

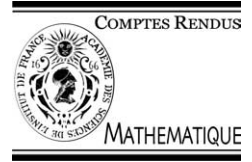


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Fast methods for the Boltzmann collision integral [☆]

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Abstract

In this Note we present methods for the development of fast numerical schemes for the Boltzmann collision integral. These schemes are based on a combination of a Carleman-like representation together with a suitable angular approximation. For the hard spheres model in dimension three, we are able to derive spectral methods that can be evaluated through fast algorithms. Estimates for the errors and spectral accuracy are also given. *To cite this article: C. Mouhot, L. Pareschi, C. R. Acad. Sci. Paris, Ser. I 339 (2004).*

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Résumé

Méthodes rapides pour l'intégrale de collision de Boltzmann. Dans cette Note nous présentons des méthodes pour le développement de schémas numériques rapides pour l'intégrale de collision de Boltzmann. Ces schémas sont basés sur la combinaison d'une représentation proche de celle de Carleman et d'une approximation angulaire appropriée. Pour le modèle des sphères dures en dimension trois, nous en déduisons des méthodes spectrales qui peuvent être évaluées par des algorithmes rapides. Nous donnons également des estimations d'erreur et un résultat de précision spectrale. *Pour citer cet article : C. Mouhot, L. Pareschi, C. R. Acad. Sci. Paris, Ser. I 339 (2004).*

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Dans cette Note nous présentons des méthodes pour le développement de schémas numériques rapides pour l'intégrale de collision de Boltzmann. L'obtention de méthodes numériques pour l'équation de Boltzmann est une question difficile en calcul scientifique, et d'une grande importance pour de nombreuses applications. L'essentiel des difficultés provient de la structure multi-dimensionnelle de l'opérateur, dont l'intégrale est prise sur une variété non plate de dimension 5.

Nous utilisons une représentation (3) de l'opérateur de collision proche de celle de Carleman pour obtenir une nouvelle façon de tronquer l'opérateur en domaine borné en vitesse par périodisation. Cette méthode préserve les

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propriétés d'invariance du noyau de collision et respecte mieux la structure de type convolution de l'opérateur que les méthodes précédentes.

Pour des interactions qui vérifient une hypothèse de découplage du noyau de collision (7), nous effectuons une approximation (6) de l'intégrale de collision par une discrétisation de la partie angulaire basée sur la méthode des rectangles pour l'intégrale des fonctions périodiques, ce qui nous permet d'obtenir des méthodes spectrales qui peuvent être évaluées par des algorithmes rapides.

Les méthodes spectrales pour l'équation de Boltzmann sont issues des travaux [12] et [13], mais contrairement à ces travaux nous tirons ici avantage de la structure de l'intégrale de collision pour obtenir un découplage des modes de Fourier (5). Ceci est le point crucial pour développer des algorithmes rapides grâce à la transformée de Fourier rapide.

La classe d'interactions considérée inclut les molécules *Maxwelliennes* en dimension deux et les molécules *sphères dures* en dimension trois (le modèle le plus pertinent physiquement pour les applications).

Nous donnons des estimations d'erreur pour les nouvelles méthodes. Celles-ci ont une précision spectrale (Théorème 5.3), c'est-à-dire d'ordre infini. Pour plus de détails et la généralisation de ces techniques à des interactions plus générales et aux modèles discrétisés en vitesse nous renvoyons à [9].

1. Introduction

Taking into account only binary interactions, the behavior of a dilute gas of particles is described by the Boltzmann equation [6,15] $\partial f / \partial t + v \cdot \nabla_x f = Q(f, f)$, where $f(t, x, v)$, $x, v \in \mathbb{R}^d$ ($d \geq 2$), is the time-dependent particle distribution function in the phase space and the collision operator Q is defined by

$$Q(f, f)(v) = \int_{v_* \in \mathbb{R}^d} \int_{\sigma \in \mathbb{S}^{d-1}} B(\cos \theta, |v - v_*|) [f'_* f' - f_* f] d\sigma dv_* \quad (1)$$

Time and position act only as parameters in Q and therefore will be omitted in its description. In (1) we used the shorthands $f = f(v)$, $f_* = f(v_*)$, $f' = f(v')$, $f'_* = f(v'_*)$. The velocities of the colliding pairs (v, v_*) and (v', v'_*) are related by $v' = \frac{v+v_*}{2} + \frac{|v-v_*|}{2}\sigma$, $v'_* = \frac{v+v_*}{2} - \frac{|v-v_*|}{2}\sigma$. The collision kernel B is a non-negative function which only depends on $|v - v_*|$ and $\cos \theta = ((v - v_*) / |v - v_*|) \cdot \sigma$.

