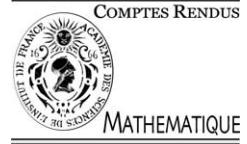




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Numerical Analysis/Mathematical Physics

Wavelet approximations of a collision operator in kinetic theory [☆]

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Abstract

This Note is devoted to the derivation of conservative and entropic fast wavelet approximations for the isotropic Fokker–Planck–Landau collision operator arising in the modeling of charged particles in plasma physics. The present approach combines the advantages of both the finite difference schemes (conservation and entropy) and the spectral methods (accuracy) which are developed in the literature. Furthermore, the wavelet approach provides a fast algorithm for the evaluation of such a collision operator. The present work is a first step to the development of wavelet approximations to more complex collision operators in kinetic theory. **To cite this article:** X. Antoine, M. Lemou, *C. R. Acad. Sci. Paris, Ser. I* 337 (2003).

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Résumé

Approximations par ondelettes d'un opérateur de collision en théorie cinétique. Cette Note présente un schéma conservatif et entropique basé sur l'utilisation des ondelettes pour l'équation de Fokker–Planck–Landau isotrope qui modélise l'évolution des particules chargées dans un plasma. La présente approche possède à la fois les propriétés des schémas aux différences finies (conservation et entropie) et celles des méthodes spectrales (essentiellement la précision) qui sont développés dans la littérature. De plus, l'approche ondelette fournit un algorithme rapide d'évaluation de l'opérateur de collision. Ce travail constitue un premier pas vers le développement d'approximations par ondelettes d'opérateurs de collision plus complexes. **Pour citer cet article :** X. Antoine, M. Lemou, *C. R. Acad. Sci. Paris, Ser. I* 337 (2003).

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Version française abrégée

L'équation de Fokker–Planck–Landau (FPL) est un modèle cinétique décrivant l'évolution des particules chargées dans un plasma. Ces particules sont décrites par une fonction de distribution $f(t, x, v)$ dépendant du temps $t \geq 0$, de la position des particules $x \in \mathbb{R}^3$ et de leurs vitesses $v \in \mathbb{R}^3$. Nous nous intéressons ici au développement de schémas conservatifs, entropiques et rapides basés sur la théorie des ondelettes pour ce type de modèle. Comme ce travail constitue, à notre connaissance, le premier développement dans cette direction, nous allons

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nous restreindre au cas homogène et isotrope, i.e. au cas où f ne dépend que du temps et du module de la vitesse. L'extension de la présente méthode à des cas plus généraux est en cours de développement. Plus précisément, nous considérons l'opérateur de collision de FPL (1), (2). Cet opérateur intégral vérifie des propriétés de conservation (de la masse, de l'impulsion et de l'énergie) et de dissipation de l'entropie données par (3). Diverses approches déterministes existent quant à la discréétisation en vitesse (ici selon $\varepsilon = |v|^2$). Ces méthodes peuvent être globalement classées en deux catégories : les méthodes à vitesse discrète et les méthodes spectrales. Parmi ce premier groupe de méthodes, citons notamment les schémas aux différences finies conservatifs et entropiques développés dans [5], ainsi que des références moins récentes qui y sont citées. Même si des algorithmes rapides de type multipôle ou multigrille peuvent être utilisés pour accélérer l'évaluation du noyau de collision [4], leur précision reste toutefois limitée. Parallèlement, des méthodes précises de type spectral ont été proposées dans [6]. Il faut noter que ces méthodes ne vérifient pas les propriétés de conservation et d'entropie de manière exacte, et que leur extension à des opérateurs de collision plus complexes ne semble pas immédiate. Nous présentons dans cette Note des schémas par ondelettes précis, conservatifs et entropiques. De plus, le coût de l'évaluation numérique de l'opérateur de collision est de l'ordre de $\mathcal{O}(-(\log \eta)N)$, où N est la dimension de l'espace d'approximation et η l'erreur tolérée par rapport à un calcul direct.

