Fast implicit schemes for the Fokker-Planck-Landau equation

Schémas implicites rapides pour l'équation Fokker-Planck-Landau

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Abstract

We propose new implicit schemes to solve the homogeneous and isotropic Fokker-Planck-Landau equation. These schemes have conservation and entropy properties. Moreover, they allow for large time steps (of the order of the physical relaxation time), contrary to usual explicit schemes. We use in particular fast linear Krylov solvers like the GMRES method. These schemes allow an important gain in terms of CPU time, with the same accuracy as explicit schemes. This work is a first step to the development of fast implicit schemes to solve more realistic kinetic models. *To cite this article: M. Lemou, L. Mieussens, C. R. Acad. Sci. Paris, Ser. I 336 (2003).*

Résumé

Nous proposons de nouveaux schémas implicites pour résoudre l'équation de Fokker-Planck-Landau homogène isotrope. Ces schémas possèdent des propriétés de conservation et d'entropie. Ils permettent l'utilisation de pas de temps de l'ordre du temps de relaxation physique, contrairement aux schémas explicites usuels. Nous utilisons en particulier des solveurs linéaires rapides de type Krylov comme la méthode GMRES. Ces schémas offrent un gain important en temps CPU avec une précision comparable à celle des schémas explicites. Ce travail constitue une première étape en vue du développement de schémas implicites rapides pour résoudre des équations cinétiques plus réalistes. *Pour citer cet article : M. Lemou, L. Mieussens, C. R. Acad. Sci. Paris, Ser. I 336 (2003).*

Version française abrégée

Dans cette Note, nous développons des schémas implicites en temps pour résoudre l'équation de Fokker-Planck-Landau homogène isotrope (1). Ce travail constitue une première étape pour construire des schémas rapides pour des modèles de collision plus complexes.

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La majorité des méthodes numériques actuelles utilisent des schémas explicites en temps souffrant d'une condition sur le pas de temps très restrictive (condition CFL). Même en utilisant des algorithmes rapides pour le calcul des collisions, cette condition induit un coût global en $O(N^3)$ pour atteindre un temps de simulation donné, N étant le nombre de points de discrétisation de la méthode [2]. Or il est connu que les schémas implicites en temps permettent de s'affranchir de la condition CFL et d'utiliser un pas de temps de l'ordre du temps de relaxation physique. Cependant, à notre connaissance, les schémas implicites existants sont soit trop coûteux en raison de l'inversion d'un grand sytème linéaire [4], soit non conservatifs [3].

Nous proposons alors différents schémas implicites qui permettent la résolution de (1) pour un coût global en $O(n_K N)$ seulement (avec $n_K \leq N$), tout en étant conservatifs et précis. Cette réduction du coût est due au fait que le pas de temps ne dépend plus de N et que les systèmes linéaires sont résolus par des algorithmes rapides.

Pour construire de tels schémas, nous proposons d'impliciter les termes de diffusion intervenant dans l'opérateur de collision (à l'origine de la condition CFL), tout en préservant la symétrie de l'opérateur nécessaire aux propriétés de conservation et d'entropie. Nous introduisons alors le schéma contracté (3) qui est un schéma implicite linéaire utilisant l'opérateur q^c donné par (4). Ensuite, nous introduisons une classe de θ-schémas (6) contenant le schéma implicite linéarisé développé dans [4]. Nous montrons dans la proposition 2.1 que tous nos schémas sont conservatifs. De plus le schéma contracté est entropique et le θ-schéma est d'ordre deux en temps pour $\theta = \frac{1}{2}$. En ce qui concerne la résolution des systèmes linéaires associés à nos schémas implicites, nous montrons que des méthodes de type Krylov permettent de les résoudre de manière approchée, tout en préservant exactement les propriétés de conservation.

Pour illustrer ces propriétés, nous présentons enfin deux tests numériques. Sur la figure 1, nous montrons que notre schéma implicite permet l'utilisation d'un pas de temps de l'ordre du temps de relaxation physique et conduit à des résultats très proches de la solution exacte. Sur la figure 2, nous constatons que le coût de calcul pour atteindre un temps de simulation donné est bien inférieur à $O(N^2)$ pour le schéma implicite contracté, alors qu'il est en $O(N^3)$ pour le schéma explicite.

