Numerical methods for kinetic equations

Lecture 4: Breaking complexity

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Lecture 4 Outline

1. Fast spectral methods
   - Carlemann-like representation
   - Fast algorithms
   - Consistency and spectral accuracy
   - Some remarks

2. Steady state preserving spectral methods
   - Long time behavior
   - Steady state preserving method

Carlemann-like representation

The computational cost of the method can be reduced to $O(n \log_2 n)$ using a different representation of the collision operator[1].
The basic identity we shall need in dimension $d = 2, 3$ is

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

Using the above identity the collision operator can be written as

Carlemann-like representation

$$Q(f,f)(v) = \int_{x,y \in \mathcal{B}_R} \tilde{B}(x,y)\delta(x \cdot y)\, [f(v+y)f(v+x) - f(v+x+y)f(v)]\, dxdy$$

with $\mathcal{B}_R = \mathcal{B}(0, 2\lambda\pi)$, $v \in [-\pi, \pi]^d$ and

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

Note that $\tilde{B}(x,y)$ is constant for Maxwell molecules ($B \equiv 1$) in dimension $d = 2$ and for hard spheres ($B \equiv |x+y|$) in dimension $d = 3$.

[1] C.Mouhot, L.Pareschi '05 - F.Filbet, C.Mouhot, L.Pareschi '06

Spectral methods

We can perform the same derivation as in the standard spectral method to obtain

$$\hat{Q}_k = \sum_{\substack{l,m=-N \\ l+m=k}}^{N} (\hat{B}(l,m) - \hat{B}(m,m))\, \hat{f}_l\, \hat{f}_m, \quad k = -N, ..., N$$

where now

New kernel modes

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

The conventional representation, in the new variables x and y, reads

$$\hat{B}(l,m) = \int_{x\in\mathcal{B}_R} \int_{y\in\mathcal{B}_R} \tilde{B}(x,y)\, \delta(x\cdot y)\, \chi_{\{|x+y|\leq R\}}\, e^{il\cdot x}\, e^{im\cdot y}\, dx\, dy.$$

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.

Fast algorithms

The search for fast deterministic algorithms consists mainly in identifying some convolution structure in the collision operator.
We make the assumption that

Decoupling assumption

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

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.
If we now change to spherical coordinates

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

Fast algorithms

In the case of hard spheres, after integrating e' on $\mathbb{S}^2 \cap e^\perp$ we get

$$\hat{B}(l,m) = \int_{e \in \mathbb{S}^2_+} \phi(l \cdot e)\, \psi\big(\Pi_{e^\perp}(m)\big)\, de$$

where $\mathbb{S}^2_+$ denotes the half-sphere, $\Pi_{e^\perp}$ is the orthogonal projection on $e^\perp$ and

$$\phi(s) = R^2\big(2\,\mathrm{Sinc}(Rs) - \mathrm{Sinc}^2(Rs/2)\big), \quad \psi(s) = \int_0^\pi \phi(s\cos\theta) d\theta.$$

Using spherical coordinates (θ, φ) and taking uniform grids of size M_1 and M_2 we get

Decoupled kernel modes

$$\hat{B}(l,m) \simeq \frac{\pi^2}{M_1 M_2} \sum_{p,q=0}^{M_1,M_2} \alpha_{p,q}(l)\alpha'_{p,q}(m)$$

Computational considerations

- Thanks to periodicity of the integrands the rectangular rule in (θ, φ) is also spectrally accurate.
- Taking $M = M_1 = M_2$ we obtain the computational cost

$$O(M^{d-1} n \log_2 n), \quad n = N^d.$$

The method is therefore faster then the classical if

$$M^{d-1} \log_2 n \ll n.$$

- The angular discretization does not affects the main physical properties of the Boltzmann equation.

Consistency and spectral accuracy

The spectral accuracy of the angular approximation is stated in the following

Lemma (Mouhot, Pareschi '05)

The error on the angular approximation of the collision operator is spectrally small, i.e. for all $r > d-1$ *such that* $f \in H^r_p$

$$\|Q(f,f) - Q^M(f,f)\|_2 \leq C_1 \frac{\|f\|^2_{H^r_p}}{M^r}.$$

Next we use the consistency result for the classical spectral method to obtain

Theorem

For all $r > d-1$ *such that* $f \in H^r_p$

$$\|Q(f,f) - Q^M_N(f_N,f_N)\|_2 \leq C_1 \frac{\|f_N\|^2_{H^r_p}}{M^r} + \frac{C_2}{N^r}\left(\|f\|_{H^r_p} + \|Q(f_N,f_N)\|_{H^r_p}\right).$$

Numerical examples

Test problems[2]:

Test#1 2D Maxwellian molecules: Exact solution

This test is used to check spectral accuracy, by comparing the error at a given time, when using $N = 8$, 16, and 32 Fourier modes for each dimension.