Boltzmann's collision operator has the fundamental properties of conserving mass, momentum and energy $\int_{v \in \mathbb{R}^d} Q(f, f) \phi(v) dv = 0$, $\phi(v) = 1, v, |v|^2$ and satisfies the well-known Boltzmann's H -theorem $-\frac{d}{dt} \int_{v \in \mathbb{R}^d} f \times \log f dv = - \int_{v \in \mathbb{R}^d} Q(f, f) \log(f) dv \geq 0$. The functional $-\int f \log f$ is the entropy of the solution. Boltzmann H -theorem implies that any equilibrium distribution function has the form of a local Maxwellian distribution $M(\rho, u, T)(v) = \frac{\rho}{(2\pi T)^{d/2}} \exp(-\frac{|u-v|^2}{2T})$, where ρ, u, T are the density, mean velocity and temperature of the gas:

$$\rho = \int_{v \in \mathbb{R}^d} f(v) dv, \quad u = \frac{1}{\rho} \int_{v \in \mathbb{R}^d} v f(v) dv, \quad T = \frac{1}{d\rho} \int_{v \in \mathbb{R}^d} |u - v|^2 f(v) dv.$$

The construction of numerical methods for Boltzmann equations represents a real challenge for scientific computing and it is of paramount importance in many applications. Most of the difficulties are due to the multidimensional structure of the collisional integral Q , as the integration runs on a $(2d - 1)$ -dimensional unflat manifold.

In this Note, for a particular class of interactions, using a Carleman-like representation of the collision operator together with a suitable angular approximation we are able to derive spectral methods that can be evaluated through fast algorithms. Related methods based on FFT have been derived in [1–3]. The class of interactions includes *Maxwellian molecules* in dimension two and *hard spheres* molecules in dimension three. The methods are strictly related to the spectral methods recently presented in [12,13], but on the contrary to the latter the new methods are able to take advantage of the structure of the Boltzmann equation in order to decouple the kernel modes. This is the central issue in the development of fast schemes. For more details and extensions of this technique to more general collision interactions and discrete velocity models we refer to [9].

2. The Boltzmann collision operator in bounded domains

Truncation of the Boltzmann collision operator in a bounded domain is the necessary preliminary stage of any deterministic method. Here we shall approximate the collision operator starting from a representation which conserves more symmetries of the collision operator when one truncates it in a bounded domain. This representation was used in [2,8] to derive finite differences schemes and it is close to the classical Carleman representation (cf. [5]).

The basic identity we shall need is

$$\frac{1}{2} \int_{\mathbb{S}^{d-1}} F(|u|\sigma - u) d\sigma = \frac{1}{|u|^{d-2}} \int_{\mathbb{R}^d} \delta(2x \cdot u + |x|^2) F(x) dx. \tag{2}$$

Using (2) the collision operator (1) can be written as $Q(f, f)(v) = 2^{d-1} \int_{x \in \mathbb{R}^d} \int_{y \in \mathbb{R}^d} B(-\frac{x \cdot (x+y)}{|x||x+y|}, |x+y|) \times \frac{1}{|x+y|^{d-2}} \delta(x \cdot y) [f(v+y)f(v+x) - f(v+x+y)f(v)] dx dy$.

Now let us consider the bounded domain $\mathcal{D}_T = [-T, T]^d$ ($0 < T < +\infty$). From now on let us write $\tilde{B}(x, y) = 2^{d-1} B(-\frac{x \cdot (x+y)}{|x||x+y|}, |x+y|) |x+y|^{-(d-2)}$. Instead of the usual reduction of the equation on the bounded domain based on removing some collisions here we consider a different approach based on periodizing the function f on the domain \mathcal{D}_T . As a consequence we have to truncate the integration in x and y since periodization would yield infinite result if not. Thus we set them to vary in \mathcal{B}_R , the ball of center 0 and radius R . For a compactly supported function f with support \mathcal{B}_S , we take $R = S$ in order to obtain all possible collisions. Then a geometrical argument (see [13]) shows that using the periodicity of the function it is enough to take $T \geq (3\sqrt{2} + 1)S/2$ to prevent intersections of the regions where f is different from zero. The operator now reads

$$Q^R(f, f)(v) = \int_{x \in \mathcal{B}_R} \int_{y \in \mathcal{B}_R} \tilde{B}(x, y) \delta(x \cdot y) [f(v+y)f(v+x) - f(v+x+y)f(v)] dx dy \tag{3}$$

for $v \in \mathcal{D}_T$. The interest of this representation is to preserve the real collision kernel and its invariance properties.

