

$$f^k - f^n = \Delta t L(f^{k-1}) f^k, \quad (4.3)$$

where  $f^k$  is the  $k^{th}$  iterate and the coefficients  $A_{i+\frac{1}{2}}$  and  $B_{i+\frac{1}{2}}$  are defined by (3.14) for  $\mathcal{S}_3$  and (3.29) for  $\mathcal{S}_1$ . At convergence we naturally obtain  $f^{n+1} = f^k$ . As we have seen above  $L(f^k)$  is an L-matrix for  $\mathcal{S}_1$  and  $\mathcal{S}_3$ , his transpose is diagonally dominant, and the kernel is the space of vectors whose all components are equal. Thus  $(Id - \Delta t L(f^k))$  is an M-matrix and the iterative procedure (4.3) preserves mass and positivity. Due to the tridiagonal form of  $(Id - \Delta t L(f^k))$ , it only requires  $\mathcal{O}(N)$  operations to compute  $f^k$  (in fact the cost is the same as the explicit method). We show on numerical examples that this fixed point method converges rather well.

### 4.2.2 The "contracted implicit" method

This scheme was developed by Lemou and Mieussens [20]. By noticing that conservation and entropy properties are a consequence of the symmetry property of the collision operator, the authors make implicit in time the diffusive term  $(f(\varepsilon') \partial_\varepsilon f(\varepsilon))$  in (2.1) without breaking the symmetry between  $\varepsilon$  and  $\varepsilon'$ . They get the following contracted implicit scheme

$$f^{n+1} - f^n = \Delta t q^{ci}(f^n, f^{n+1}), \quad (4.4)$$

with  $q^{ci}(f, g) = \frac{1}{\sqrt{\varepsilon}} \frac{\partial}{\partial \varepsilon} \int_0^\infty k(\varepsilon, \varepsilon') \left( f(\varepsilon') \frac{\partial g(\varepsilon)}{\partial \varepsilon} - f(\varepsilon) \frac{\partial g(\varepsilon')}{\partial \varepsilon'} \right) d\varepsilon'$ . This scheme conserves mass, energy, see [20], and discrete Maxwellians but it can produce negative solution. In our case this time discretization writes as

$$f_i^{n+1} - f_i^n = \frac{\Delta t}{c_i} \left( E_{i+\frac{1}{2}}^{n+1} f_{i+\frac{1}{2}}^n + D_{i+\frac{1}{2}}^n \frac{f_{i+1}^{n+1} - f_i^{n+1}}{\Delta \varepsilon_{i+\frac{1}{2}}} - E_{i-\frac{1}{2}}^{n+1} f_{i-\frac{1}{2}}^n - D_{i-\frac{1}{2}}^n \frac{f_i^{n+1} - f_{i-1}^{n+1}}{\Delta \varepsilon_{i-\frac{1}{2}}} \right), \quad (4.5)$$

for  $\mathcal{S}_1$  and for  $\mathcal{S}_3$  we just have to replace  $f_{i+\frac{1}{2}}^n$  by  $f_{i+1}^n \frac{\overline{\Delta\varepsilon}_{i+\frac{1}{2}}}{\Delta\varepsilon_{i+\frac{1}{2}}}$  (see (3.25)) and  $D_{i+\frac{1}{2}}^n$  by  $\overline{D}_{i+\frac{1}{2}}^n$ .

For the sake of simplicity we write them in the compact form  $(Id - \Delta t L^{ci}(f^n))f^{n+1} = f^n$ . Using the definition of the drift coefficients  $E_{i+\frac{1}{2}}$  it is obvious that  $Id - \Delta t L^{ci}(f^n)$  is a non-sparse matrix, the drift term fills the matrix with his coefficients and we get a  $N \times N$  matrix. The procedure to solve (4.4) by a direct method requires  $\mathcal{O}(N^3)$  operations (note that  $L^{ci}$  is nearly a lower triangular matrix, thus the cost can be reduced to  $\mathcal{O}(N^2)$  operations). To bring the matrix sparse (and in fact band diagonal with the last column if the unknowns are stored correctly) the idea is to introduce the drift coefficient  $E$  as unknown associated with the equation (2.10). Namely we rewrite the "contracted implicit" scheme as

