Analysis and numerical simulations of the Boltzmann’s equation - Multi-scale problems

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The Boltzmann’s equation for rarefied gas dynamics

**Aim**: develop accurate and stable numerical schemes to approximate the evolution of the solution to the Boltzmann’s equation.

**Description of the mathematical model**: the Boltzmann’s equation for a monoatomic gas is given by

\[
\frac{\partial f}{\partial t} + v \cdot \nabla_x f = Q(f, f), \quad x, v \in \mathbb{R}^d,
\]

where \(Q(f, f)\) is the collision operator and reads

\[
Q(f, f)(v) = Q^+(f, f) - L[f]f,
\]

with for \(v \in \mathbb{R}^d\)

\[
Q^+(f, f) = \int_{\mathbb{R}^d} \int_{S^{d-1}} B(|v - v_*|, \theta) f(v') f(v'_*) d\omega dv_*,
\]

\[
L[f] = \int_{\mathbb{R}^d} \int_{S^{d-1}} B(|v - v_*|, \theta) f(v_*) d\omega dv_*.
\]
Properties of the solution to the Boltzmann’s equation

- The collision operator preserves positivity of the distribution function
  \[ f(0, x, v) \geq 0 \quad \Rightarrow \quad f(t, x, v) \geq 0 \]

- The collision operator preserves local mass, momentum and energy
  \[ \int_{v \in \mathbb{R}^d} Q(f, f) \phi(v) \, dv = 0, \quad \phi(v) = 1, v, |v|^2 \]

- The solution satisfies the famous \( H \) theorem or entropy production
  \[ -\frac{d}{dt} \int_{\mathbb{R}^d} f(t, v) (\log(f(t, v)) - 1) \, dv \geq 0 \]

- Equilibrium states are characterized by Maxwellian distribution functions
  \[ \mathcal{M}(v) = \frac{\rho}{(2\pi T)^{d/2}} \exp\left( -\frac{|v - u|^2}{2T} \right), \]
  where \( \rho, u, T \) respectively represent the density, mean velocity and temperature of the gas.
Plan of the talk

1. General framework: spectral methods

2. Part I: What’s about stability of such methods? (collab. with C. Mouhot)

3. Part II: Asymptotic Preserving Schemes (collab with S. Jin)

Part of this project is related to the ERC Starting Grant 2009:

everybody is very welcome to the University of Lyon!
A general framework for spectral methods

We consider the space homogeneous case and write the Boltzmann’s equation in the form

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

where $Q$ is given by

$$Q(f, f)(t, v) = \int_{C} B(y) (f'f' - f*f) \, dy, \quad v \in \mathbb{R}^d$$

with $f' = f(v'),...$

$$v' = v + \Theta'(y), \quad v'_* = v + \Theta'_*(y), \quad v_* = v + \Theta_*(y).$$

In the equations above: $C$ is the domain of integration, which is usually an unbounded domain. Functions $\Theta, \Theta', \Theta'_*$ are given functions describing the collision mechanism.

Remark : We easily check via a change of variable that the Boltzmann’s equation can indeed be written in this form.
Fourier-Galerkin Methods

We describe the main steps:

- reduce the domain of integration $C$ to a bounded domain $C^R$ and compute an appropriate bounded set for the velocity $v \in D_L$, where $R$ and $L$ are two different parameters (linked together);
- approximate the distribution function by $f_N$, which represents its truncated Fourier series

$$f_N(v) = \sum_{k=-N}^{N} \hat{f}_k e^{i \frac{\pi}{L} k \cdot v}, \quad \hat{f}_k := \frac{1}{(2L)^d} \int_{D_L} f(v) e^{-i \frac{\pi}{L} k \cdot v} dv;$$

- substitute $f_N$ in the collision operator $Q^R$, which simply gives

$$Q^R(f_N, f_N) = \int_{C^R} B(y) (f_N' f_N^* - f_N^* f_N) \, dy, \quad v \in D_L$$