Nous pensons que la stratégie présentée peut s'étendre au cas tridimensionnel ainsi qu'à d'autres opérateurs de collision. Dans ces cas, des techniques de calcul rapide des collisions comme celles développées dans [6,1], et des méthodes de préconditionnement des systèmes linéaires pourront être utilisées. Ceci fait l'objet d'un travail futur.

1. Introduction

The Fokker-Planck-Landau (FPL) is a kinetic collisional model used to describe a system of particles in plasma physics. The particles are described through a distribution function $f(t, x, v)$ depending on time t, particle position x, and their velocity v. In this note, we focus on the isotropic case, that is the case where the distribution function only depends on time, and on the particle kinetic energy $\varepsilon = |v|^2$. In this case, the FPL equation writes

$$\partial_t f(t,\varepsilon) = Q(f) = \frac{1}{\sqrt{\varepsilon}} \frac{\partial}{\partial \varepsilon} \int_0^{+\infty} K(\varepsilon, \varepsilon_*) \left(f_* \partial_\varepsilon f - f \partial_\varepsilon f_* \right) d\varepsilon_*, \tag{1}$$

with $K(\varepsilon, \varepsilon_*) = \frac{16}{3} \pi \inf(\varepsilon^{3/2}, \varepsilon_*^{3/2})$ for Coulombian interactions, and $K(\varepsilon, \varepsilon_*) = \frac{16}{3} \pi \varepsilon^{3/2} \varepsilon_*^{3/2}$ for Maxwellian interactions. Here, we set $f = f(\varepsilon)$ and $f_* = f(\varepsilon_*)$ to simplify the notations.

For any distribution function f, the collision operator $Q(f)$ satisfies the following weak formulation

$$\int_0^{+\infty} Q(f) \phi(\varepsilon) \sqrt{\varepsilon}\, d\varepsilon = -\frac{1}{2} \int_0^{+\infty} \int_0^{+\infty} K(\varepsilon, \varepsilon_*) \left(f_* \partial_\varepsilon f - f \partial_\varepsilon f_* \right) \left(\partial_\varepsilon \phi - \partial_\varepsilon \phi_* \right) d\varepsilon d\varepsilon_*, \tag{2}$$

ϕ being any test function. From this formulation, one can immediately derive the following conservation and entropy properties

$$\int_0^{+\infty} (1,\varepsilon)^T Q(f)\sqrt{\varepsilon}\, d\varepsilon = 0, \qquad \int_0^{+\infty} Q(f)\log(f)\sqrt{\varepsilon}\, d\varepsilon \leq 0.$$

Numerous works have been concerned with constructing a discretization of the collision operator that obeys the physical properties of conservation and entropy listed above, and that does not require too much computational time. In most of these works, the time discretization is explicit and induces a severe CFL condition of the form $\Delta t \leq C\Delta\varepsilon^2$, [2], where Δt is the time step and $\Delta\varepsilon = N^{-1}$ is the step of the energy grid of N points. To reach a given simulation time, a large number of iterations n_{it} is then required. In that case, even with fast evaluation of the collision operator in $O(N)$, these explicit schemes require a total simulation cost of the order of $n_{it}O(N) = O(N^3)$.

Consequently, it is attractive to use time implicit schemes, since they are known to be free of a restrictive time step condition. However, even if the number of iterations is reduced, implicit schemes usually induce an additional computational cost (non-sparse matrix inversion [4]). This may also affect the properties of conservation and entropy [3].

In this note we develop a strategy leading to fast and conservative implicit schemes in which large time steps of the order of the physical relaxation time can be used. One of our schemes (called contracted) is proved to have an entropy dissipation property, and another one is proved to be second order in time. Both of them preserve the total mass and energy of particles. Iterative Krylov solvers are used to rapidly solve the linear systems involved in the implicit schemes. This strategy is also proved to be conservative, even if the linear systems are only solved approximately, and an important gain in terms of computational cost is obtained.