$$\begin{cases} f^{n+1} - f^n - \Delta t \tilde{q}^{ci}((f^n, E^n), (f^{n+1}, E^{n+1})) = f^{n+1} - f^n - \Delta t q^{ci}(f^n, f^{n+1}) = 0, \\ f^{n+1} - R(E^{n+1}) = 0. \end{cases} \quad (4.6)$$

where  $R(E^{n+1}) = \frac{2}{3} \frac{1}{\sqrt{\varepsilon}} \frac{\partial E^{n+1}}{\partial \varepsilon}$ . If one discretizes in energy by the Chang and Cooper type scheme we get from (3.17)

$$\begin{cases} f_i^{n+1} - f_i^n - \frac{\Delta t}{c_i} (E_{i+\frac{1}{2}}^{n+1} f_{i+\frac{1}{2}}^n + D_{i+\frac{1}{2}}^n \frac{f_{i+1}^{n+1} - f_i^{n+1}}{\Delta\varepsilon_{i+\frac{1}{2}}} - E_{i-\frac{1}{2}}^{n+1} f_{i-\frac{1}{2}}^n - D_{i-\frac{1}{2}}^n \frac{f_i^{n+1} - f_{i-1}^{n+1}}{\Delta\varepsilon_{i-\frac{1}{2}}}) = 0, \\ f_i^{n+1} - f_N^{n+1} - \frac{E_{i+\frac{1}{2}}^{n+1} - E_{i-\frac{1}{2}}^{n+1}}{\Delta\varepsilon_i^{\frac{3}{2}}} = 0. \end{cases} \quad (4.7)$$

To solve (4.7) the number of arithmetic operations required is  $\frac{N-1}{2}$  operations (subtractions) to eliminate the last column and  $m^2 \times (2N-1)$  operations to solve one  $m$ -diagonal system by  $LU$  factorization (here  $m=5$ ). We can also substitute the function distribution  $f_i^{n+1}$  in the first equation of (4.7) by his expression in the drift term given by the second equation. Thus the operator is a  $N \times N$  sparse matrix and the number of operations required to solve the scheme reduces to  $\mathcal{O}(N)$  and the number of diagonal is now  $m=5$  (as done by Decoster for the Newton's method [7]). Therefore we gain a factor 2 in terms of CPU time. For the equilibrium scheme  $\mathcal{S}_3$  we just have to replace  $f_{i+\frac{1}{2}}^n$  by  $f_{i+1}^n \frac{\overline{\Delta\varepsilon}_{i+\frac{1}{2}}}{\Delta\varepsilon_{i+\frac{1}{2}}}$  (see (3.25)) and  $D_{i+\frac{1}{2}}^n$  by

$$\overline{D}_{i+\frac{1}{2}}^n.$$

It is obvious that the scheme (4.7) is still conservative in mass and energy. This type of procedure can be easily extended to all variants of the "Log" scheme. It is also straightforward to generalize it to Maxwellian potential since in this case we have recurrences relation to evaluate drift and diffusion coefficients. It is also interesting to notice that the "contracted implicit" method applied to  $\mathcal{S}_1$ ,  $\mathcal{S}_3$  or the "Log" scheme depicted by Dellacherie in [11] gives exactly the same system to solve for uniform grid. The only differences is in the manner to compute the diffusion coefficients from the distribution function. Obviously, at equilibrium, the diffusion coefficients are the same.

### 4.2.3 The Newton's method

The last method uses a Newton algorithm to solve equation (4.2).

Introducing  $F(f) = f - f^n - \Delta t Q(f)$  the resulting iteration procedure is

$$F'(f^{k-1}) \cdot (f^k - f^{k-1}) = -F(f^{k-1}), \quad (4.8)$$

where  $F'(f^{k-1})$  is the Jacobian and we choose the starting point  $f^0$  with the same mass and energy as  $f^n$ . Introducing the linearized operator  $Q^l$  around  $f$  we have

$$Q^l(f, g) = \frac{1}{\sqrt{\varepsilon}} \frac{\partial}{\partial \varepsilon} \int_0^\infty k(\varepsilon, \varepsilon') \left( f(\varepsilon') \frac{\partial g(\varepsilon)}{\partial \varepsilon} - f(\varepsilon) \frac{\partial g(\varepsilon')}{\partial \varepsilon'} + g(\varepsilon') \frac{\partial f(\varepsilon)}{\partial \varepsilon} - g(\varepsilon) \frac{\partial f(\varepsilon')}{\partial \varepsilon'} \right) d\varepsilon', \quad (4.9)$$

and thus we can write

$$F'(f^{k-1}) \cdot (f^k - f^{k-1}) = f^k - f^{k-1} - \Delta t Q^l(f^{k-1}, f^k - f^{k-1}).$$

