FAST ALGORITHMS FOR COMPUTING
THE BOLTZMANN COLLISION OPERATOR

CLÉMENT MOUHOT AND LORENZO PARESCHI

ABSTRACT. The development of accurate and fast numerical schemes for the five-fold Boltzmann collision integral represents a challenging problem in scientific computing. For a particular class of interactions, including the so-called *hard spheres model* in dimension three, we are able to derive spectral methods that can be evaluated through fast algorithms. These algorithms are based on a suitable representation and approximation of the collision operator. Explicit expressions for the errors in the schemes are given and spectral accuracy is proved. Parallelization properties and adaptivity of the algorithms are also discussed.

1. INTRODUCTION

The Boltzmann equation describes the behavior of a dilute gas of particles when the only interactions taken into account are binary elastic collisions. It reads for $x, v \in \mathbb{R}^d$ $(d \geq 2)$

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

where $f(t, x, v)$ is the time-dependent particle distribution function in the phase space. The Boltzmann collision operator Q is a quadratic operator local in (t, x). The time and position acts only as parameters in Q and therefore will be omitted in its description

$$(1.1) \qquad Q(f, f)(v) = \int_{\mathbb{R}^d \times \mathbb{S}^{d-1}} B(|v - v_*|, \cos\theta) \ (f'_* f' - f_* f) \ dv_* \, d\sigma.$$

In (1.1) we used the shorthand $f = f(v)$, $f_* = f(v_*)$, $f' = f(v')$, $f'_* = f(v'_*)$. The velocities of the colliding pairs (v, v_*) and (v', v'_*) are related by

$$v' = \frac{v + v_*}{2} + \frac{|v - v_*|}{2}\sigma, \qquad v'_* = \frac{v + v^*}{2} - \frac{|v - v_*|}{2}\sigma.$$

The collision kernel B is a nonnegative function which by physical arguments of invariance only depends on $|v - v_*|$ and $\cos\theta = \hat{g} \cdot \sigma$ (where $\hat{g} = (v - v_*)/|v - v_*|$).

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The Boltzmann collision operator has the fundamental properties of conserving mass, momentum, and energy,

$$\int_{\mathbb{R}^d} Q(f,f)\phi(v)\,dv = 0, \quad \phi(v) = 1, v_1, \ldots, v_d, |v|^2,$$

and satisfies the well-known Boltzmann H theorem

$$-\frac{d}{dt}\int_{\mathbb{R}^d} f \log f\, dv = -\int_{\mathbb{R}^d} Q(f,f)\log(f)\,dv \geq 0.$$

The functional $-\int f \log f$ is the entropy of the solution. The Boltzmann H theorem implies that any equilibrium distribution function, i.e., any function which is a maximum of the entropy, has the form of a locally Maxwellian distribution

$$M(\rho, u, T)(v) = \frac{\rho}{(2\pi T)^{d/2}} \exp\left\{ -\frac{|u-v|^2}{2T} \right\},$$

where ρ, u, T are the density, mean velocity, and temperature of the gas, defined by

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

respectively. For further details on the physical background and derivation of the Boltzmann equation, we refer to [15, 49].

The construction of numerical methods for Boltzmann equations represents a real challenge for scientific computing, and it is of paramount importance in many applications, ranging from rarefied gas dynamics (RGD) [15], plasma physics [18], granular flows [2, 3], semiconductors [29], and quantum kinetic theory [20].

Most of the difficulties are due to the multidimensional structure of the collisional integral Q, as the integration runs on a five-dimensional unflat manifold. In addition to the unpracticable computational cost of deterministic quadrature rules, the integration has to be handled carefully since it is at the basis of the macroscopic properties of the equation. Additional difficulties are represented by the stiffness induced by the presence of small scales, like the case of small mean free path [25] or the case of large velocities [22].

For such reasons realistic numerical computations are based on probabilistic Monte Carlo techniques at different levels. The most famous examples are the direct simulation Monte Carlo (DSMC) methods by Bird [4] and by Nanbu [35]. These methods preserve the conservation properties of the equation in a natural way and avoid the computational complexity of a deterministic approach. However, avoiding the low accuracy and the fluctuations of the results becomes extremely expensive in presence of nonstationary flows or close to continuum regimes.

Among deterministic approximations, one of the most popular methods in RGD is represented by the discrete velocity models (DVM) of the Boltzmann equation. These methods [10, 30, 9, 17, 38, 47] are based on a regular grid in the velocity field and construct a discrete collision mechanics on the points of the grid in order to preserve the main physical properties. Unfortunately DVM have the same computational cost of a product quadrature rule, and due to the particular choice of the nodes imposed by the conservation properties the accuracy of the schemes seems to be less than first order [37, 36, 38].

More recently a new class of methods based on the use of spectral techniques in the velocity space has attracted the attention of the scientific community. The method was first developed for kinetic equations in [42], inspired from spectral

methods in fluid mechanics [11] and the use of Fourier transform tools in the analysis of the Boltzmann equation [6]. It is based on a Fourier–Galerkin approximation of the equation. Generalizations of the method and spectral accuracy have been given in [43, 44]. This method, thanks to its generality, has been applied also to nonhomogeneous situations [24], to the Landau equation [22, 40], and to the case of granular gases [34, 23]. A related numerical strategy based on the direct use of the fast Fourier transform (FFT) has been developed in [5, 7].

The lack of discrete conservations in the spectral scheme (mass is preserved, whereas momentum and energy are approximated with spectral accuracy) is compensated by its higher accuracy and efficiency. In fact it has been shown that these spectral schemes permit us to obtain spectrally accurate solutions with a reduction of the computational cost strictly related to the particular structure of the collision operator. A reduction from $O(N^2)$ to $O(N \log_2 N)$ is readily deducible for the Landau equation, whereas in the Boltzmann case such a reduction had been obtained until now only at the price of poor accuracy (in particular the loss of the spectral accuracy); see [5, 7].

Finally we mention that spectral methods have been successfully applied also to the study of *noncutoff* Boltzmann equations, like for RGD in the grazing collision limit [41] and for granular flows in the quasi-elastic limit [34]. In particular, during these asymptotic processes it is possible to obtain intermediate approximations that can be evaluated with fast algorithms which bring the overall computational cost to $O(N \log_2 N)$. This idea has been used in [39] to obtain fast approximated algorithms for the Boltzmann equation.

For a recent introduction to numerical methods for the Boltzmann equation and related kinetic equations we refer the reader to [19].

In this paper we shall focus on the two main questions in the approximation of the Boltzmann equation by deterministic schemes; that is the computational complexity and the accuracy of the numerical schemes for computing the collision operator Q.