2. A class of implicit schemes

In this section, we do not discretize the energy variable ε. We only focus on the time discretization. Indeed, any conservative and entropic discretization in ε would lead to completely discrete schemes with the same properties. The main idea is to note that the CFL constraint on the time step for explicit schemes is due to the diffusive terms. On the other hand, the conservation and entropy properties are a consequence of the symmetry property of the collision operator. Therefore, our strategy consists in making implicit in time the diffusive term ($f_*\partial_\varepsilon f$ in (1)), without destroying the original symmetry of the operator. This leads to the following contracted implicit (CI) scheme

$$\frac{f^{n+1} - f^n}{\Delta t} = q^c(f^n, f^{n+1}), \quad \text{with} \tag{3}$$

$$q^c(f,g) = \frac{1}{\sqrt{\varepsilon}}\frac{\partial}{\partial\varepsilon}\int_0^{+\infty} K(\varepsilon,\varepsilon_*)\left(f_*\partial_\varepsilon g - f\partial_\varepsilon g_*\right) d\varepsilon_*. \tag{4}$$

Note that this operator q^c is not the linearization of $Q(g)$ around f. This linearized operator is in fact

$$q(f,g) = \frac{1}{\sqrt{\varepsilon}}\frac{\partial}{\partial\varepsilon}\int_0^{+\infty} K(\varepsilon,\varepsilon_*)\left(f_*\partial_\varepsilon g - f\partial_\varepsilon g_* + g_*\partial_\varepsilon f - g\partial_\varepsilon f_*\right) d\varepsilon_*.$$

Therefore, the CI scheme (3) is not the usual linearized implicit (LI) scheme as used by Epperlein in [4]. The q^c operator is contracted in the sense that we only keep the terms that are necessary to ensure the symmetry between ε and ε_* in the linearized operator q. Therefore, q^c satisfies the following weak form

$$\int_0^{+\infty} q^c(f,g)\phi(\varepsilon)\sqrt{\varepsilon}\, d\varepsilon = -\frac{1}{2}\int_0^{+\infty}\int_0^{+\infty} K(\varepsilon,\varepsilon_*)\left(f_*\partial_\varepsilon g - f\partial_\varepsilon g_*\right)\left(\partial_\varepsilon\phi - \partial_\varepsilon\phi_*\right) d\varepsilon d\varepsilon_*. \tag{5}$$

Moreover, we consider the following implicit schemes (θ-LI), derived from the linearized operator q

$$\frac{f^{n+1}-f^n}{\Delta t} = \theta q(f^n, f^{n+1}) + (\frac{1}{2}-\theta) q(f^n, f^n), \tag{6}$$

for any $\theta \in [0,1]$. Note that the CI scheme is not a θ-LI scheme and that the linearized implicit scheme used in [4] is obtained for $\theta = 1$. Now we give the main properties of these schemes.

Proposition 2.1 *(i) The CI and $\theta - LI$ schemes, respectively given by (3) and (6), are conservative:*

$$\int_0^{+\infty} (1,\varepsilon)^T q^c(f,g)\sqrt{\varepsilon}\, d\varepsilon = 0, \qquad \int_0^{+\infty} (1,\varepsilon)^T \Big(\theta q(f,g) + (1-\theta) q(f,f)\Big)\sqrt{\varepsilon}\, d\varepsilon = 0.$$

(ii) The θ-LI scheme is second order in time if and only if $\theta = \frac{1}{2}$.

(iii) The CI scheme is entropic in the following sense:

$$\int_0^{+\infty} q^c(f,g) h(f,g)\sqrt{\varepsilon}\, d\varepsilon \le 0, \quad \textit{with} \qquad h(f,g) = \int_0^{\varepsilon} \frac{1}{f_*} \partial_\varepsilon g_*\, d\varepsilon_*.$$

(iv) The operator $g \mapsto q^c(f,g)$ satisfies the following inequality

$$\langle q^c(f,g), g\rangle_{L^2(\sqrt{\varepsilon}d\varepsilon)} \le C_f \|g\|^2_{L^2(\sqrt{\varepsilon}d\varepsilon)}. \tag{7}$$

Sketch of the proof: properties (i) and (iii) are direct consequences of weak formulations (2) and (5). A straightforward Taylor expansion leads to Property (ii). Estimate (7) is a bit more technical. We refer to [7] for details.