This is the method used by Epperlein in [15]. The Newton's sequence becomes

$$f^k - f^n = \Delta t \left( Q^l(f^{k-1}, f^k) - Q(f^{k-1}, f^{k-1}) \right).$$

Because  $Q^l$  and  $Q$  have a symmetric weak form, the Newton's process conserves mass and energy at each iteration. Now we assume that the discretization in energy is provided by the Chang and Cooper type scheme. This scheme is naturally expensive because it generates a  $N \times N$  non-sparse matrix when we discretize in energy. The cost is then in  $\mathcal{O}(N^3)$  at each iteration. In the case where potentials are Coulombian an other strategy is to remember the equations satisfied by the drift and the diffusive terms, namely (2.9), and to introduce  $E$  and  $D$  as unknowns [7]. Thus the implicit scheme writes

$$\begin{cases} \frac{f^{n+1} - f^n}{\Delta t} = Q(f^{n+1}) = \tilde{Q}(f^{n+1}, E(f^{n+1}), D(f^{n+1})) = \tilde{Q}(f^{n+1}, E^{n+1}, D^{n+1}), \\ f^{n+1} = R(E(f^{n+1})) = R(E^{n+1}), \\ f^{n+1} = -S(D(f^{n+1})) = -S(D^{n+1}), \end{cases}$$

where the unknowns are now  $f^{n+1}$ ,  $E^{n+1}$  and  $D^{n+1}$  and  $S(D) = \frac{2}{3} \frac{\partial}{\partial \varepsilon} \frac{1}{\sqrt{\varepsilon}} \frac{\partial D}{\partial \varepsilon}$ . We solve the previous system by the Newton's method. The Jacobian matrix involved in the method is now a sparse matrix. If one discretizes in energy by the Chang and Cooper type scheme this yields to

$$\begin{cases} f_i - f_i^n - \frac{\Delta t}{c_i} (E_{i+\frac{1}{2}} f_{i+\frac{1}{2}} + D_{i+\frac{1}{2}} \frac{f_{i+1} - f_i}{\Delta \varepsilon_{i+\frac{1}{2}}} - E_{i-\frac{1}{2}} f_{i-\frac{1}{2}} - D_{i-\frac{1}{2}} \frac{f_i - f_{i-1}}{\Delta \varepsilon_{i-\frac{1}{2}}}) = 0, \\ f_i - f_N - \frac{E_{i+\frac{1}{2}} - E_{i-\frac{1}{2}}}{\Delta \varepsilon_i^{\frac{3}{2}}} = 0, \\ f_{i+\frac{1}{2}} + \frac{1}{\Delta \varepsilon_{i+\frac{1}{2}}} \left( \frac{D_{i+\frac{3}{2}} - D_{i+\frac{1}{2}}}{\Delta \varepsilon_{i+1}^{\frac{3}{2}}} - \frac{D_{i+\frac{1}{2}} - D_{i-\frac{1}{2}}}{\Delta \varepsilon_i^{\frac{3}{2}}} \right) = 0, \end{cases}$$

where  $f_{i+\frac{1}{2}}$  is given by the Chang and Cooper average (3.10) for  $\mathcal{S}_1$ . Note that  $f_{i+\frac{1}{2}}$  depends on  $E$ ,  $D$  and  $f = \{f_i\}_{1 \leq i \leq N}$ . Thus we can write the above system in  $f, E, D$  as

$$\begin{cases} f - f^n - \Delta t \tilde{Q}(f, E, D) = 0, \\ f - R(E) = 0, \\ h(f, E, D) + S(D) = 0. \end{cases} \quad (4.10)$$

Starting from  $(f^0, E^0, D^0)$  verifying the second and third equation of (4.10) the iteration procedure is defined as:

**Iteration process 1.** *Steps:*

1. we solve

$$\begin{cases} f^k - f^n = \Delta t \left( \partial_{f,E,D} \tilde{Q}(f^{k-1}, E^{k-1}, D^{k-1}) \cdot (f^k - f^{k-1}, E^k - E^{k-1}, D^k - D^{k-1}) \right. \\ \quad \left. - \tilde{Q}(f^{k-1}, E^{k-1}, D^{k-1}) \right) \\ f^k - R(E^k) = 0, \\ \partial_{f,E,D} h(f^{k-1}, E^{k-1}, D^{k-1}) \cdot (f^k - f^{k-1}, E^k - E^{k-1}, D^k - D^{k-1}) + S(D^k) \\ \quad = -h(f^{k-1}, E^{k-1}, D^{k-1}) \end{cases} \quad (4.11)$$

where  $\partial_{f,E,D} \tilde{Q}^1(f, E, D)$  is the linearized of  $\tilde{Q}(f, E, D)$ , and we have taken into account all the simplifications coming from the fact that  $R$  and  $S$  are linear operators.

2. Set  $D^k$  as the solution of  $h(f^k, E^k, D^k) - S(D^k) = 0$ .

**Proposition 5.** *The sequence  $f^k$  defined by the iteration process (1) is conservative in mass and energy.*

*Proof.* We proceed by induction. By construction  $f^{k-1}, E^{k-1}, D^{k-1}$  satisfy the second and third equations of (4.10). Thus the second and third equations of (4.11) give  $E^k - E^{k-1} = \partial_f E(f^{k-1}) \cdot (f^k - f^{k-1})$  and  $D^k - D^{k-1} = \partial_f D(f^{k-1}) \cdot (f^k - f^{k-1})$ . Plugging these relations in the first equation of (4.11), we have nothing else than the sequence of the Newton's method (4.8) with only the unknown  $f$ , which is conservative in mass and energy since the linearized operator  $Q(f)$  defined by (3.6) is too. Thus  $f^k$  and  $f^{k-1}$  have the same mass and energy. Since  $(f^0, E^0, D^0)$  verify the second and third equation of (4.10) that ends the proof. The starting point  $f^0$  is obviously chosen such that it has the same mass and energy as  $f^n$ .  $\square$

The linear system involved by (4.11) when the vector of the unknowns is stored as

$$((f_i, E_{i+\frac{1}{2}}, D_{i+\frac{1}{2}})_{i=1, N-1}, f_N)$$

gives a  $(3N - 2) \times (3N - 2)$  matrix like a block-tridiagonal matrix where  $3(N - 1)$  blocks represent a square matrix of order 3 and the last row (respectively column) is a  $3N - 2$  vector (respectively column-vector). The last row can be easily eliminated by subtracting lines and that gives a band diagonal system which can be solved by a direct method like LU in  $\mathcal{O}((3N - 2)m^2)$  operations,  $m = 11$  is the number of diagonals.

Applied to the equilibrium scheme  $\mathcal{S}_3$  this strategy is more simple since the function  $h$  becomes linear: the second step of the iteration process (1) is useless.

Additional optimization can be done in the case of Coulombian potentials, by replacing the  $f_i$ ;  $i = 1, N - 1$  by  $E_{i+\frac{1}{2}}$  and by rearranging a little bit the linear system involved by the Newton's method, the matrix is then only  $(2N - 1) \times (2N - 1)$ , the number of diagonals is  $m = 9$  and we gain approximately a factor 2 in terms of CPU time. This the Newton's implementation of Decoster [7] for  $\mathcal{S}_2$  for which we have a substantial gain since the last row is null.

Such a strategy can be also be applied with "Log" schemes. It can also be applied for Maxwellian potentials even for the full 3-D Landau equation. The key point is still the fact that in these cases drift and diffusion coefficients can be computed through recurrences relations. But for the full Landau equation with Coulombian potentials the question remains open.

## 5 Numerical results

We compare  $\mathcal{S}_1$  and  $\mathcal{S}_3$  and the various implicit schemes on two numerical test cases: the first one is the classical Rosenbluth test [24] and the second one is a  $\delta$  function in energy.