Let us mention that a major problem associated with deterministic methods that use a fixed discretization in the velocity domain is that the velocity space is approximated by a finite region. Physically the domain for the velocity is $\mathbb{R}^d$. But, as soon as $d \geq 2$, the property of having compact support is not conserved by the collision operator (in fact for some Boltzmann models in dimension $d = 1$, like granular models, the support is conserved [34]). In general the collision process "spreads" the support by a factor $\sqrt{2}$ (see [46, 31]). As a consequence, for the continuous equation in time, the function f is immediately positive in the whole velocity domain $\mathbb{R}^d$.

Thus at the numerical level some nonphysical condition has to be imposed to keep the support of the function at velocity uniformly bounded. In order to do this there are two main strategies, which we shall make more precise later in this paper.

(1) One can remove the physical binary collisions that will lead outside the bounded velocity domain, which means a possible increase of the number of local invariants. If this is done properly (i.e., "without removing too many collisions"), the scheme remains conservative (and without spurious invariants). However, this truncation breaks down the convolution-like structure of the collision operator, which requires the invariance in velocity. Indeed the modified collision kernel depends on v through the boundary

conditions. This truncation is the starting point of most schemes based on discrete velocity models in a bounded domain.

(2) One can add some nonphysical binary collisions by periodizing the function and the collision operator. This implies the loss of some local invariants (some nonphysical collisions are added). Thus the scheme is not conservative anymore, except for the mass if the periodization is done carefully (and possibly the momentum if some symmetry properties are satisfied by the function). In this way the structural properties of the collision operator are maintained and thus they can be exploited to derive fast algorithms. This periodization is the basis of the spectral method.

Note that in both cases by enlarging the computational domain enough the number of removed or added collisions can be made negligible (as it is usually done for removing the aliasing error of the FFT; see, e.g., [11]) as well as the error in the local invariants.

In this paper we shall focus on the second approach, which means that the schemes have to deal with some aliasing error introduced by the periodization. In this way for a particular class of interactions, using a Carleman-like representation of the collision operator, we are able to derive spectral methods that can be evaluated through fast algorithms. The class of interactions includes *Maxwellian molecules* in dimension two and *hard spheres* molecules in dimension three.

The rest of the paper is organized in the following way. In Section 2 we introduce a Carleman-like representation of the collision operator which is used as a starting point for the development of our methods. After the derivation of the schemes the details of the fast spectral algorithm together with its accuracy properties are given in Section 3. In a separate Appendix we show a possible way to extend the present fast schemes to general collision interactions.

2. CARLEMAN-LIKE REPRESENTATION AND APPROXIMATION OF THE COLLISION OPERATOR

In this section we shall approximate the collision operator starting from a representation which somehow conserves more symmetries of the collision operator when one truncates it in a bounded domain. This representation was used in [5, 7, 8, 28] and it is close to the classical Carleman representation (cf. [12]). Also the kind of periodization inspired from this representation was implicitly used in [7].

2.1. **The Boltzmann collision operator in bounded domains.** The basic identity we shall need is

$$(2.1) \qquad \frac{1}{2} \int_{\mathbb{S}^{d-1}} F(|u|\sigma - u) \, d\sigma = \frac{1}{|u|^{d-2}} \int_{\mathbb{R}^d} \delta(2\, x \cdot u + |x|^2) \, F(x) \, dx,$$

and can be verified easily by completing the square in the delta Dirac function, taking the spherical coordinate $x = r\, \sigma$ and performing the change of variable $r^2 = s$.

Setting $u = v - v_*$, we can write the collision operator in the form

$$Q(f,f)(v) = \int_{v_* \in \mathbb{R}^d} \left\{ \int_{\sigma \in \mathbb{S}^{d-1}} B(|u|, \cos\theta) \right.$$
$$\left. \left[f\left(v_* - \frac{|u|\sigma - u}{2}\right) f\left(v + \frac{|u|\sigma - u}{2}\right) - f(v_*) f(v) \right] d\sigma \right\} dv_*,$$

and thus equation (2.1) yields

$$Q(f,f)(v) = 2 \int_{v_* \in \mathbb{R}^d} \left\{ \int_{x \in \mathbb{R}^d} B\left(|u|, \frac{x \cdot u}{|x||u|}\right) \frac{1}{|u|^{d-2}} \delta(2\,x \cdot u + |x|^2) \right.$$
$$\left. \left[f(v_* - x/2)\, f(v + x/2) - f(v_*)\, f(v) \right] dx \right\} dv_*.$$

Now let us make the change of variable $x \to x/2$ in x to get

$$Q(f,f)(v) = 2^{d+1} \int_{v_* \in \mathbb{R}^d} \int_{x \in \mathbb{R}^d} B\left(|u|, \frac{x \cdot u}{|x||u|}\right) \frac{1}{|u|^{d-2}} \delta(4\,x \cdot u + 4|x|^2)$$
$$[f(v_* - x)\, f(v + x) - f(v_*)\, f(v)]\, dx\, dv_*.$$

Then setting $y = v_* - v - x$ in v_*, we obtain

$$Q(f,f)(v) = 2^{d+1} \int_{y \in \mathbb{R}^d} \int_{x \in \mathbb{R}^d} B\left(|u|, \frac{x \cdot u}{|x||u|}\right) \frac{1}{|u|^{d-2}} \delta(-4x \cdot y)$$
$$[f(v + y)\, f(v + x) - f(v + x + y)\, f(v)]\, dx\, dy,$$

where now $u = -(x + y)$. Thus in the end we have

$$Q(f,f)(v) = 2^{d-1} \int_{x \in \mathbb{R}^d} \int_{y \in \mathbb{R}^d} B\left(|x + y|, -\frac{x \cdot (x + y)}{|x||x + y|}\right) \frac{1}{|x + y|^{d-2}}$$
$$\delta(x \cdot y)\, [f(v + y)\, f(v + x) - f(v + x + y)\, f(v)]\, dx\, dy.$$

Figure 1 sums up the different geometrical quantities of the usual representation and the one we derived from the Carleman-like representation.
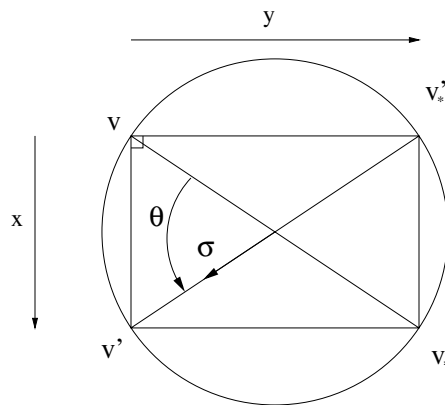

FIGURE 1. Geometry of the collision $(v, v_*) \leftrightarrow (v', v'_*)$.