About the conservation properties one can show that: (i) The mass is locally conserved but not necessarily the momentum and the energy. (ii) When f is even there is *global* conservation of momentum, which is 0 in this case. (iii) The collision operator Q^R satisfies formally the H -theorem. (iv) As long as f has compact support included in \mathcal{B}_S with $T \geq (3\sqrt{2} + 1)S/2$ (no aliasing condition, see [13] for a detailed discussion) and $R = S$, then no unphysical collisions occur and thus mass, momentum and energy are preserved.

3. Spectral methods

Now we use the representation Q^R to derive new spectral methods. The spectral methods for kinetic equations originated in the works [12] and [13], and were further developed in [14] and [7]. The main difference compared to the usual spectral method is in the way we truncate the collision operator. In fact this yields better decoupling properties between the arguments of the operator.

To simplify notations let us take $T = \pi$. Hereafter we use just one index to denote the d -dimensional sums of integers.

The approximate function f_N is represented as the truncated Fourier series $f_N(v) = \sum_{k=-N}^N \hat{f}_k e^{ik \cdot v}$, $\hat{f}_k = \frac{1}{(2\pi)^d} \int_{\mathcal{D}_\pi} f(v) e^{-ik \cdot v} dv$. The spectral equation is the projection of the collision equation in \mathbb{P}^N , the $(2N + 1)^d$ -dimensional vector space of trigonometric polynomials of degree at most N in each direction, i.e. $\frac{\partial f_N}{\partial t} = \mathcal{P}_N Q^R(f_N, f_N)$, where \mathcal{P}_N denotes the orthogonal projection on \mathbb{P}^N in $L^2(\mathcal{D}_\pi)$. A straightforward computation leads to the following set of ordinary differential equations on the Fourier coefficients

$$\frac{d\hat{f}_k(t)}{dt} = \sum_{\substack{l+m=k \\ l,m=-N}}^N \hat{\beta}(l, m) \hat{f}_l \hat{f}_m, \quad k = -N, \dots, N, \tag{4}$$

where $\hat{\beta}(l, m)$ are the so-called *kernel modes*, given by $\hat{\beta}(l, m) = \beta(l, m) - \beta(m, m)$ where $\beta(l, m) = \int_{x \in \mathcal{B}_R} \int_{y \in \mathcal{B}_R} \tilde{B}(x, y) \delta(x \cdot y) e^{il \cdot x} e^{im \cdot y} dx dy$. In the sequel we shall focus on β , and one easily checks that $\beta(l, m)$ depends only on $|l|$, $|m|$ and $|l \cdot m|$.

Note that the usual way to truncate the Boltzmann collision operator for periodic functions originates the following form of the kernel modes in the x, y notation (see [13]) $\hat{\beta}_{\text{usual}}(l, m) = \int_{x \in \mathcal{B}_R} \int_{y \in \mathcal{B}_R} \tilde{B}(x, y) \delta(x \cdot y) \times \chi_{\{|x+y| \leq R\}} [e^{il \cdot x} e^{im \cdot y} - e^{im \cdot (x+y)}] dx dy$. One can notice that here x and y are also restricted to the ball \mathcal{B}_R but the condition $|x + y|^2 = |x|^2 + |y|^2 \leq R^2$ couples the two modulus, such that the ball is not completely covered (for instance, if x and y are orthogonal both with modulus R , the condition is not satisfied, since $|x + y| = \sqrt{2}R$).

4. Fast algorithms

The search for fast deterministic algorithms for the collision operator, i.e. algorithms with a cost lower than $O(N^{2d+\varepsilon})$ (with typically $\varepsilon = 1$), consists mainly in identifying some convolution structure in the operator (see for example [2,10,11]). If this is trivial for the loss part of the operator, for the gain part this is rather contradictory with the search for a conservative scheme in a bounded domain, since the boundary condition needed to prevent for the outgoing or ingoing collisions breaks the invariance.