### 5.1 Test 1: the classical Rosenbluth test

This numerical test is extracted from the work of Rosenbluth *et al.* [24]. The initial data is a gaussian velocity distribution given by  $f_0(\varepsilon) = 0.01 \exp(-10((\sqrt{\varepsilon} - 0.3)/0.3)^2)$ . We use a regular velocity discretization. Thus the discrete energy points are  $\varepsilon_i = (\frac{i}{N})^2$  for  $i = 1$  to  $N$ . Let  $\Delta t_{exp}$  the largest step ensuring the stability of the explicit scheme. As the grid is irregular, the time step of the explicit scheme is constrained by the smallest step size of the mesh. We denote  $\tau$  the characteristic collision time. In figure (1) we plot the numerical kinetic entropy  $\sum_{i=1}^N f_i^n \log f_i^n c_i$  as a function of time, obtained by the "contracted implicit" method (4.4) and the full implicit method (4.11). Tolerance for the iterative schemes is  $10^{-12}$ . We consider three time steps namely:  $\Delta t = 10^{-1}\tau$ ,  $\Delta t = \tau$  and  $\Delta t = 10\tau$ . The final physical time corresponds to  $20\tau$ . We observe that the equilibrium state is reached in only four collision times. The results given by the full implicit method are the more accurate. This is clear also in figure (2) where the fourth moment  $\sum_{i=1}^N f_i^n \varepsilon_i^2 c_i$  is plotted as a function of time or for the distribution function in figure (3). The time step  $\Delta t = 10\tau$  gives a *CFL* of about 23000. For our two schemes we show in table (1), for all the time discretization, the CPU time required to attain a final time of  $30\tau$ . The "contracted implicit" scheme is the cheaper method but gives poor results as the time step exceed  $\tau$  and it could give negative solutions.

	Explicit	Contracted implicit	Fixed point	Newton
$\mathcal{S}_1, \Delta t = 10^{-1}\tau$	6	7.9E-002	0.26	0.24
$\mathcal{S}_1, \Delta t = \tau$	6	9.6E-003	7.32E-002	2.46E-002
$\mathcal{S}_1, \Delta t = 10\tau$	5.7	1.6E-003	5.1E-002	3.9E-003
$\mathcal{S}_3, \Delta t = 10^{-1}\tau$	.6	3.0E-002	6.6E-002	0.16
$\mathcal{S}_3, \Delta t = \tau$	0.75	4.2E-003	1.7E-002	1.7E-002
$\mathcal{S}_3, \Delta t = 10\tau$	0.78	1.0E-003	1.0E-002	1.7E-003

Table 1: Test 1. Comparison of the total costs involved by  $\mathcal{S}_1$  and  $\mathcal{S}_3$  for three values of the time step,  $\Delta t = 10^{-1}\tau, \tau, 10\tau$ , and a final time  $T = 30\tau$ .

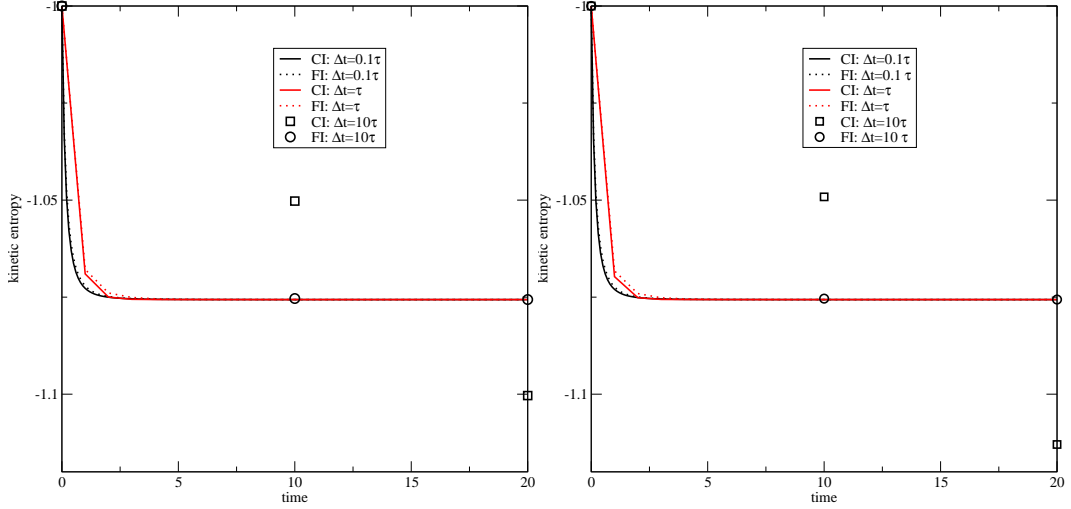


Figure 1: Test 1. Kinetic entropy for contracted implicit scheme (CI) and full implicit (FI),  $\mathcal{S}_1$  vs  $\mathcal{S}_3$ .