Using the mathematical properties of the function $e^{i \frac{\pi}{L} k \cdot v}$ and the particular form of the collision operator, it yields for the gain term:

$$Q^R_+(f_N, f_N) = \sum_{l,m=-N}^{N} \left( \int_{C^R} B(y) e^{i \frac{\pi}{L} (l \cdot \Theta' + m \cdot \Theta')} \, dy \right) \hat{f}_l \hat{f}_m e^{i \frac{\pi}{L} (l+m) \cdot v} \cdot \beta(l,m).$$
Fourier-Galerkin Method

Then using orthogonality property of trigonometric polynomials, we get the following differential system of ODEs for the Fourier coefficients

$$\frac{d\hat{f}_k}{dt} = \sum_{l,m=-N}^{N} [\beta(l,m) - \beta(m,m)] \hat{f}_l \hat{f}_m.$$

Finally, we can also write

$$\begin{cases}
\frac{\partial f_N}{\partial t} = P_N Q^R(f_N, f_N), & (t, v) \in \mathbb{R}^+ \times \mathcal{D}_L \\
f_N(0, v) = f_{0,N}(v), & v \in \mathcal{D}_L
\end{cases}$$

A short review of spectral methods for Boltzmann’s equation

- Classical spectral method: it has been first proposed by B. Perthame, L. Pareschi (92), A. Bobylev & S. Rjasanow, G. Russo & L. Pareschi (00) and F. Filbet & G. Russo (03), I. Gamba & S. H. Tharkabhushanam (09).

- Fast spectral method with a computational cost for the evaluation of the collision operator of order $N \log(N)$, where $N$ is the total number of degree of freedom: Bobylev-Rjasanow, recently proposed by C. Mouhot & L. Pareschi...
Convergence to equilibrium for the space dependent Boltzmann’s equation

Let us consider the nonhomogeneous Boltzmann’s equation

\[
\begin{aligned}
\frac{\partial f}{\partial t} + v \cdot \nabla_x f &= Q(f, f), \quad x \in \mathbb{T}, v \in \mathbb{R}^2, \\
\end{aligned}
\]

\[
\begin{aligned}
f(0, x, v) &= f_0(x, v),
\end{aligned}
\]

with periodic boundary conditions in space.

We define hydrodynamic quantities: local density, local mean velocity

\[
\rho_l(t, x) = \int_{\mathbb{R}^2} f(t, x, v) dv, \quad u_l(t, x) = \frac{1}{\rho_l} \int_{\mathbb{R}^2} v f(t, x, v) dv
\]

and local temperature

\[
T_l(t, x) = \frac{1}{d \rho_l} \int_{\mathbb{R}^d} |u_l - v|^2 f(t, x, v) dv.
\]
Consider an initial datum such that the global temperature $T_g = 1$, global mean velocity $u_g$ is zero and the global density $\rho_g = 1$, hence using $H$-theorem we can prove that\(^1\)

$$H_g(t) = H_I(t) + \int_T \rho_I(t,x) \log(\rho_I(t,x)/T_I(t,x))dx.$$  

where

$$H_I(t) = \int f \log(f/M_I)dx dv, \quad H_g(t) = \int f \log(f/M_g)dx dv,$$

with $M_I(t,x,v)$ and $M_g(v)$ are respectively the Maxwellians obtained from local and global equilibria.

Moreover,

$$H_I(t) \leq H_g(t), \quad \forall t \geq 0.$$

Influence of the length box: $\text{diam}(\mathcal{T}) = \pi; \, 3\pi/2$ and $2\pi$
Analysis of the linearized Boltzmann’s around global equilibrium (Ellis & Pinsky)

Some fastidious (but explicit!) calculations show that at first order with respect to the parameter \( \varepsilon = 1 / \text{diam}(\mathbb{T}) \), all eigenvalues are vanishing except for two of them

\[
\lambda_1 = i \varepsilon \sqrt{1 + 2/d} + O(\varepsilon^2), \quad \lambda_2 = -i \varepsilon \sqrt{1 + 2/d} + O(\varepsilon^2).
\]

These eigenvalues are related to the speed of sound\(^2\).