The aim is to approximate each $\hat{\beta}(l, m)$ by a sum

$$\beta(l, m) \simeq \sum_{p=1}^A \alpha_p(l) \alpha'_p(m). \tag{5}$$

This gives a sum of A discrete convolutions and so the algorithm can be computed in $O(A N^d \log_2 N)$ operations by means of standard FFT techniques [4]. To this purpose we shall use a further approximated collision operator where the number of possible directions of collision is reduced to a finite set.

We start from representation (3) and write x and y in spherical coordinates

$$Q^R(f, f)(v) = \frac{1}{4} \int_{e \in \mathbb{S}^{d-1}} \int_{e' \in \mathbb{S}^{d-1}} \delta(e \cdot e') de de' \times \left\{ \int_{-R}^R \int_{-R}^R \rho^{d-2} (\rho')^{d-2} \tilde{B}(\rho, \rho') [f(v + \rho' e') f(v + \rho e) - f(v + \rho e + \rho' e') f(v)] d\rho d\rho' \right\}.$$

Let us denote with \mathcal{A} a discrete set of orthogonal couples of unit vectors (e, e') , which is even, i.e. $(e, e') \in \mathcal{A}$ implies that $(-e, e')$, $(e, -e')$ and $(-e, -e')$ belong to \mathcal{A} (this property on the set \mathcal{A} is required to preserve the conservation properties of the operator). Now we define $Q^{R, \mathcal{A}}$ to be

$$Q^{R, \mathcal{A}}(f, f)(v) = \frac{1}{4} \int_{(e, e') \in \mathcal{A}} \left\{ \int_{-R}^R \int_{-R}^R \rho^{d-2} (\rho')^{d-2} \tilde{B}(\rho, \rho') [f(v + \rho' e') f(v + \rho e) - f(v + \rho e + \rho' e') f(v)] d\rho d\rho' \right\} d\mathcal{A}, \tag{6}$$

where $d\mathcal{A}$ denotes a discrete measure on \mathcal{A} which is also even in the sense that $d\mathcal{A}(e, e') = d\mathcal{A}(-e, e') = d\mathcal{A}(e, -e') = d\mathcal{A}(-e, -e')$. It is easy to check that $Q^{R, \mathcal{A}}$ has the same conservations properties as Q_R .

We make the *decoupling assumption* that

$$\tilde{B}(x, y) = a(|x|)b(|y|). \tag{7}$$

This assumption is obviously satisfied if \tilde{B} is constant. This is the case of Maxwellian molecules in dimension two, and hard spheres in dimension three (the most relevant kernel for applications). Extensions to more general interactions are discussed in [9].

We describe the method in dimension $d = 3$ with \tilde{B} satisfying the decoupling assumption (7) (see [9] for other dimensions). First we change to spherical coordinates

$$\beta(l, m) = \frac{1}{4} \int_{e \in \mathbb{S}^2} \int_{e' \in \mathbb{S}^2} \delta(e \cdot e') \left[\int_{-R}^R |\rho| a(\rho) e^{i\rho(l \cdot e)} d\rho \right] \left[\int_{-R}^R |\rho'| b(\rho') e^{i\rho'(m \cdot e')} d\rho' \right] de de'$$