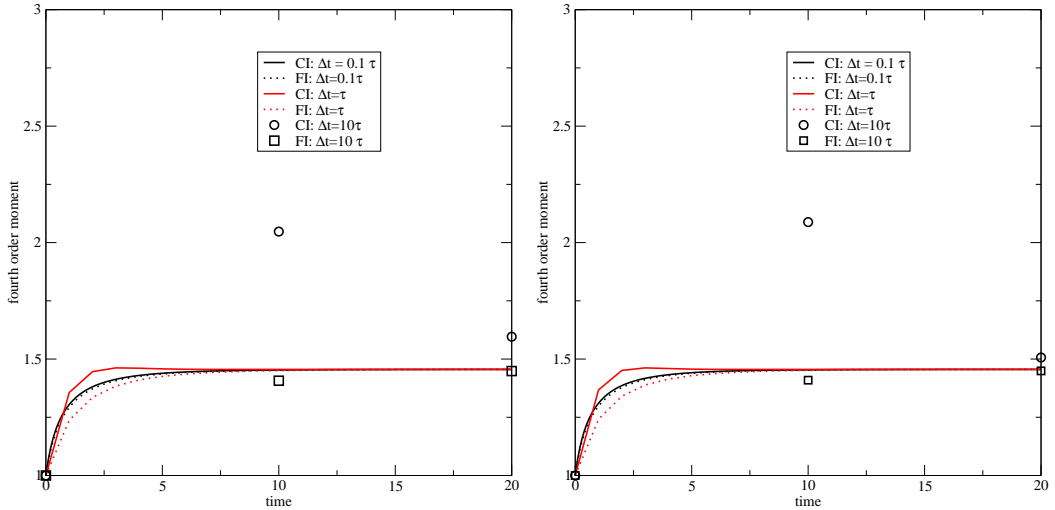


Figure 2: Test 1. Fourth order moment for contracted implicit scheme (CI) and full implicit (FI),  $\mathcal{S}_1$  vs  $\mathcal{S}_3$ .

## 5.2 Test 2: a mono-energetic initial data

This is typically a test that can't be handle by "Log" schemes : either the scheme is not defined [10] or the initial data don't evolve through time [4, 11]. One consider thus the initial data  $f_0(\varepsilon) = \delta_{\varepsilon=0.3}$  and we do the same computations as for the Rosenbluth test case, that is with the same parameters. Now the time step  $\Delta t = 10\tau$  gives a  $CFL$  of about 23000. As for test 1, the full implicit scheme via fixed point method or the Newton method gives the more accurate results even if the time step is much larger: see figures (6) and (5) where the fourth moment  $\sum_{i=1}^N f_i^n \varepsilon_i^2 c_i$  is plotted as a function of time. The contracted implicit scheme is still the cheaper but to give the right relaxation, the time step would not exceed  $10^{-1}\tau$ , see

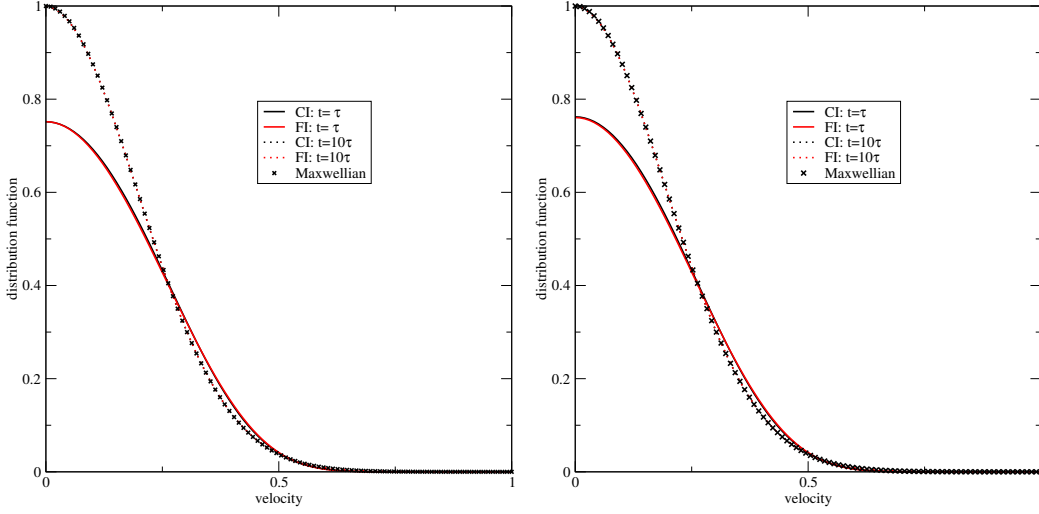


Figure 3: Test 1. Distribution function,  $\Delta t = 0.1\tau$ ,  $\mathcal{S}_1$  vs  $\mathcal{S}_3$ .

figure (4). And it could produce negative solutions even with large time steps. At contrary the full implicit scheme using fixed point iteration or Newton method gives always a positive solution and a better relaxation despite their extra cost.