Test#2 3D VHS molecules: sum of two Gaussians

This test is used compare the relaxation to equilibrium of the stress tensor for Maxwellian molecules, with the relaxation of other VHS molecules.

Number of points	Classical spectral	Fast spectral with $M = 4$	Fast spectral with $M = 6$	Fast spectral with $M = 8$
16	2 $sec.$ 40	1 $sec.$ 15	1 $sec.$ 70	2 $sec.$ 30
32	38 $sec.$ 01	5 $sec.$ 55	8 $sec.$ 47	11 $sec.$ 10
64	616 $sec.$	35 $sec.$ 50	54 $sec.$ 66	71 $sec.$ 27

Comparison of the computational time in $2D$ between the classical spectral method and the fast spectral method with different numbers of discrete angles and with a second order Runge-Kutta time discretization.

[2] F.Filbet, C.Mouhot, L.Pareschi, '05

Cost and accuracy

Number of points	Classical spectral	Fast spectral with $M = 4$	Fast spectral with $M = 6$	Fast spectral with $M = 8$
16	1 $m.$ 14$s.$	3 $m.$ 31$s.$	7 $m.$ 45 $s.$	13 $m.$ 44 $s.$
32	118 $m.$ 02 $s.$	50 $m.$ 31$s.$	105 $m.$ 19 $s.$	186 $m.$ 18$s.$
64	125h 54 $m.$	8h 45 $m.$ 22$s.$	21h 39 $m.$	35h 01 $m.$ 28$s.$

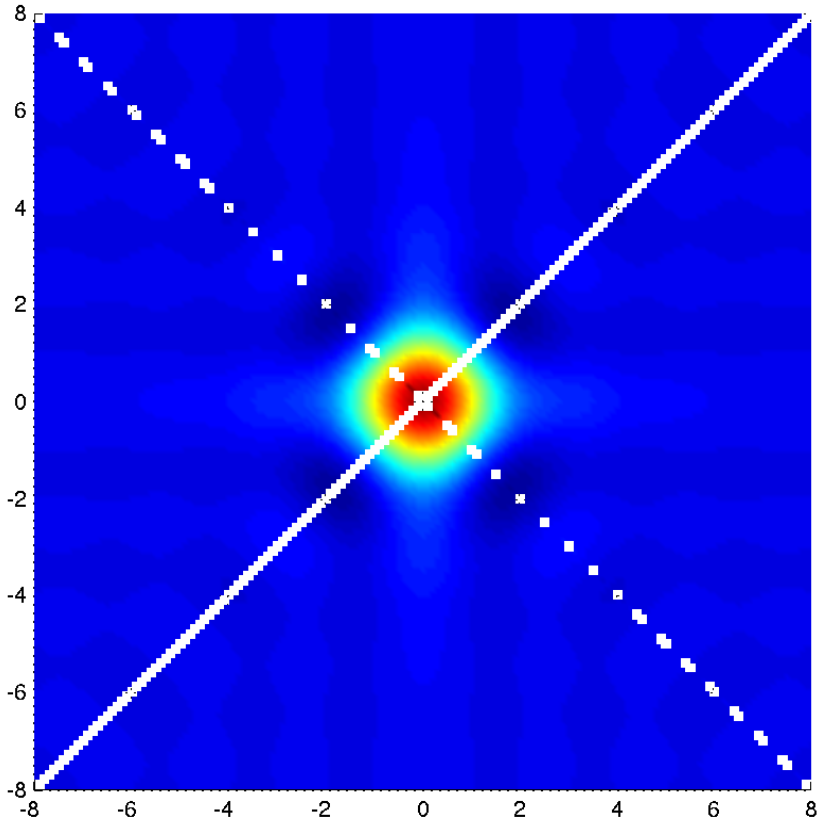
Comparison of the computational time in $3D$ between the classical spectral method and the fast spectral method with different numbers of discrete angles and with a second-order Runge-Kutta time discretization.

Number of points	Classical spectral	Fast spectral with $M = 4$	Fast spectral with $M = 6$	Fast spectral with $M = 8$
8	0.02013	0.02778	0.02129	0.02112
16	0.00204	0.00329	0.00238	0.00224
32	1.405E-5	2.228E-5	1.861E-5	1.772E-5

Comparison of the L^1 error in $2D$ between the classical spectral method and the fast spectral method with different numbers of discrete angles and with a second-order Runge-Kutta time discretization at time $T_{end} = 1$.

Other computational reduction approaches

- Other fast algorithms can be introduced introducing a selective multiscale approximation of the kernel modes, the simplest case is given by the *hyperbolic cross approximation* [3].