Now let us consider the bounded domain $\mathcal{D}_T = [-T, T]^d$ $(0 < T < +\infty)$. There are two possibilities of truncation to reduce the collision process in a box. From now on let us write

$$\tilde{B}(x, y) = 2^{d-1} B\left(|x+y|, -\frac{x \cdot (x+y)}{|x||x+y|}\right) |x+y|^{-(d-2)}.$$

One can easily see that on the manifold defined by $x \cdot y = 0$, a simpler formula (using the parities of the collision kernel) is

(2.2)

$$\tilde{B}(x, y) = \tilde{B}(|x|, |y|) = 2^{d-1} B\left(\sqrt{|x|^2 + |y|^2}, \frac{|x|}{\sqrt{|x|^2 + |y|^2}}\right) (|x|^2 + |y|^2)^{-\frac{d-2}{2}}.$$

First one can remove the collisions connecting with some points out of the box. This is the natural preliminary stage for deriving conservative schemes based on the discretization of the velocity. In this case there is no need for a truncation on the modulus of x and y since we impose them to stay in the box. It yields

$$Q^{\mathrm{tr}}(f, f)(v) = \int \int_{\left\{x,\, y \in \mathbb{R}^d \ \mid\ v+x,\, v+y,\, v+x+y \in \mathcal{D}_T\right\}} \tilde{B}(x, y)\, \delta(x \cdot y)$$
$$[f(v+y)\, f(v+x) - f(v+x+y)\, f(v)]\, dx\, dy$$

defined for $v \in \mathcal{D}_T$. One can easily check that the following weak form is satisfied by this operator

(2.3)

$$\int Q^{\mathrm{tr}}(f, f)\, \varphi(v)\, dv = \frac{1}{4} \int \int \int_{\left\{v,\, x,\, y \in \mathbb{R}^d \ \mid\ v,\, v+x,\, v+y,\, v+x+y \in \mathcal{D}_T\right\}} \tilde{B}(x, y)\, \delta(x \cdot y)$$
$$f(v+x+y)\, f(v)\, [\varphi(v+y) + \varphi(v+x) - \varphi(v+x+y) - \varphi(v)]\, dv\, dx\, dy,$$

and this implies conservation of mass, momentum, and energy as well as the H theorem on entropy. Note that at this level this formulation gives no advantage with respect to the usual one obtained from (1.1) by restricting $v, v_*, v', v_*' \in \mathcal{D}_T$ (except that consistency results for discrete velocity models seem easier to prove when they are derived by quadrature on this formulation; see [38]). The problem of this truncation on a bounded domain is the fact that we have changed the collision kernel itself by adding some artificial dependence on v, v_*, v', v_*'. In this way convolution-like properties are broken.

A different approach consists in periodizing the function f on the domain $\mathcal{D}_T$. This amounts in adding some nonphysical collisions by connecting some points in the domain $\mathcal{D}_T$ which are geometrically included in a collision circle "modulo $2T$" (i.e., up to a translation of $2T$ of certain points in certain directions). Here we have to truncate the integration in x and y since periodization would yield infinite results 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 $R = 2S$ in order to obtain all possible collisions. Then a geometrical argument (see [43]) shows that by using the periodicity of the function it is enough to take $T \geq (1 + 3\sqrt{2})S/2$ to prevent intersections of the regions where f is different from zero. Note that here this so-called dealiasing condition is slightly worse from the one in [43], since the truncation on the modulus of x and y in the ball $\mathcal{B}_R$ implies only a truncation in the ball $\mathcal{B}_{\sqrt{2}R}$ for the relative velocity.

The operator now reads

$$(2.4) \quad Q^R(f,f)(v) = \int_{x \in \mathcal{B}_R} \int_{y \in \mathcal{B}_R} \tilde{B}(x,y)\,\delta(x \cdot y)$$
$$[f(v+y)f(v+x) - f(v+x+y)f(v)]\,dx\,dy$$

for $v \in \mathcal{D}_T$ (the expression for $v \in \mathbb{R}^d$ is deduced by periodization). The interest of this representation is to preserve the real collision kernel and its properties.

By making some translation changes of variable on v (by x, y and $x+y$), using the changes $x \to -x$ and $y \to -y$, and the fact that

$$\tilde{B}(-x,y)\,\delta(-x \cdot y) = \tilde{B}(x,y)\,\delta(x \cdot y) = \tilde{B}(x,-y)\,\delta(x \cdot -y),$$

one can easily prove that for any function φ *periodic* on $\mathcal{D}_T$ the following weak form is satisfied:

$$(2.5) \quad \int_{\mathcal{D}_T} Q^R(f,f)\,\varphi(v)\,dv = \frac{1}{4} \int_{v \in \mathcal{D}_T} \int_{x \in \mathcal{B}_R} \int_{y \in \mathcal{B}_R} \tilde{B}(x,y)\,\delta(x \cdot y)$$
$$f(v+x+y)f(v)\,[\varphi(v+y) + \varphi(v+x) - \varphi(v+x+y) - \varphi(v)]\,dv\,dx\,dy.$$

About the conservation properties one can show the following.

(1) The only invariant φ is 1: it is the only periodic function on $\mathcal{D}_T$ such that

$$\varphi(v+y) + \varphi(v+x) - \varphi(v+x+y) - \varphi(v) = 0$$

for any $v \in \mathcal{D}_T$ and $x \perp y \in \mathcal{B}_R$ (see [13] for instance). It means that the mass is locally conserved but not necessarily the momentum and energy.

(2) When f is even there is *global* conservation of momentum, which is 0 in this case. Indeed Q^R preserves the parity property of the solution, which can be checked using the change of variable $x \to -x$, $y \to -y$.

(3) The collision operator satisfies formally the H theorem

$$\int_{\mathbb{R}^d} Q^R(f,f) \log(f)\,dv \le 0.$$

(4) If f has compact support included in $\mathcal{B}_S$, and we have $R = 2S$ and $T \ge (3\sqrt{2}+1)S/2$ (no aliasing condition, see [43] for a detailed discussion), then no unphysical collisions occur, and thus mass, momentum, and energy are preserved. Obviously this compactness is not preserved with time since the collision operator spreads the support of f by a factor $\sqrt{2}$.

To sum up, one could say that the lack of conservation originates from the fact that the geometry of the collision does not respect the periodization.

Finally we give the Cauchy theorems for the homogeneous Boltzmann equations in $\mathcal{D}_T$ computed with Q^{tr} or Q^R.