At this point, we want to emphasize that, our schemes  $\mathcal{S}_1$  and  $\mathcal{S}_3$  are robust whatever the time discretization. This point out the interest of designing positive schemes for the FPL equation, not as the "Log" schemes rightly. This last class of scheme is very useless with the "contracted implicit" method or the Newton method since they used Logarithm of the distribution function. And the fixed point iterative method cannot be defined in general for them. This is in relationship with the fact that for them, excepted for the Berezin and Pekker one on uniform grid in energy, it is impossible to exhibit a condition on the time step to ensure the positivity (see [3, 4]).

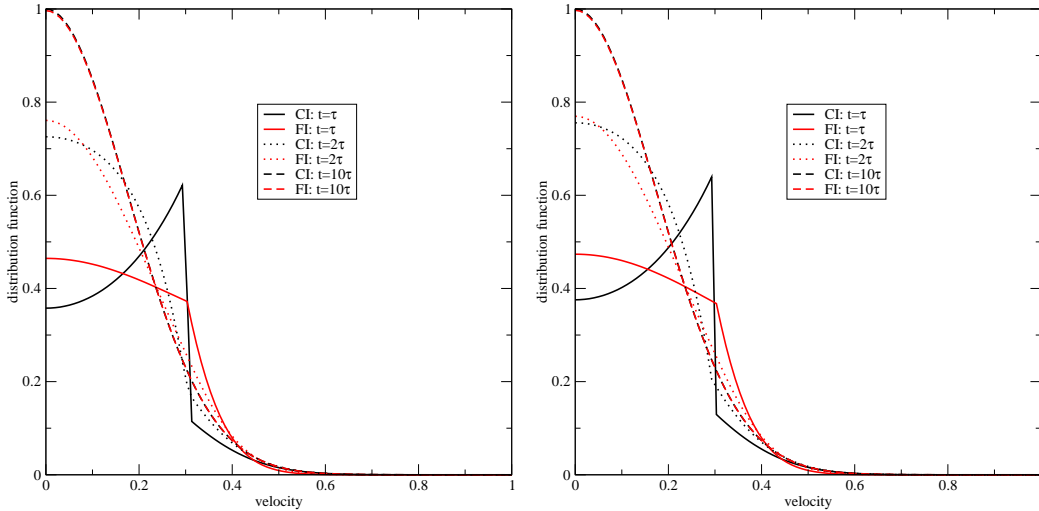


Figure 4: Test 2. Distribution function,  $\Delta t = \tau$ ,  $\mathcal{S}_1$  vs  $\mathcal{S}_3$ .