Plot of the kernel modes for Maxwell molecules with $d = 2$

[3] E. Fonn, P. Grohs, R. Hiptmair '14

Some remarks

- *Fast spectral solvers* have been developed also for other collisional kinetic equations, like the *Landau equation* of collisional plasma physics [4], the *inelastic Boltzmann equation* [5] and the *quantum Boltzmann equation* [6].
- The spectral method is well-defined for any physical collision kernel of the Boltzmann equation and, at variance with Monte Carlo methods, does not require any truncation over the angular cross section $b_\alpha(\theta)$.
- In the case of *Coulomb collisions* it can be shown that the kernel modes converge (in the *grazing limit*) to the corresponding kernel modes of the Landau equation and that the resulting spectral method is uniformly spectrally accurate with respect to the grazing collision parameter[7].
- Related methods based on the use of the discrete Fourier transform have been proposed by other authors[8].

[4] L.Pareschi, G.Russo, G.Toscani '00
[5] L.Pareschi, G.Toscani '04
[6] J.Hu, L. Ying '12
[7] L.Pareschi, G.Toscani, C.Villani '03
[8] A.V.Bobylev, S.Rjasanow '99 - I.Gamba, S. Tharkabhushanam '09

Long time behavior

- Spectral methods are therefore capable to produce spectrally accurate solution of the Boltzmann equation at a reduced computational cost which makes them competitive with Monte Carlo methods.
- A major drawback of spectral methods is the lack of exact conservations and entropy dissipation, and, as a consequence, the incapacity of the scheme to preserve the Maxwellian steady states of the system.
- We will show how to overcome this drawback thanks to a new reformulation of the method which permits to preserve the spectral accuracy and to capture the long time behavior of the system [9].

[9] F.Filbet, L.Pareschi, T.Rey '14

Theorem (Filbet, Mouhot '14)

Consider any nonnegative initial datum $f_0 \in H^r_p([-\pi,\pi]^3)$. Then there exists N_0 (depending on the mass and $\|f\|_{H^r_p}$) such that for all $N \geq N_0$:

(i) *there is a unique global solution $f_N = f_N(\cdot,t)$ to the following problem*

$$\frac{\partial f_N}{\partial t} = Q_N^L(f_N),$$
$$f_N(v, t=0) = f_{0,N}(v);$$

(ii) *for any $k < r$, there exists $C > 0$ such that*

$$\forall\, t \geq 0, \quad \|f_N(\cdot,t)\|_{H^k_p} \leq C;$$

(iii) *this solution is everywhere positive for time large enough, and the mass of its negative values can be made uniformly (in times) L^∞ small as $N \to \infty$;*

(iv) *this solution f_N converges to $f(t)$, the periodized solution in $[-\pi,\pi]^3$, with spectral accuracy, uniformly in time;*

(v) *this solution converges exponentially in time to a constant solution prescribed by the mass conservation law.*

Steady state preserving method

The idea is to start from the decomposition

$$g = f - M,$$

with M the local Maxwellian equilibrium and g such that $\int_{\mathbb{R}^3} g\,\phi\,dv = 0$, $\phi = 1, v, |v|^2$. When inserted into the collision operator gives

$$Q(f,f) = \mathcal{L}(M,g) + Q(g,g),$$

where $\mathcal{L}(M,g) = Q(g,M) + Q(M,g)$ and we used the fact that $Q(M,M) = 0$. We get the equilibrium preserving formulation

$$\frac{\partial g}{\partial t} = \mathcal{L}(M,g) + Q(g,g).$$

Note that:

- The steady state of the system is again given by $g \equiv 0$.
- Discretizing $Q(f,f)$ and discretizing $\mathcal{L}(M,g) + Q(g,g)$ is not equivalent.

Steady state preserving spectral methods

We can write the Fourier-Galerkin approximation as

Equilibrium preserving spectral method

$$\mathcal{L}_N(M_N, g_N) + Q_N(g_N, g_N),$$
$$f_N = M_N + g_N,$$

where M_N is the local equilibrium in our approximation space

$$M_N := \mathcal{P}_N M, \quad g_N := \mathcal{P}_N g, \quad \mathcal{L}_N(M_N, g_N) := \mathcal{P}_N \mathcal{L}(M_N, g_N).$$

It is immediate to see that $g_N \equiv 0$ is an admissible local equilibrium of the spectral scheme and therefore $f_N = M_N$ is a local equilibrium state.
It is interesting to relate the steady state preserving method with the usual spectral method. We have

$$Q_N(f_N, f_N) = \underbrace{\mathcal{L}_N(M_N, g_N) + Q_N(g_N, g_N)}_{\text{equilibrium preserving scheme}} + \underbrace{Q_N(M_N, M_N)}_{\text{perturbation}},$$

so that the only difference is due to the *non zero* term

$$Q_N(M_N, M_N) \neq 0.$$

Spectral accuracy

It is easy to prove that $Q_N(M_N, M_N)$ is spectrally close to 0 since we have

Lemma (Filbet, Pareschi, Rey '14)

$$||Q_N(M_N, M_N)||_2 \leq \frac{C}{N^{r-2}} \left(||M||_{H^r_p} + ||Q(M_N, M_N)||_{H^r_p} \right), \quad \forall\, r \geq 2.$$

- Therefore consistency and spectral accuracy follow in a straightforward way sing the analogous results for the standard spectral methods.
- The implementation can be done using the underlying fast method. Simply by removing $Q_N(M_N, M_N)$ at each time step in the usual spectral method we avoid the accumulation of errors and can take advantage of the fact that $f_N = M_N$ is the steady state of the numerical scheme.