Theorem 2.1. *Let $f_0 \in L^1(\mathcal{D}_T)$ be a nonnegative function. Then there exists a unique solution $f \in C^1(\mathbb{R}_+, L^1(\mathcal{D}_T))$ to the Cauchy problems*

$$(2.6) \qquad \frac{\partial f}{\partial t} = Q^{\mathrm{tr}}(f,f), \quad f(t=0,\cdot) = f_0,$$

$$(2.7) \qquad \frac{\partial f}{\partial t} = Q^R(f,f), \quad f(t=0,\cdot) = f_0,$$

which is nonnegative and has constant mass (and so constant L^1 norm). If f_0 has finite entropy, the entropy is finite and nondecreasing for all time. Moreover

in the case of (2.6), *if f_0 has finite momentum (respectively energy) on $\mathcal{D}_T$, the momentum (respectively energy) is conserved with time.*

Remark. When the initial data f_0 is nonnegative and has finite mass and entropy, it is possible to show by the Dunford-Pettis compactness theorem that the solution f converges weakly in $L^1(\mathcal{D}_T)$, as t goes to infinity, to the unique maximum of the entropy functional compatible with the conservation law(s) (and the periodicity in the case (2.7)). In the case (2.6) this equilibrium state is a sort of truncated Maxwellian on $\mathcal{D}_T$ defined by the conservation laws (see [13]). In the case (2.7) this equilibrium state is a constant defined by the mass of the initial data, which is due to the effect of aliasing in the very long-time. We omit the proof for brevity.

Proof of Theorem 2.1. For clarity we briefly sketch the main lines of the proof. The existence and uniqueness are proved by the method of Arkeryd for bounded collision kernels; see [1, Part I, Proposition 1.1]. In our case the collision kernel is bounded because of the boundedness of the domain. The only a priori estimate required in [1, Part I, Proposition 1.1] is the mass conservation, valid for the two equations under consideration. This method is based on a monotonicity argument to prove propagation of the sign of the solution. The argument relies on a splitting of the collision operator Q into a gain part Q^+ which is monotonic (i.e., $Q^+(f, f)$ is nonnegative when f is nonnegative), and a loss part Q^- which writes $Q^-(f, f) = L(f)f$ with L is a linear operator such that $\|L(f)\|_\infty \leq C \|f\|_{L^1}$. One can check easily that this splitting is still valid for the two collision operators Q^{tr} and Q^R. For brevity we omit the details and refer to the article [1]. The conservation law(s) and the H theorem are deduced from the weak forms (2.3) and (2.5) (see the proof of [1, Part I, Proposition 1.2] and [1, Part I, Theorem 2.1]).   □

2.2. **Application to spectral methods.** In this section we use the representation Q^R to derive new spectral methods. The spectral methods for kinetic equations originated in [42] and [43], and were further developed in [44] and [24]. Before they had a long history in fluid mechanics; see [11].

The main change compared to the usual spectral method is in the way we truncate the collision operator. In fact as we shall see in the next section this yields better decoupling properties between the arguments of the operator.

To simplify notation, 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

$$\begin{cases} f_N(v) = \displaystyle\sum_{k=-N}^{N} \hat{f}_k e^{ik \cdot v}, \\ \hat{f}_k = \dfrac{1}{(2\pi)^d} \displaystyle\int_{\mathcal{D}_\pi} f(v) e^{-ik \cdot v} \, dv. \end{cases}$$

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

$$(2.8) \qquad \hat{f}'_k(t) = \sum_{\substack{l,m=-N \\ l+m=k}}^{N} \hat{\beta}(l,m)\, \hat{f}_l\, \hat{f}_m, \quad k = -N, \dots, N,$$

where $\hat{\beta}(l,m)$ are the so-called *kernel modes*, given by

$$\hat{\beta}(l,m) = \int_{x\in\mathcal{B}_R} \int_{y\in\mathcal{B}_R} \tilde{B}(x,y)\, \delta(x\cdot y) \left[e^{il\cdot x}\, e^{im\cdot y} - e^{im\cdot(x+y)} \right]\, dx\, dy.$$

The kernel modes can be written as

$$\hat{\beta}(l,m) = \beta(l,m) - \beta(m,m),$$

where

$$\beta(l,m) = \int_{x\in\mathcal{B}_R} \int_{y\in\mathcal{B}_R} \tilde{B}(x,y)\, \delta(x\cdot y)\, e^{il\cdot x}\, e^{im\cdot y}\, dx\, dy.$$

Therefore, later in this paper 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 function starts from the representation (see [43])

$$(2.9) \quad Q(f,f) = \int_{u\in\mathbb{R}^d} \int_{\sigma\in\mathbb{S}^{d-1}} B(|u|,\cos\theta)$$
$$\left[f\big(v - (u - |u|\sigma)/2\big) f\big(v - (u + |u|\sigma)/2\big) - f(v)f(v-u) \right] d\sigma\, du,$$

and then truncates the parameter $u = x + y$ in order that $u \in \mathcal{B}_R$. Thus we have

$$Q_{\text{usual}}^R(f,f)(v) = \int_{x\in\mathbb{R}^d} \int_{y\in\mathbb{R}^d} \tilde{B}(x,y)\, \delta(x\cdot y)\, \chi_{\{|x+y|\le R\}}$$
$$[f(v+y)f(v+x) - f(v+x+y)f(v)]\, dx\, dy,$$

where $\chi_{\{|x+y|\le R\}}$ denotes the characteristic function of the set $\{|x+y| \le R\}$. One can notice that here x and y are also restricted to the ball $\mathcal{B}_R$ but the condition $|x+y|^2 = |x|^2 + |y|^2 \le R^2$ couples the two modulus, such that the ball is not completely covered (for instance, if x and y both have modulus R, the condition is not satisfied, since $|x+y| = \sqrt{2}R$).

Finally let us compare the new kernel modes with the usual ones. As a consequence of representation (2.9), the usual kernel modes (cf. [43]) are

$$\hat{\beta}_{\text{usual}}(l,m) = \int_{u\in\mathcal{B}_R} \int_{\sigma\in\mathbb{S}^{d-1}} B(|u|,\cos\theta) \left[e^{-i\frac{u\cdot(l+m)+|u|\sigma\cdot(m-l)}{2}} - e^{-i(u\cdot m)} \right] d\sigma\, du,$$

and hence coming back to the representation in x and y,

$$\hat{\beta}_{\text{usual}}(l,m) = \int_{x\in\mathcal{B}_R} \int_{y\in\mathcal{B}_R} \tilde{B}(x,y)\, \delta(x\cdot y)\, \chi_{\{|x+y|\le R\}} \left[e^{il\cdot x}\, e^{im\cdot y} - e^{im\cdot(x+y)} \right] dx\, dy.$$

Thus the usual representation contains more coupling between x and y and it is less appropriate for the construction of fast algorithms.