Le choix de la base d'approximation s'est porté sur les multi-ondelettes interpolantes introduites récemment par Alpert et al. [1]. Ces bases définissent une structure multi-échelle dans $L^2([0, 1])$, décrite plus en détails dans la Section 2. Elles sont construites à partir de fonctions « scalings » définies par le biais des polynômes d'interpolation de Lagrange aux racines des polynômes de Legendre d'ordre $M + 1$ et des poids de Gauss-Legendre grâce à la formule (4). Les bases multi-ondelettes associées possèdent respectivement les propriétés de concentration et d'annulation des M premiers moments donnés par les formules (5). Ces propriétés fournissent des formules de quadratures localisantes, contrairement à une approximation par transformée de Fourier standard. Ceci permet également d'approcher spectralement la projection multi-ondelettes d'une fonction f de $L^2([0, 1])$ par la formule (6) et de définir ainsi une approximation \bar{f} . La structure des schémas ondelettes ainsi obtenus est semblable à celle des discréétisations par différences finies développées dans [5], permettant ainsi de satisfaire toutes les propriétés de conservation et d'entropie, tout en gardant une précision élevée. De plus, un des points essentiels de cette approximation est l'introduction d'un algorithme multi-niveaux qui permet d'obtenir, par une troncature adéquate du noyau K donné par (2), une évaluation en $\mathcal{O}(N)$ de l'opérateur de collision, à comparer au coût $\mathcal{O}(N^2)$ lié à une approche directe. Dans le cas d'un opérateur de collision isotrope (1), (2), on écrit alors un schéma d'approximation de type multi-ondelette conservatif et entropique avec une précision spectrale. Ce résultat est décrit dans la Proposition 3.1 de la Section 3. De plus, ce schéma est rapide grâce à l'utilisation d'un algorithme d'évaluation multiniveaux. Des résultats numériques présentés dans la dernière section mettent en avant l'efficacité de l'approche proposée en testant les cas de potentiels coulombiens et maxwelliens. Nous représentons notamment sur la Fig. 1 les entropies des systèmes pour différents niveaux de résolution n et ordres M des bases multi-ondelette. En outre, ces résultats montrent que l'utilisation d'un noyau tronqué lors des simulations n'affecte que très peu la précision. Finalement, la Table 1 donne des temps de calculs effectifs qui illustrent et confirment les coûts de calculs prévus par la théorie. Les extensions de cette approche au cas multidimensionnel semblent possibles et leurs développements sont en cours. Cette Note est une version courte des travaux développés dans [2].

1. Introduction

The FPL operator arises in the modeling of charged particles. Let f be the distribution function of particles assumed to be isotropic, that is f only depends on time $t \geq 0$ and on the particle energy $\varepsilon = |v|^2/2$. The collision operator Q is given by

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

where the kernel K is given by

$$\begin{aligned} K(\varepsilon, \varepsilon') = & \frac{-8\pi}{(\gamma+2)(\gamma+4)(\gamma+6)} ((\varepsilon^{1/2} + \varepsilon'^{1/2})^{\gamma+4} (\varepsilon - (\gamma+4)\varepsilon^{1/2}\varepsilon'^{1/2} + \varepsilon') \\ & - |\varepsilon^{1/2} - \varepsilon'^{1/2}|^{\gamma+4} (\varepsilon + (\gamma+4)\varepsilon^{1/2}\varepsilon'^{1/2} + \varepsilon')) \end{aligned} \quad (2)$$

Real number γ leads to the usual classification in Maxwellian molecules ($\gamma = 0$), hard ($\gamma > 0$) and soft ($\gamma < 0$) potentials. The FPL operator has the following physical properties (mass-energy conservation and entropy dissipation):

$$\int_0^{+\infty} Q(f)(\varepsilon) \left(\frac{1}{\varepsilon} \right) \sqrt{\varepsilon} d\varepsilon = 0 \quad \text{and} \quad \int Q(f)(\varepsilon) \ln f(\varepsilon) \sqrt{\varepsilon} d\varepsilon \leq 0, \quad \forall f. \quad (3)$$

Moreover, this last inequality becomes an equality if and only if f is a Maxwellian distribution: $f = \exp(A\varepsilon + B)$, for some constants $A < 0$ and $B \in \mathbb{R}$.