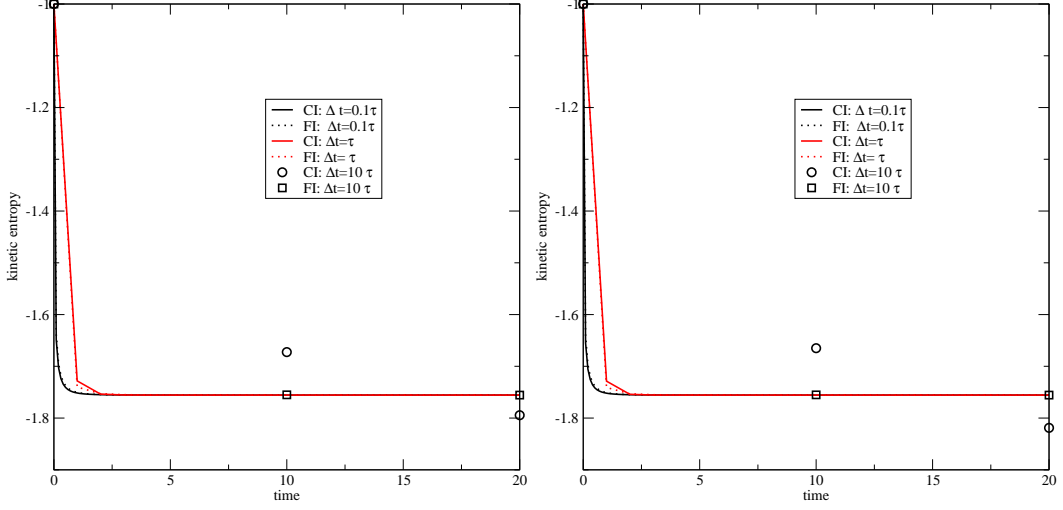


Figure 5: Test 2. Kinetic entropy for contracted implicit scheme (CI) and full implicit (FI),  $\mathcal{S}_1$  vs  $\mathcal{S}_3$ .

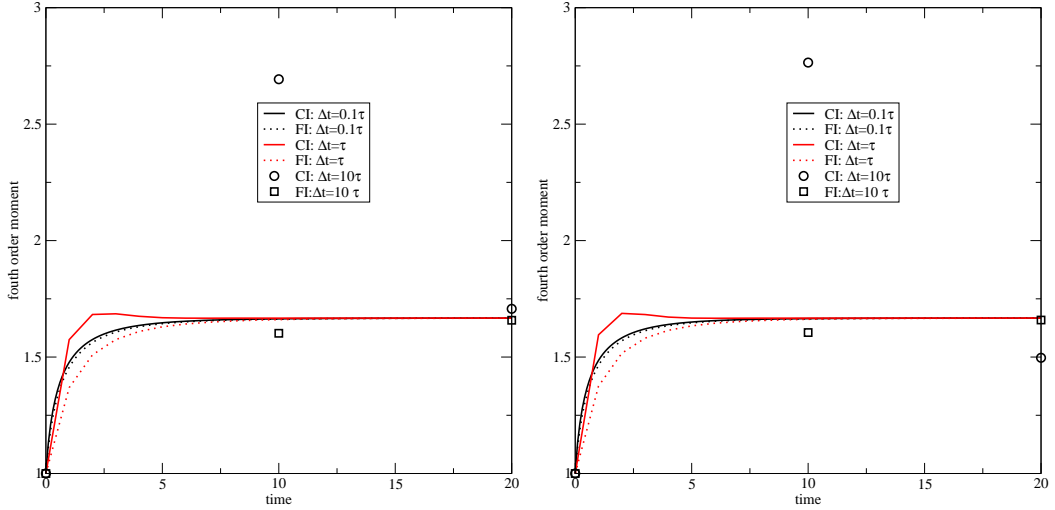


Figure 6: Test 2. Fourth order moment for contracted implicit scheme (CI) and full implicit (FI),  $\mathcal{S}_1$  vs  $\mathcal{S}_3$ .

## 6 Conclusions

In this work, we have introduced a new variant of the Chang and Cooper method  $\mathcal{S}_1$  for the isotropic FPL equation and also a new scheme called equilibrium scheme  $\mathcal{S}_3$ . These two methods, on non-uniform grid, are both positive, conservative in mass and energy and preserve the discrete Maxwellians, contrary to other existing methods for the isotropic FPL equation. This last method is cheaper than the Chang and Cooper one. Nevertheless this one could be more precise if the temperature of the plasma becomes low compared to the mesh size. These two schemes should apply to the full 3-D Landau equation.

We have also shown that time discretization like the "contracted implicit" method and the Newton's method can be formulate in such a manner so that they lead to the inversion of

a band diagonal system which can be solved by direct method with a linear cost. Let us also emphasize that if such technics could be also applied to "Log" schemes, they will be more expensive due to the more complex structure of such algorithms. Despite it's lack of conservation of energy, the fixed point approach method works well on numerical tests and it has a cost comparable to the "contracted implicit" method or the Newton's method. Moreover since we have positive scheme, we are able to give a time step restriction for the explicit scheme which could be the cheaper if the number of points is of the order of 20 and if the time step is little compared to the collision time (approximately  $10^{-2}\tau$ ). With these four time's discretization it could be possible, by switching between them, to minimize the cost of a time step according to the number of points and the ratio  $\frac{\Delta t}{\tau}$ . In conclusion, through this study we have also emphasized the importance of positive schemes, especially when time discretization is approached. The extension of these tools to the full Landau equation will be the subject of a future work.

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