3. Fast spectral algorithm for a class of collision kernels

As soon as one is searching for fast deterministic algorithms for the collision operator, i.e., algorithms with a cost lower than $O(N^{2d+\varepsilon})$ (which is the cost of a usual discrete velocity model, with typically $\varepsilon = 1$), one has to find some way to compute the collision operator *without going through all the couples of collision points* during the computation. This leads naturally to search for some convolution structure (discrete or continuous) in the operator. Unfortunately, as discussed in the previous sections, this is rather contradictory with the search for a conservative scheme in a bounded domain, since the boundary condition needed to prevent the outgoing or ingoing collisions breaks the invariance. Thus fast algorithms seem more adapted to spectral methods, or more in general to methods where the invariance is conserved thanks to the periodization.

Here we search for a convolution structure in equation (2.8). The aim is to approximate each $\hat{\beta}(l, m)$ by the sum

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

This gives the 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 [11, 16]. Obviously this is equivalent to obtaining such a decomposition on β. To this purpose we shall use a further approximated collision operator where the number of possible directions of a collision is reduced to a finite set.

The starting point of our study is an idea of [7]: use the Carleman-like representation (2.4) to obtain a convolution structure for every fixed direction of the vectors x and y. In [7] the corresponding set of directions

$$S = \left\{ (e, e') \in \mathbb{S}^{N-1} \times \mathbb{S}^{N-1} \mid e \perp e' \right\}$$

is very difficult to discretize in a way that preserves the symmetry properties of the collision operator. No systematic process is available, and the discretization is done only for some particular number of grid points. Then the FFT is used in each couple of directions and finally a correction is imposed at the end to preserve the conservation laws. However no consistency result is available and the accuracy suggested by the numerical simulation is of order 1. The two main new ingredients of our method follow.

- First we project the collision operator on the Fourier basis. This enables us to integrate one of the two coordinates of the manifold S and to reduce the discretization of the sphere $\mathbb{S}^{N-1}$. This discretization is straightforward and can be made easily to preserve the symmetries of the collision operator. Moreover it reduces the complexity of the algorithm by suppressing $N - 2$ degrees of freedom to discretize.
- Second we choose to discretize $\mathbb{S}^{N-1}$ by the rectangular rule. Indeed the periodization shall imply that this quadrature rule is of infinite order. This point will allow us to obtain a spectrally accurate scheme and adaptativity properties.

3.1. **A semi-discrete collision operator.** We write x and y in spherical coordinates

$$Q^R(f,f)(v) = \frac{1}{4} \int_{e \in \mathbb{S}^{d-1}} \int_{e' \in \mathbb{S}^{d-1}} \delta(e \cdot e') \, de \, de'$$

(3.1)
$$\left\{ \int_{-R}^{R} \int_{-R}^{R} \rho^{d-2} \, (\rho')^{d-2} \, \tilde{B}(\rho, \rho') \right.$$

$$\left. \big[f(v+\rho'e')f(v+\rho e) - f(v+\rho e + \rho'e')f(v) \big] \, d\rho \, d\rho' \right\}.$$

Let us take $\mathcal{A}$ a set of orthogonal couples of unit vectors (e, e'), which is even: $(e, e') \in \mathcal{A}$ 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

$$Q^{R,\mathcal{A}}(f,f)(v) = \frac{1}{4} \int_{(e,e') \in \mathcal{A}}$$

$$\left\{ \int_{-R}^{R} \int_{-R}^{R} \rho^{d-2} \, (\rho')^{d-2} \, \tilde{B}(\rho, \rho') \right.$$

$$\left. \big[f(v+\rho'e')f(v+\rho e) - f(v+\rho e + \rho'e')f(v) \big] \, d\rho \, d\rho' \right\} d\mathcal{A},$$

where $d\mathcal{A}$ denotes a measure on $\mathcal{A}$ which is also even in the sense that $d\mathcal{A}(e, e') = d\mathcal{A}(-e, e') = d\mathcal{A}(e, -e') = d\mathcal{A}(-e, -e')$. Using translation changes of variable on v by ρe, $\rho'e'$, and $\rho e + \rho'e'$ and the symmetries of the set $\mathcal{A}$, one can easily derive the following weak form on $Q^{R,\mathcal{A}}$. For any function φ *periodic* on $\mathcal{D}_T$,

$$\int_{\mathcal{D}_T} Q^{R,\mathcal{A}}(f,f)\, \varphi(v) \, dv = \frac{1}{16} \int_{v \in \mathcal{D}_T} \int_{(e,e') \in \mathcal{A}} \int_{-R}^{R} \int_{-R}^{R} \rho^{d-2} \, (\rho')^{d-2} \, \tilde{B}(\rho, \rho')$$

$$f(v+\rho e + \rho'e')f(v) \big[\varphi(v+\rho'e') + \varphi(v+\rho e) - \varphi(v+\rho e + \rho'e') - \varphi(v) \big] \, d\rho \, d\rho' \, d\mathcal{A} \, dv.$$

This immediately gives the same conservation properties as Q^R. Of course one could also prove exactly as for Q^R:

Theorem 3.1. *Let $f_0 \in L^1(\mathcal{D}_T)$ be a nonnegative function. Then there exists a unique solution $f \in C^1(\mathbb{R}_+, L^1(\mathcal{D}_T))$ to the Cauchy problem*

$$\frac{\partial f}{\partial t} = Q^{R,\mathcal{A}}(f,f), \quad f(t=0, \cdot) = f_0,$$

which is nonnegative and has constant mass (and so constant L^1 norm). Moreover, if f_0 has finite entropy, the entropy is nondecreasing with time.

3.2. **Expansion of the kernel modes.** We make the *decoupling assumption* that

(3.2)
$$\tilde{B}(x, y) = a(|x|) \, b(|y|).$$

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 the Appendix.

First let us deal with dimension two with $\tilde{B} = 1$ to explain the method. Here we write x and y in spherical coordinates $x = \rho e$ and $y = \rho' e'$ to get

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

Let us denote

$$\phi_R^2(s) = \int_{-R}^{R} e^{i\rho s} \, d\rho,$$

for $s \in \mathbb{R}$. It is easy to see that ϕ_R^2 is even and we can give the explicit formula

$$\phi_R^2(s) = 2 \, R \, \mathrm{Sinc}(Rs)$$

with $\mathrm{Sinc}(\theta) = (\sin \theta)/\theta$.

Thus we have

$$\beta(l, m) = \frac{1}{4} \int_{e \in \mathbb{S}^1} \int_{e' \in \mathbb{S}^1} \delta(e \cdot e') \, \phi_R^2(l \cdot e) \, \phi_R^2(m \cdot e') \, de \, de',$$

and thanks to the parity property of ϕ_R^2 we can adopt the periodic parametrization

$$\beta(l, m) = \int_0^\pi \phi_R^2(l \cdot e_\theta) \, \phi_R^2(m \cdot e_{\theta + \pi/2}) \, d\theta.$$

The function $\theta \to \phi_R^2(l \cdot e_\theta) \, \phi_R^2(m \cdot e_{\theta + \pi/2})$ is periodic on $[0, \pi]$ and thus the rectangular quadrature rule is of infinite order and optimal. A regular discretization of M equally spaced points thus gives

$$\beta(l, m) = \frac{\pi}{M} \sum_{p=0}^{M-1} \alpha_p(l) \alpha'_p(m)$$

with

$$\alpha_p(l) = \phi_R^2(l \cdot e_{\theta_p}), \qquad \alpha'_p(m) = \phi_R^2(m \cdot e_{\theta_p + \pi/2}),$$

and $\theta_p = \pi p/M$.