Several works are devoted to the velocity discretization of the FPL collisional operator (1) and of its three-dimensional form. We are only interested here in deterministic approaches (and not probabilistic as for Monte Carlo simulation techniques) that we can roughly classify into two categories: the *finite velocity* schemes and the *spectral* methods. Concerning the first approach, conservative and entropic finite difference schemes have been proposed in [5]. However, even if multigrid or multipole algorithms can be used to accelerate the evaluation of the collisional operator [4], the accuracy remains limited. To circumvent this problem, spectral discretizations have been developed in [6]. However, these methods are not exactly conservative or entropic, and their extension to collision operators involving different geometries or more physics (relativistic and quantum effects for instance) is an open problem. We propose here a velocity discretization scheme of the FPL operator based on the multiwavelet method [1]. We construct conservative, entropic and accurate schemes combining thus the advantages of discrete velocity approximations and spectral discretizations. Furthermore, the evaluation of the collision operator has a cost of the order of $\mathcal{O}(N)$, where N is the dimension of the approximation space. This Note is a short version of [2].

2. Interpolating multiwavelet bases

Let M be an integer and $\{q_i\}_{0 \leq i \leq M}$ an $L^2([0, 1])$ -orthonormal basis of polynomial functions of degree less than or equal to M . We define the scaling functions $\{\varphi_i\}_{0 \leq i \leq M}$ on \mathbb{R} by: $\varphi_i(x) := q_i(x)$ on $[0, 1]$ and 0 otherwise. Let V_0 be the space of vanishing functions outside $[0, 1]$ and whose restrictions to $[0, 1]$ are polynomials of degree less or equal to M . Then we have $V_0 = \text{Span}\{\varphi_i\}_{0 \leq i \leq M}$. We briefly recall the multilevel structure of wavelet-type algorithms. For a level n of resolution, we introduce V_n as the space of piecewise polynomial functions vanishing outside $[0, 1]$ and whose restriction to each interval $[2^{-n}l, 2^{-n}(l+1)]$ is a polynomial of degree less or equal to M , for $0 \leq l \leq 2^n - 1$. We then define the dilated-translated scaling functions $\varphi_I^{(n)}(x) = 2^{n/2} \varphi_i(2^n x - l)$, where $I = (i, l)$ and $\mathcal{I} = \{(i, l) \mid 0 \leq i \leq M, 0 \leq l \leq 2^n - 1\}$. We have $V_n = \text{Span}\{\varphi_I^{(n)}\}_{I \in \mathcal{I}}$ and $V_j \subset V_{j+1}$, for $j \geq 0$. Moreover, $\{\varphi_I^{(n)}\}_{I \in \mathcal{I}}$ is an orthonormalized basis of V_n (and $\dim V_n = N = (M+1)2^n$). Let us now introduce the corrective space W_n of V_n as the orthogonal complement of V_n in V_{n+1} : $V_n \oplus W_n = V_{n+1}$. Another construction of spaces W_n can be also described from W_0 as follows. Consider an orthonormal basis $\{\psi_i\}_{0 \leq i \leq M}$ spanning W_0 which is the orthogonal of V_0 in V_1 . We define the dilated-translated multiwavelet functions, and get $W_n = \text{Span}\{\psi_I^{(n)}\}_{I \in \mathcal{I}}$, for $n \geq 1$.

Up to now, the orthonormal families $\{\varphi_i\}_{0 \leq i \leq M}$ and $\{\psi_i\}_{0 \leq i \leq M}$ are not specified. We are going to give a suitable basis for our approximation. This basis was recently introduced by Alpert et al. [1], and our choice is motivated by the localizing property (5) of these functions and by their “easy to use” character. Let \mathbb{P}_{M+1} be the

Legendre polynomial of degree $M + 1$ on $[-1, 1]$ and (x_0, \dots, x_M) its roots. Consider the Lagrange interpolating polynomials $\{l_i\}_{0 \leq i \leq M}$ at the Gauss points $\{x_i\}_{0 \leq i \leq M}$ and $\{\omega_i\}_{0 \leq i \leq M}$ as the Gauss–Legendre weights, and define the following orthonormal family of scaling functions

$$\varphi_i(x) := \sqrt{\frac{2}{\omega_i}} l_i(2x - 1), \quad \forall x \in [0, 1], \quad 0 \leq i \leq M. \quad (4)$$