□

Remark 1 The quantity $h(f,g)$ is in fact an approximation of $\log f$ *when g is close to f. This shows that our inequality is a discrete version of the usual entropy dissipation property of Q.*

3. Solving the linear systems

In this section, we present some strategies to solve the linear systems involved in the above implicit schemes. For brevity, only the CI scheme (3) is explained in details.

For the energy discretization, consider for instance the one used in [2]: they use the regular energy discretization $\varepsilon_i = (i-1)\Delta\varepsilon$, $i = 1..N$, and the following discrete collision operator $Q(f)$

$$Q_i(f) = -\frac{1}{c_i} D^* \sum_{j=1}^{N-1} K_{i,j} \left(f_j Df_i - f_i Df_j\right),$$

where D is the one-sided difference operator $Df_i = f_{i+1} - f_i$, and D^* is its formal adjoint, f_i stands for an approximation of $f(\varepsilon_i)$, and c_i is an approximation of the measure $\sqrt{\varepsilon}d\varepsilon$. We also set $K_{i,j} = K(\varepsilon_i, \varepsilon_j)$ with the convention $K_{1,.} = K_{N,.} = 0$. This discretization has been proved in [2] to be conservative and entropic. Then, we associate to this definition the discrete operators $q_i^c(f,g)$ as in the continuous case. Discrete analogue properties of proposition 2.1 can be proved (see [7] for details).

Consequently, the CI scheme (3) reads

$$L^c(f^n) f^{n+1} = \Big(I - \Delta t\, q^c(f^n, .)\Big) f^{n+1} = f^n. \tag{8}$$

Note that property (iv) of proposition 2.1 implies that there exists a time step Δt such that $L^c(f^n)$ is invertible.

To solve this linear system, we use Krylov iterative methods. This strategy has been first proposed in [3] in a slightly different frame. Here, we believe that Krylov solvers can also be used with many more advantages that are described below.

First - this has been noticed in [3] in a slightly different context - matrix $L^c(f^n)$ does not need to be neither formed nor stored: only the matrix-vector product $L^c(f^n)g = g - \Delta t\, q^c(f^n, g)$ has to be made. This is done by applying the discretized form of (4).

A new advantage is that a Krylov solver is necessarily *conservative* in the sense that each iterate k has the same mass and energy as f^n. This can easily be seen: let M be the $2 \times N$ matrix such that the matrix-vector product Mf is the mass and energy of f. Since q^c is conservative, then $Mq^c(f^n, .) = 0$ and thus $ML^c(f^n) = M$. Each k^{th} iterate of the Krylov solver belongs to the affine space $f^n + \mathcal{K}^k$ where $\mathcal{K}^k = \text{span}\{r_0, L^c(f^n)r_0, \ldots, L^c(f^n)^{k-1}r_0\}$ and where the residual is $r_0 = f^n - L^c(f^n)f^n$ (see [8] for introduction to Krylov solvers). Therefore, each element of this affine space has the same mass and energy as f^n since $M\mathcal{K}^k = \{0\}$. It is remarkable that this conservation property holds even if linear system (8) is not exactly solved.

For Coulombian and Maxwellian potentials, the matrix-vector product can be done in $O(N)$ operations. On the other hand, the time step Δt_{imp} used in the implicit scheme is independent of N ($\Delta t_{imp} = O(1)$). Therefore, to reach a given simulation time t_{max}, the use of Krylov solvers (with n_K iterations) leads to a total complexity of the order of $O(n_K N \frac{t_{max}}{\Delta t_{imp}}) \leq O(N^2)$, since $n_K \leq N$. At the contrary, the explicit scheme requires a time step $\Delta t_{exp} = O(N^{-2})$ which leads to a total cost of the order of $O(N \frac{t_{max}}{\Delta t_{exp}}) = O(N^3)$. This is clearly much larger than the cost of our implicit schemes.

Finally, this analysis also applies to the θ-LI scheme (6).