More generally under the decoupling assumption (3.2) on $\tilde{B}$, we get the decomposition formula

$$\beta(l, m) = \frac{\pi}{M} \sum_{p=0}^{M-1} \alpha_p(l) \alpha'_p(m),$$

where

$$\alpha_p(l) = \phi_{R,a}^2(l \cdot e_{\theta_p}), \qquad \alpha'_p(m) = \phi_{R,b}^2(m \cdot e_{\theta_p + \pi/2})$$

and

$$\phi_{R,a}^2(s) = \int_{-R}^{R} a(\rho) \, e^{i\rho s} \, d\rho, \qquad \phi_{R,b}^2(s) = \int_{-R}^{R} b(\rho') \, e^{i\rho' s} \, d\rho'$$

with $\theta_p = \pi p/M$.

Remark. In the symmetric case $a = b$ (for instance for hard spheres) it is possible to parametrize $\beta(l, m)$ as

$$\beta(l, m) = 2 \int_0^{\pi/2} \phi_{R,a}^2(l \cdot e_\theta) \, \phi_{R,a}^2(m \cdot e_{\theta + \pi/2}) \, d\theta,$$

and the function $\theta \to \phi_{R,a}^2(l \cdot e_\theta) \, \phi_{R,a}^2(m \cdot e_{\theta + \pi/2})$ is periodic on $[0, \pi/2]$. Thus the decomposition can be obtained by applying the rectangular rule on this interval. At the numerical level it yields a reduction of the cost by a factor 2.

Now let us deal with dimension $d = 3$ with $\tilde{B}$ satisfying the decoupling assumption (3.2). First we change to the 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 $e^{\perp}$,

$$\beta(l, m) = \frac{1}{4} \int_{e \in \mathbb{S}^2} \phi_{R,a}^3(l \cdot e) \left[\int_{e' \in \mathbb{S}^2 \cap e^{\perp}} \phi_{R,b}^3(m \cdot e')\, de' \right]\, de,$$

where

$$\phi_{R,a}^3(s) = \int_{-R}^{R} |\rho|\, a(\rho)\, e^{i\rho s}\, d\rho, \qquad \phi_{R,b}^3(s) = \int_{-R}^{R} |\rho|\, b(\rho)\, e^{i\rho s}\, d\rho.$$

Thus we get the following decoupling formula with two degrees of freedom

$$\beta(l, m) = \int_{e \in \mathbb{S}_+^2} \phi_{R,a}^3(l \cdot e)\, \psi_{R,b}^3\big(\Pi_{e^{\perp}}(m) \big)\, de,$$

where $\mathbb{S}_+^2$ denotes the half-sphere and

$$\psi_{R,b}^3\big(\Pi_{e^{\perp}}(m) \big) = \int_0^{\pi} \phi_{R,b}^3\big(|\Pi_{e^{\perp}}(m)| \cos\theta \big)\, d\theta$$

(this formula can be derived performing the change of variable $de' = \sin\theta\, d\theta\, d\varphi$ with the basis $(e, u = \Pi_{e^{\perp}}(m)/|\Pi_{e^{\perp}}(m)|, e \times u)$).

Again in the particular case where $\tilde{B} = 1$ (hard spheres model), we can compute explicitly the functions ϕ_R^3 (in this case $a = b = 1$),

$$\phi_R^3(s) = R^2 \left[2\mathrm{Sinc}(Rs) - \mathrm{Sinc}^2(Rs/2) \right].$$

Now the function $e \to \phi_{R,a}^3(l \cdot e)\, \psi_{R,b}^3\big(\Pi_{e^{\perp}}(m) \big)$ is periodic on $\mathbb{S}_+^2$ and so the rectangular rule is of infinite order and optimal. Taking a spherical parametrization (θ, φ) of $e \in \mathbb{S}_+^2$ and uniform grids of respective size M_1 and M_2 for θ and φ we get

$$\beta(l, m) = \frac{\pi^2}{M_1 M_2} \sum_{p,q=0}^{M_1, M_2} \alpha_{p,q}(l) \alpha_{p,q}'(m),$$

where

$$\alpha_{p,q}(l) = \phi_{R,a}^3\big(l \cdot e_{(\theta_p, \varphi_q)} \big), \qquad \alpha_{p,q}'(m) = \psi_{R,b}^3\Big(\Pi_{e_{(\theta_p, \varphi_q)}^{\perp}}(m) \Big)$$

and

$$(\theta_p, \varphi_q) = \left(\frac{p\,\pi}{M_1}, \frac{q\,\pi}{M_2} \right).$$

From now on we shall consider this expansion with $M = M_1 = M_2$ to avoid anisotropy in the computational grid.

Remarks. 1. It is possible to give more general exact formulas in dimension two and three when $a(r) = |r|^t$, $b(r) = |r|^{t'}$ with $t, t' \in \mathbb{N}$ by computing derivatives along s of the two quantities

$$\int_0^R \sin(\rho s)\, d\rho, \qquad \int_0^R \cos(\rho s)\, d\rho.$$

2. For any dimension, we can construct as above an approximated collision operator $Q^{R,\mathcal{A}_M}$ with

$$\mathcal{A}_M = \left\{(e, e') \in \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \mid e \in \mathbb{S}^{d-1}_{M,+}, \ e' \in e^\perp \cap \mathbb{S}^{d-1}\right\},$$

where $\mathbb{S}^{d-1}_{M,+}$ denotes a uniform angular discretization of the half sphere with M points in each angular coordinate (the other half sphere is obtained by parity). Let us remark that this discretization contains exactly M^{d-1} points. From now on we shall denote

$$Q^{R,M} = Q^{R,\mathcal{A}_M} = \sum_{p=1}^{M^{d-1}} Q_p^{R,M}.$$

3.3. **Spectral accuracy.** In this paragraph we are interested in computing the accuracy of the scheme according to the three parameters N (the number of modes), R (the truncation parameter), and M (the number of angular directions for each angular coordinate). Instead of looking at the error on each kernel mode it is more convenient to look at the error on the global operator. Here the Lebesgue spaces L^p, $p = 1, \cdots, +\infty$, and the periodic Sobolev spaces H_p^k, $k = 0, \cdots, +\infty$ refer to $\mathcal{D}_\pi$.