Then we construct the spaces V_n and W_n as previously. The scaling and multiwavelet functions respectively fulfill at a fixed level of resolution n the *concentration* and the *vanishing* properties

$$\int_0^1 f(x) \varphi_I^{(n)}(x) dx = \alpha_{n,i} f\left(\frac{y_i + k}{2^n}\right) \quad \text{and} \quad \int_0^1 f(x) \psi_I^{(n)}(x) dx = 0, \quad \forall f \in V_n \quad (5)$$

with $I = (i, k) \in \mathcal{I}$, $\alpha_{n,i} = 2^{-n/2} \sqrt{\omega_i/2}$ and $y_i = (x_i + 1)/2$. Let $f \in L^2([0, 1])$ and $P_n f$ the orthogonal projection of f onto V_n . Then we have the following approximation \bar{f} of $P_n f$

$$P_n f \sim \bar{f} = \sum_{I \in \mathcal{I}} \bar{f}_I \varphi_I^{(n)}, \quad \text{with } \bar{f}_I = \alpha_{n,i} f\left(\frac{y_i + k}{2^n}\right) \sim \int_0^1 f(x) \varphi_I^{(n)}(x) dx. \quad (6)$$

To discretize $Q(f)$ given by (1), we first define the product $\bar{f} \otimes \bar{g}$, the logarithm $\overline{\ln}(\bar{f})$ and the exponential $\overline{\exp}(\bar{f})$ of two approximations \bar{f} and \bar{g} by their components as follows

$$(\bar{f} \otimes \bar{g})_I = \frac{1}{\alpha_{n,i}} \bar{f}_I \bar{g}_I \overline{\ln}(\bar{f})_I = \alpha_{n,i} \ln\left(\frac{\bar{f}_I}{\alpha_{n,i}}\right) \quad \text{and} \quad \overline{\exp}(\bar{f})_I = \alpha_{n,i} \exp\left(\frac{\bar{f}_I}{\alpha_{n,i}}\right). \quad (7)$$

We also need to define the derivative operator. Following [1] we introduce the right decentered derivative operator D defined by the relations

$$[D \bar{f}]_k = R_0 [\bar{f}]_k - R_1^T [\bar{f}]_{k+1}, \quad 0 \leq k \leq 2^n - 2, \quad \text{and} \quad [D \bar{f}]_{2^n-1} = R_{0,r} [\bar{f}]_{2^n-1}, \quad (8)$$

for a function $\bar{f} = ([\bar{f}]_k)_{k=0}^{2^n-1} \in V_n$, where the block vectors $[\bar{f}]_k$ are defined by $[\bar{f}]_k = (\bar{f}_{i,k})_{i=0}^M$. Blocks R_0 , R_1 and $R_{0,r}$ are $(M+1) \times (M+1)$ matrices given by

$$(R_0)_{i,j} = 2^n \left[-\varphi_i(1)\varphi_j(1) + \sqrt{\frac{\omega_i}{2}} \varphi'_j(y_i) \right], \quad (R_1)_{i,j} = -2^n \varphi_i(0)\varphi_j(1) \quad \text{and} \quad (R_{0,r})_{i,j} = 2^n \sqrt{\frac{\omega_i}{2}} \varphi'_j(y_i),$$

for $0 \leq i, j \leq M$ and where the derivatives of the scaling functions are exactly computed. We also introduce the adjoint (or transposed) operator D^* of D . Note that all the above approximations have spectral accuracy thanks to the localizing property (5) (see [1] and [2] for details).

To proceed with the approximation of the collision operator, we restrict the integration domain to $[0, 1]$ and keep the same notation for $Q(f)$

$$\sqrt{\varepsilon} Q(f)(\varepsilon) = \frac{\partial}{\partial \varepsilon} \left[\frac{\partial \ln f}{\partial \varepsilon}(\varepsilon) f(\varepsilon) (Tf)(\varepsilon) - f(\varepsilon) T \left[\frac{\partial \ln f}{\partial \varepsilon} f \right](\varepsilon) \right], \quad (9)$$

with

$$Tg(\varepsilon) = \int_0^1 K(\varepsilon, \varepsilon') g(\varepsilon') d\varepsilon'. \quad (10)$$