A numerical example

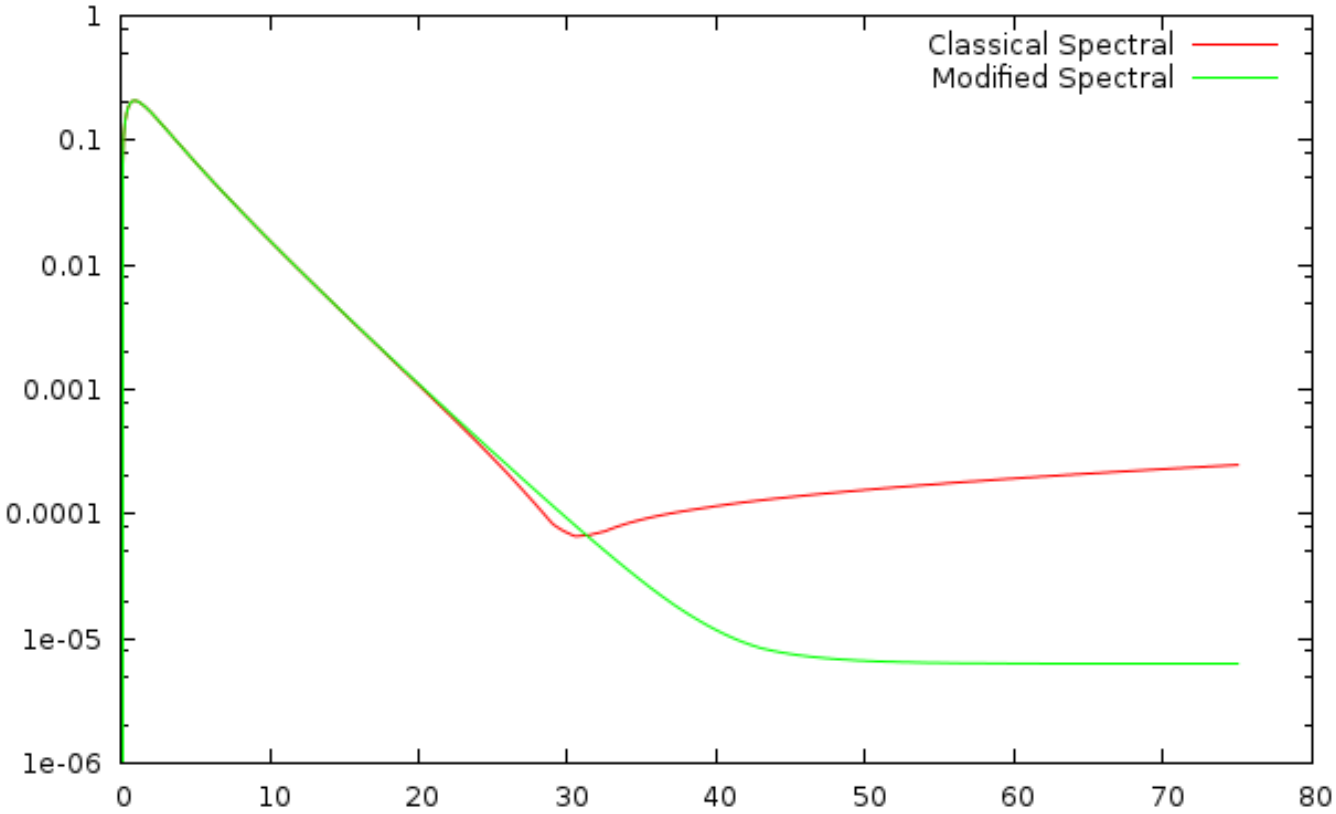


Figure: Long time behavior of the L_1-error for the space homogeneous equation in the case of Maxwell molecules in dimension $d = 2$.

Final considerations

- Compared to DSMC techniques, *deterministic methods* offer clear advantages for problems where high accuracy and low noise are required.
- The possibility to compute accurate solutions makes them an important source of validation for large-scale simulations and analytical conjectures.
- The *equilibrium preserving method* is fully general and in principle can be extended to any numerical discretization of PDE possessing explicit stationary states[10].

[10] L.Pareschi, T.Rey '15