In order to give a consistency result, the first step will be to prove a consistency result for the approximation of Q^R by $Q^{R,M}$.

Lemma 3.2. *The error on the approximation of the collision operator is spectrally small, i.e., for all $k > d-1$ such that $f \in H_p^k$,*

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

Proof of Lemma 3.2. Starting from (3.1), one gets

$$Q^R(g,f)(v) = \frac{1}{2} \int_{e \in \mathbb{S}^{d-1}_+} \left[\int_{e' \in \mathbb{S}^{d-1} \cap e^\perp} \int_{-R}^{R} \int_{-R}^{R} \rho^{d-2} (\rho')^{d-2} \tilde{B}(\rho, \rho') \right.$$

$$\left. [g(v + \rho'e')f(v + \rho e) - g(v + \rho e + \rho'e')f(v)] \, d\rho \, d\rho' \, de' \right] de.$$

As the function in the brackets is a periodic function of e on $\mathbb{S}^{d-1}_+$ with period π in each coordinate, one can apply the error estimate for the rectangular rule (see, e.g., [48, Theorem 19.10]). This error estimate is valid for $k > d-1$ and depends on the derivative along e of this functional in the following way:

$$\|Q^R(g,f) - Q^{R,M}(g,f)\|_{L^2}$$

$$\leq \frac{C}{2^k M^k}$$

$$\sum_{i=1}^{d-1} \left\| \int_{e \in \mathbb{S}^{d-1}_+} \left| \partial_{e_i}^k \int_{e' \in \mathbb{S}^{d-1} \cap e^\perp} \int_{-R}^{R} \int_{-R}^{R} \rho^{d-2} (\rho')^{d-2} \right.\right.$$

$$\left.\left. \tilde{B}(\rho, \rho') \left[g(v+\rho'e')f(v+\rho e) - g(v+\rho e+\rho'e')f(v)\right] \, d\rho \, d\rho' \, de' \right| de \right\|_{L^2_v},$$

where the constant is independent on k and $\partial_{e_i}^k$ is the derivative of order k along the coordinate e_i. Then a straightforward computation gives

$$\|Q^R(g,f) - Q^{R,M}(g,f)\|_{L^2}$$

$$\leq \frac{CR^k}{2^k M^k} \sum_{i=1}^{d-1} \left[\sum_{k'+k''=k} \binom{k}{k'} \left(\|Q^{R,+}(|\partial^{k'}g|, |\partial^{k''}f|)\|_{L^2} + \|Q^{R,-}(|\partial^{k'}g|, |\partial^{k''}f|)\|_{L^2} \right) \right],$$

where $\partial^{k'}$ and $\partial^{k''}$ denote some derivatives of order k' and k''. Then using the estimates

$$\|Q^{R,+}(g,f),\ Q^{R,-}(g,f)\|_{L^2} \leq C \, \|g\|_{L^2} \|f\|_{L^2}$$

proved in [25],[1] we get

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

which concludes the proof. $\qquad\square$

For the second step we shall use the consistency result [43, Corollary 5.4] on the operator Q^R, which we quote here for the sake of clarity.

Lemma 3.3. *For all $k \in \mathbb{N}$ such that $f \in H_p^k$,*

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

Combining these two results, one gets the following consistency result.

Theorem 3.4. *For all $k > d-1$ such that $f \in H_p^k(\mathcal{D}_\pi)$,*

$$\|Q^R(f,f) - \mathcal{P}_N Q^{R,M}(f_N, f_N)\|_{L^2}$$

$$\leq C_1 \frac{R^k \|f_N\|_{H_p^k}^2}{M^k} + \frac{C_2}{N^k} \left(\|f\|_{H_p^k} + \|Q^R(f_N, f_N)\|_{H_p^k} \right).$$

Proof of Theorem 3.4. By triangular inequality

$$\|Q^R(f,f) - \mathcal{P}_N Q^{R,M}(f_N, f_N)\|_{L^2}$$

$$\leq \|\mathcal{P}_N \big(Q^R(f_N f_N) - Q^{R,M}(f_N, f_N) \big)\|_{L^2} + \|Q^R(f,f) - \mathcal{P}_N Q^R(f_N, f_N)\|_{L^2}.$$

The first term on the right-hand side is controlled by Lemma 3.2:

$$\|\mathcal{P}_N \big(Q^R(f_N, f_N) - Q^{R,M}(f_N, f_N) \big)\|_{L^2}$$

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

The second term in the right-hand side is controlled by Lemma 3.3, which concludes the proof. $\qquad\square$

Now 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. First with Lemma 3.2 at hand one can establish the estimate

$$\|Q^{R,M}(g,f)\|_{L^2} \leq C \, \|g\|_{H_p^d} \|f\|_{H_p^d},$$

---

[1]Which are consequences of the L^p estimates proved in [26, 27], and revisited in [33].

for a constant uniform in M. Then following the method of [43, Remark 5.4] and using this estimate, we obtain the following spectral accuracy result

$$
\begin{aligned}
\big|\langle Q^{R,M}(f,f),\varphi\rangle &- \langle \mathcal{P}_N Q^{R,M}(f_N,f_N),\varphi\rangle\big|_{L^2} \\
&\leq \frac{C_3}{N^k}\,\|\varphi\|_{L^2}\left(\|f\|_{H_p^{k+d}} + \|Q^{R,M}(f_N,f_N)\|_{H_p^k}\right),
\end{aligned}
$$

where φ can be replaced by $v, |v|^2$. Indeed there is no need to compare the momenta of $\mathcal{P}_N Q^{R,M}(f_N,f_N)$ with those of $Q^R(f,f)$ since $Q^{R,M}$ is also conservative, and so they can be compared directly to those of $Q^{R,M}$. Thus the error on momentum and energy is independent of M and is spectrally small according to N even for very small value of the parameter M.

3.4. **Implementation of the algorithm.** The final spectral scheme depends on the three parameters N, R, and M. The only condition on these parameters is the no-aliasing condition that relates R and the size of the box T (here π). A detailed study of the influence of the choices of N and R was done in [43]. Here we are interested only in the influence of M over the computations, since M controls the computations speed-up.

The method of the previous subsections yields a decomposition of the collision operator, which after projection on $\mathbb{P}^N$ gives the following decomposition

$$
(3.3) \qquad \mathcal{P}_N Q^{R,M} = \sum_{p=1}^{M^{d-1}} \mathcal{P}_N Q_p^{R,M}.
$$

Each $\mathcal{P}_N Q_p^{R,M}$ can be computed with a cost $O(N^d \log_2 N)$. Thus for a general choice of M and N we obtain the cost $O(M^{d-1}N^d \log_2 N)$. The decomposition (3.3) is completely parallelizable and thus the cost can be strongly reduced on a parallel machine (theoretically up to $O(N^d \log_2 N)$). One just has to make independent computations for the M^{d-1} terms of the decomposition.