The operator T is represented on V_n by the matrix $T^{(n)}$ whose coefficients are approximated by

$$T_{I,J}^{(n)} = \iint_0^1 K(\varepsilon, \varepsilon') \varphi_I^{(n)}(\varepsilon) \varphi_J^{(n)}(\varepsilon') d\varepsilon d\varepsilon' \sim \alpha_{n,i} \alpha_{n,j} K\left(\frac{y_i + k}{2^n}, \frac{y_j + l}{2^n}\right) = T_{I,J}^{(n)}. \quad (11)$$

We denote this last approximation by $\mathcal{T} = (\mathcal{T}_{I,J}^{(n)})_{(I,J) \in \mathcal{I}^2}$. Of course, a direct evaluation of $\mathcal{T} \bar{f}$ would require $\mathcal{O}(N^2)$ operations. However, this cost is reduced to $\mathcal{O}(N)$ operations using a multiscale algorithm [3] and a suitable truncation of the kernel K . Indeed it is well known in the wavelet approximation theory that integral operators as T can be rapidly evaluated. We refer to [2] for a detailed presentation of this algorithm and for some error estimates.

3. Conservative and entropic multiwavelet schemes for the isotropic FPL operator

Under the previous notations, we have the following multiwavelet approximation for the FPL operator.

Proposition 3.1. *Let \bar{f} be the approximation of the unknown distribution function f defined by (6), $\bar{\ln}$ be the logarithm function on V_n given by (7) and consider the approximation \mathcal{T} of the integral operator T defined by (11). Under these notations, we introduce the following operator on the space V_n*

$$\mathcal{Q}(\bar{f}) = -D^*[(D \bar{\ln}(\bar{f})) \otimes \bar{f} \otimes (\mathcal{T} \bar{f}) - \bar{f} \otimes \mathcal{T}((D \bar{\ln}(\bar{f})) \otimes \bar{f})], \quad (12)$$

where D is the derivative operator (8) and D^* its adjoint operator. The operator (12) is the multiwavelet approximation of $\sqrt{\varepsilon} Q(f)$ given by (9). Furthermore, this approximation satisfies the following weak discrete formulation

$$\sum_{I \in \mathcal{I}} [\mathcal{Q}(\bar{f})]_I \Theta_I = -\frac{1}{2} \sum_{I, J \in \mathcal{I}^2} \mathcal{T}_{I,J} \bar{f}_I \bar{f}_J \left[\frac{1}{\alpha_{n,i}} (D\Theta)_I - \frac{1}{\alpha_{n,j}} (D\Theta)_J \right] \left[\frac{1}{\alpha_{n,i}} (D \bar{\ln}(\bar{f}))_I - \frac{1}{\alpha_{n,j}} (D \bar{\ln}(\bar{f}))_J \right], \quad (13)$$

for all element $\Theta \in V_n$. From this weak formulation, we deduce the conservation of the discrete mass and energy and the discrete entropy dissipation property respectively given by

$$\sum_{I \in \mathcal{I}} [\mathcal{Q}(\bar{f})]_I \bar{\Theta}_I = 0, \quad \text{for } \Theta = 1, \varepsilon \quad \text{and} \quad \sum_{I \in \mathcal{I}} [\mathcal{Q}(\bar{f})]_I (\bar{\ln}(\bar{f}))_I \leq 0, \quad \forall \bar{f} \in V_n, \quad \bar{f}_i \geq 0, \quad (14)$$

with equality for this last relation if and only if \bar{f} is a Maxwellian: $\bar{f} = \overline{\exp}(A\bar{\varepsilon} + B\bar{1})$, where $(A, B) \in \mathbb{R}^2$.

The scheme (13) is a generalization of that obtained in [5]. Indeed, taking $M = 1$ in the definition of the approximation space V_n , (13) coincides with the finite difference scheme developed in [5]. The scheme (13) allows high accuracy on a non-regular grid.