and then we integrate first e' on the intersection of the unit sphere with the plane e^\perp , $\beta(l, m) = \frac{1}{4} \int_{e \in \mathbb{S}^2} \phi_{R,a}^3(l \cdot e) [\int_{e' \in \mathbb{S}^2 \cap e^\perp} \phi_{R,b}^3(m \cdot e') de'] de$, where $\phi_{R,a}^3(s) = \int_{-R}^R |\rho| a(\rho) e^{i\rho s} d\rho$, $\phi_{R,b}^3(s) = \int_{-R}^R |\rho| b(\rho) e^{i\rho s} d\rho$. Thus we get the following decoupling formula with two degrees of freedom $\beta(l, m) = \int_{e \in \mathbb{S}_+^2} \phi_{R,a}^3(l \cdot e) \psi_{R,b}^3(\Pi_{e^\perp}(m)) de$, where \mathbb{S}_+^2 denotes the half-sphere and $\psi_{R,b}^3(\Pi_{e^\perp}(m)) = \int_0^\pi \phi_{R,b}^3(|\Pi_{e^\perp}(m)| \cos \theta) d\theta$. In the particular case where $\tilde{B} = 1$ (hard spheres model), we can compute the functions ϕ_R^3 and ψ_R^3 : $\phi_R^3(s) = R^2 [2 \text{Sinc}(Rs) - \text{Sinc}^2(Rs/2)]$, $\psi_R^3(s) = \int_0^\pi \phi_R^3(s \cos \theta) d\theta$. Now the function $e \rightarrow \phi_{R,a}^3(l \cdot e) \psi_{R,b}^3(\Pi_{e^\perp}(m))$ is periodic on \mathbb{S}_+^2 . Taking a spherical parametrization (θ, φ) of $e \in \mathbb{S}_+^2$ and taking for the set \mathcal{A} uniform grids of respective size M_1 and M_2 for θ and φ we get $\beta(l, m) \simeq \frac{\pi^2}{M_1 M_2} \sum_{p,q=0}^{M_1, M_2} \alpha_{p,q}(l) \alpha'_{p,q}(m)$, where $\alpha_{p,q}(l) = \phi_{R,a}^3(l \cdot e_{(\theta_p, \varphi_q)})$, $\alpha'_{p,q}(m) = \psi_{R,b}^3(\Pi_{e_{(\theta_p, \varphi_q)}^\perp}(m))$ and $(\theta_p, \varphi_q) = (p\pi/M_1, q\pi/M_2)$.

We shall consider this expansion with $M = M_1 = M_2$ to avoid anisotropy in the computational grid. The computational cost of the algorithm is then $O(M^2 N^3 \log_2 N)$, compared to $O(M^2 N^6)$ of a direct discretization on the grid and $O(N^6)$ of the usual spectral method.

5. Error estimates

In order to give a consistency result, the first step will be to prove a consistency result for the approximation of Q^R by $Q^{R,M} = Q^{R, \mathcal{A}_M}$ where \mathcal{A}_M is the uniform spherical grid with M points for each angular coordinate (see [9]). Here H_p^k denotes the periodic Sobolev space on \mathcal{D}_π .

Lemma 5.1. *The error on the approximation of the collision operator is spectrally small, i.e. for all $k > d - 1$ such that $f \in H_p^k$*

$$\|Q^R(f, f) - Q^{R,M}(f, f)\|_{L^2} \leq C_1 \frac{R^k \|f\|_{H_p^k}^2}{M^k}.$$

For the second step we use the consistency result [13, Corollary 5.4] on the operator Q^R , which we quote here for the sake of clarity.

Lemma 5.2. *For all $k \in \mathbb{N}$ such that $f \in H_p^k$*

$$\|Q^R(f, f) - \mathcal{P}_N Q^R(f_N, f_N)\|_{L^2} \leq \frac{C_2}{N^k} (\|f\|_{H_p^k} + \|Q^R(f_N, f_N)\|_{H_p^k}).$$

Combining these two results, one gets the following consistency result of spectral accuracy [9]

Theorem 5.3. For all $k > d - 1$ such that $f \in H_p^k$

$$\|Q^R(f, f) - \mathcal{P}_N Q^{R,M}(f_N, f_N)\|_{L^2} \leq C_1 \frac{R^k \|f_N\|_{H_p^k}^2}{M^k} + \frac{C_2}{N^k} (\|f\|_{H_p^k} + \|Q^R(f_N, f_N)\|_{H_p^k}).$$

Finally let us focus briefly on the macroscopic quantities. In fact here no additional error (related to M) occurs, compared with the usual spectral method, since the approximation of the collision operator that we are using is still conservative. Following the method of [13, Remark 5.4], we have the following spectral accuracy result

$$\|Q^{R,M}(f, f), \varphi) - (\mathcal{P}_N Q^{R,M}(f_N, f_N), \varphi)\|_{L^2} \leq \frac{C_3}{N^k} \|\varphi\|_{L^2} (\|f\|_{H_p^{k+d}} + \|Q^{R,M}(f_N, f_N)\|_{H_p^k}),$$

where φ can be replaced by $v, |v|^2$. Thus the error on momentum and energy is independent on M and it is spectrally small according to N .

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