Moreover the formula of decomposition is naturally adaptive (that is, the number M can be made space dependent), which can be quite useful in the inhomogeneous setting, where some regions deserve less accuracy than others. Since it relies on the rectangular formula, whose adaptivity property is well known, one can easily double the number of directions M if needed, without computing again those points already computed.

Finally the decomposition can be also interesting from the storage viewpoint, as the classical spectral method requires the storage of an $N^d \times N^d$ matrix whereas our method requires the storage of $2M^{d-1}$ vectors of size N^d. In dimension two the classical method requires a storage of order $O(N^4)$ and our method requires a storage of order $O(MN^2)$. In dimension three the classical method requires a storage of order $O(N^4)$ (thanks to the symmetries of the matrix of kernel modes, see [25]), and our method requires a storage of order $O(M^2 N^3)$.

As a numerical example we report the results obtained in the case of space homogeneous two-dimensional Maxwellian molecules using as a comparison the exact analytic solution (see [43]). The results for the relative L_1 norm of the error at time $t = 0.01$ are reported in Table 1.

Although further extensive testing is necessary, the results are very promising and seem to indicate a very low influence of the number of directions over the accuracy of the scheme. For $M = 2$ the angle error dominates, but as soon as

TABLE 1. Relative L_1 norm of the error for different values of N and M for the fast spectral method.

N	$M = 2$	$M = 4$	$M = 8$	$M = 16$
32	$2.129E - 4$	$1.993E - 05$	$2.153E - 05$	$2.262E - 5$
64	$2.109E - 4$	$7.122E - 10$	$6.830E - 10$	$6.843E - 10$
128	$2.112E - 4$	$3.116E - 12$	$3.117E - 12$	$3.117E - 12$

$M = 4$ the error in N is dominating. Note that the number of angle directions will indirectly influence the aliasing effect through the slight change in the relaxation times. This may explain the slight error variations that we observe taking $M \geq 4$.

Finally, in view of space nonhomogeneous computations, we will have the additional advantage of taking a larger number of gridpoints without increasing too much the computational cost, thus allowing the computations of flows at larger Mach number compared to conventional deterministic schemes. Further numerical results are under development and will be presented in [21].

4. CONCLUSIONS

We have presented a deterministic way for computing the Boltzmann collision operator with fast algorithms, for a class of interactions which includes the case of hard spheres in dimension three. The method is based on a Carleman-like representation of the operator that allows us to express it as a combination of convolutions (this is trivially true for the loss part but it is not trivial for the gain part). A suitable periodized truncation of the operator is then used to derive new spectral methods computable with a high speed up in computation times. This brings the overall cost in dimension d to $O(M^{d-1}N^d \log_2 N)$, where N is the number of velocity parameters and M the number of angular directions in each angular coordinate. Consistency and accuracy of the proposed schemes are also presented, and it is shown to be spectrally accurate. Moreover the error on the momentum and energy is spectrally small and independent of the value of the speed-up parameter M. The first numerical results seem to indicate the validity and flexibility of the present approach that, in our opinion, will make deterministic schemes much more competitive with Monte Carlo methods in several situations.

In a related work [32] we will extend the fast algorithms described here to the case of discrete velocity methods.

APPENDIX: REMARKS ON ADMISSIBLE COLLISION KERNELS AND AN EXTENSION TO THE "NONDECOUPLED" CASE

Let us study the cases where assumption (3.2) is satisfied. For hard spheres in dimension three, or Maxwellian molecules in dimension two, one has equation (3.2) with $a = b = 1$. Formally for the Coulomb potential in dimension three, we have

$$B(\theta, |u|) = |u|^{-3} \sin^{-4}(\theta/2),$$

and thus, thanks to formula (2.2)

$$\tilde{B}(x, y) = 2^{d-1} |x|^{-4}.$$

This suggests, in dimension three, that we consider the following family of "variable hard sphere" collision kernels

(0.4) $$B_\gamma(\theta, |u|) = \sin^{\gamma-1}(\theta/2) \, |u|^\gamma.$$

Indeed simple computations give

$$\tilde{B}_\gamma(x, y) = 2^{d-1} \, |x|^{\gamma-1},$$

and thus they satisfy the decoupling assumption (3.2). In the case where $\gamma \in (-1, 1]$, the angular part of the collision kernel remains integrable. On the contrary, for $\theta \sim 0$, the equivalent derived from the physical nonexplicit formula in [14] for inverse-power laws kernels (for a potential $1/|d|^{n-1}$ with n such that $\gamma = (n-5)/(n-1)$) is of the form

$$B_\gamma^{\mathrm{exact}}(\theta, |u|) \sim_{\theta \sim 0} \sin^{\frac{\gamma-5}{2}}(\theta/2) \, |u|^\gamma$$

with $\gamma \in [-3, 1)$. It is therefore always nonintegrable at $\theta \sim 0$.

The model (0.4) coincides with the hard spheres model for $\gamma = 1$ and, formally, coincides with the kernel of the Coulomb potential for $\gamma = -3$. Moreover for $\gamma \in (-1, 1]$ (i.e., for hard potentials and the so-called moderately soft potentials) it remains integrable for $\theta \sim 0$. Thus it seems quite reasonable to consider it to be a model for cutoff hard and moderately soft potentials, as well as hard spheres.

In dimension two the same arguments and computations lead to the following cutoff hard and moderately soft potentials model:

$$B_\gamma(\theta, |u|) = \sin^\gamma(\theta/2) \, |u|^\gamma,$$

valid for $\gamma \in (-1, 1]$, which coincides with the case of Maxwellian molecules for $\gamma = 0$.

For the spectral method the other situation where one obtains naturally a fast algorithm is the case where collisions concentrate on the grazing part; see [45] and [41] for a fast algorithm to compute the Fokker–Planck–Landau collision operator, which is the limit of the Boltzmann collision operator in the grazing collision limit. Indeed in this case one of the two variables x or y of the representation (2.4) disappears in the limit process, which "decouples" the kernel modes. Thus it may be possible to construct fast algorithms for noncutoff models by splitting the collision operator into a cutoff part treated by the method presented in this paper, and a noncutoff part restricted to very small deviation angles, which would be close to the grazing collision limit and thus could be computed by the fast algorithm of [45] and [41].

Acknowledgments

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UMPA, ENS Lyon, 46 allée d'Italie, 69364 Lyon Cedex 07, France
E-mail address: cmouhot@umpa.ens-lyon.fr

Dipartimento di Matematica, Università di Ferrara, Via Machiavelli 35, 44100 Ferrara, Italy
E-mail address: lorenzo.pareschi@unife.it