For a time step $\Delta t > 0$, \bar{f}^p denotes an approximation of the projection on V_n of the distribution function f at time $p\Delta t$. For an initial datum f_0 represented on V_n , we solve the classical FPL equation by the explicit time discretization scheme

$$\bar{f}^{p+1} = \bar{f}^p + \Delta t \mathcal{Q}(\bar{f}^p), \quad (15)$$

$\mathcal{Q}(\bar{f}^p)$ is given by (12). If the discrete operator \mathcal{T} given by (11) is used then we shall say that the computation is direct. If we rather use its representation in a basis of V_n involving the multiwavelet functions ψ_I^k , then \mathcal{T} can be approximated by a highly sparse matrix with a sparsity depending on a truncation parameter b and we say that we

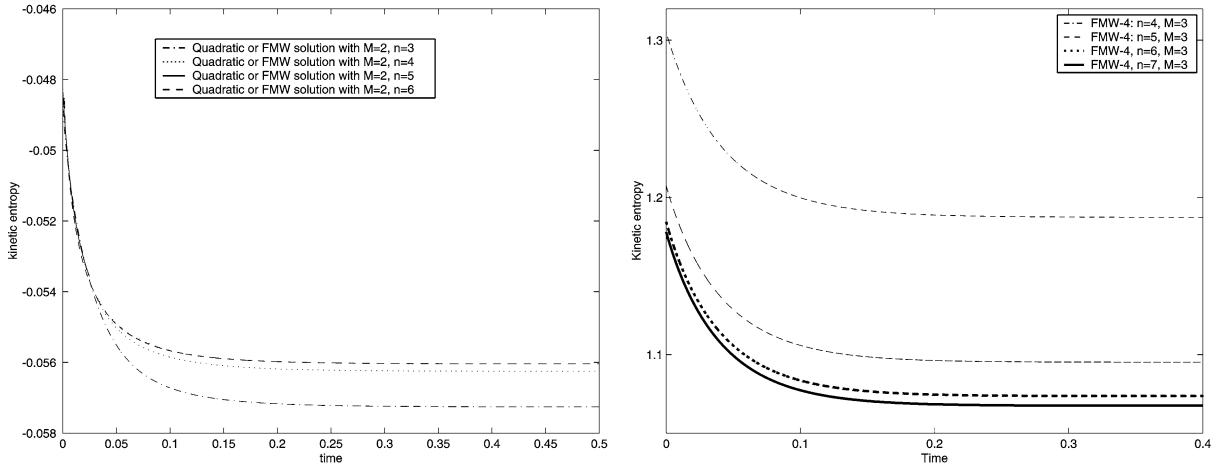


Fig. 1. Left: Kinetic entropies for different levels of resolution n using the direct or FMW-2 algorithms with the second-order ($M = 2$) multiwavelet basis for the Coulombian case. Right: Kinetic entropies for different values of the level of resolution n using direct and FMW algorithms with the third-order multiwavelet basis for the Maxwellian case.

Table 1

Coulombian case: computational time (in seconds) for one thousand iterations using the direct and FMW schemes

Level n	$M = 2$				$M = 3$				$M = 4$			
	6	7	8	9	6	7	8	9	6	7	8	9
Direct	0.27	2.03	8.02	32.23	0.82	5.40	21.23	89.0	1.88	7.36	30.0	180.0
FMW-2	0.42	0.85	1.80	3.55	0.60	1.18	2.70	6.10	0.87	1.82	3.75	8.50
FMW-4	0.46	0.99	2.16	4.35	0.70	1.47	3.60	8.30	1.02	2.25	5.10	11.20

use the FMW- b method. For more details, we refer to [2]. We consider two test cases, the coulombian ($\gamma = -3$) and the Maxwellian ($\gamma = 0$) ones, corresponding respectively to the two initial data

$$f_0(\varepsilon) = \exp\left(-10\left[\frac{(\varepsilon - 0.3)}{0.6}\right]^2\right) \quad \text{and} \quad f_0(\varepsilon) = \frac{2}{(2\pi 0.01)^{3/2}} \exp\left(-\frac{R}{2}\right)\left(1 + \frac{11}{120}(R^2 - 10R + 15)\right),$$

with $R = \varepsilon/(0.01)$. We present on Fig. 1 the discrete kinetic entropies to show the accuracy and report on Table 1 some computational times. We see that the FMW- b methods become more and more faster for levels $n \geq 6, 7$. Moreover, the computational cost increases linearly with the dimension of the approximation space ($\mathcal{O}(2^n)$) for the FMW- b methods, while it increases quadratically for the direct method ($\mathcal{O}(2^{2n})$). The method has also been applied with success in [2] to a quantum version of the FPL operator.

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