4. Numerical tests

First, in the case of Maxwellian potential, it is proved in [5] that

$$f^{exact}(t, \varepsilon) = \frac{\rho}{(2\pi T)^{3/2}} \exp(-\frac{\varepsilon}{2T}) \left(1 + \frac{11}{120}((\frac{\varepsilon}{T})^2 - 10\frac{\varepsilon}{T} + 15) \exp(-8\rho t)\right)$$

is an exact solution of (1). Then, in figure 1, we compare the numerical solution obtained with the second order in time θ-LI scheme (6) ($\theta = 1$) to this exact solution. The energy domain is $[0, 2]$ discretized with 500 points. The parameters of the exact solution are $\rho = 2$ and $T = 0.01$. The time step used with the implicit scheme is about 300 times the time step required by an explicit computation. We observe that the numerical solution is very close to the exact one, and the equilibrium is reached in only ten iterations, which corresponds to a final physical time equal to $t_{max} = 10$. This shows that the dynamics described by the exact FPL equation can efficiently be simulated with a much larger time step than those of usual explicit schemes.

The second test case uses Coulombian potential with the same initial data as in [2]. On figure 2, we plot the computational cost versus the number N of energy points for explicit and CI schemes for a simulation time $t_{max} = 40$. For the CI scheme, the GMRES method is stopped when the residual is lower than 10^{-6}, and the time step is 0.3. We see that our implicit scheme is more and more advantageous as N increases. As expected, figure 2 confirms that the CPU of the implicit scheme (to reach t_{max}) is less than $O(N^2)$, as opposed to $O(N^3)$ for the explicit scheme.

5. Conclusion

As we pointed in the introduction, the present work is a first step toward the development of time implicit schemes for multidimensional collision operators. In this case, the involved linear systems are much larger, and suitable preconditioners are needed. We recall that in a Krylov method with a good

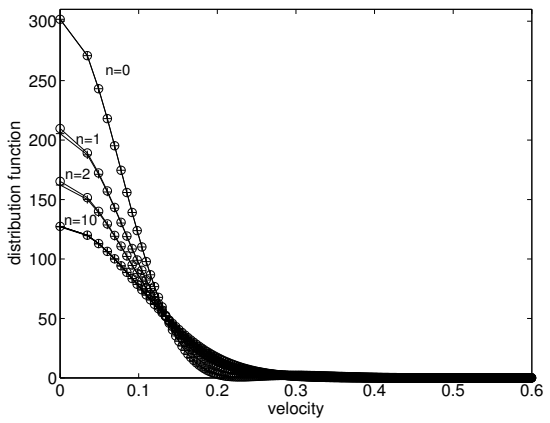

Figure 1. Exact solution (+) and implicit scheme (o) for Maxwellian potential (iterates $n = 0, 1, 2$ and 10).
Figure 1. Solution exacte (+) et schéma implicite (o) pour le potentiel maxwellien (itérations $n = 0, 1, 2$ et 10).

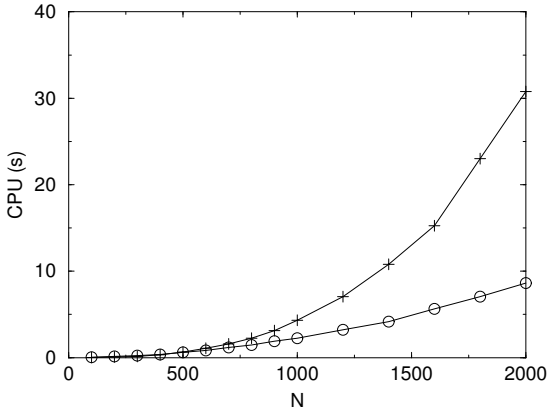

Figure 2. CPU cost of explicit (+) and CI implicit (o) schemes for Coulombian potential vs the number N of energy points.
Figure 2. Temps CPU des schémas explicite (+) et implicite CI (o) pour le potentiel coulombien en fonction du nombre de points N.

preconditioner, the number of iterations is independent of N. Thus the complexity of our implicit schemes could be reduced to $O(N)$ only.

Moreover, the rapid matrix-vector product that has been used in the isotropic case cannot be applied to the multidimensional cases. Therefore, to get a fast implicit solver in several dimensions, other acceleration techniques are required. We believe that this can be done using multipole or wavelets techniques [6,1].

Finally, the extension of our strategy to other collision operators (e.g. relativistic or quantum Landau operators) is an interesting question which we defer to future investigation.

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