<table>
<thead>
<tr>
<th>Lenght</th>
<th>period (2\pi/\omega)</th>
<th>(2\pi\varepsilon/\omega)</th>
<th>rate (\alpha)</th>
<th>(-\alpha/\varepsilon^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(d(\mathbb{T}) = \pi/2)</td>
<td>02.25</td>
<td>1.432</td>
<td>-2.202</td>
<td>21.71</td>
</tr>
<tr>
<td>(d(\mathbb{T}) = \pi)</td>
<td>04.50</td>
<td>1.432</td>
<td>-0.641</td>
<td>25.26</td>
</tr>
<tr>
<td>(d(\mathbb{T}) = 3\pi/2)</td>
<td>06.61</td>
<td>1.142</td>
<td>-0.285</td>
<td>25.31</td>
</tr>
<tr>
<td>(d(\mathbb{T}) = 2\pi)</td>
<td>08.78</td>
<td>1.140</td>
<td>-0.160</td>
<td>25.27</td>
</tr>
<tr>
<td>(d(\mathbb{T}) = 8\pi)</td>
<td>17.57</td>
<td>1.140</td>
<td>-0.040</td>
<td>25.35</td>
</tr>
</tbody>
</table>

Tab.: Influence of the length box using a mesh in phase space \(64 \times 64 \times 64\) with an initial perturbation of amplitude \(A_0 = 0.1\).

\(^2\)Thanks to Ph. J. Morrison!
What’s about stability of such methods?

- **Results**: the method preserves mass. But, we lose other conservations: momentum, energy; $H$-theorem does not hold true for entropy production, positivity of the distribution function is not conserved at all!

- **L. Pareschi & G. Russo** introduced some filters allowing to preserve positivity $\Rightarrow$ the method becomes first order accurate.

- It seems difficult to analyze directly the spectral method by evaluating the qualitative behavior of the approximation $f_N$.

**Theorem** Let $f \in L^2([−\pi, \pi]^3)$, then

$$
\|Q^R(f, f) - Q^R_N(f_N, f_N)\|_{L^2} \leq C_{fN} \left(\|f - f_N\|_{L^2} + \frac{\|Q^R(f_N, f_N)\|_{H^r_p}}{|N|^r}\right).
$$

Let $f \in H^r_p([−\pi, \pi]^3)$, $r \geq 0$ then

$$
\|Q^R(f, f) - Q^R_N(f_N, f_N)\|_{L^2} \leq \frac{C_{fN}}{|N|^r} \left(\|f\|_{H^r_p} + \|Q^R(f_N, f_N)\|_{H^r_p}\right).
$$
New formulation for stability analysis

The spectral scheme for $f_\varepsilon$ can be written as:

\[
\begin{aligned}
\frac{\partial f_\varepsilon}{\partial t} &= Q^R(f_\varepsilon, f_\varepsilon) + P_\varepsilon(f_\varepsilon), \quad v \in \mathcal{D}_L, \\
f_\varepsilon(0, v) &= f_0(v), \quad v \in \mathcal{D}_L,
\end{aligned}
\]

(1)

where the perturbation $P_\varepsilon$ satisfies the following properties:

well-balanced

\[\int_{\mathcal{D}_L} P_\varepsilon(f) \, dv = 0.\]  

(2)

and preserve smoothness

\[
\begin{aligned}
\|P_\varepsilon(f)\|_{H^k} &\leq C_k \|f\|_{L^1} \|f\|_{H^k}, \\
\|P_\varepsilon(f)\|_{H^p} &\leq \varphi(\varepsilon),
\end{aligned}
\]

(3)

where $\varphi(\varepsilon)$ depends on $\|f\|_{H^k}$ for $k > p$ and converges towards zero, when $\varepsilon$ converges towards zero.
Consider the perturbed Boltzmann’s equation (1) where \((P_\varepsilon)_\varepsilon\) satisfies (2)-(3). Assume that the initial datum is nonnegative, non zero everywhere in the bounded domain and \(f_0 \in H^k(D_L)\), with \(k > d/2\). We consider a sequence of smooth balanced perturbations \(f_0,\varepsilon\) of the initial datum for the perturbed problem. Then, there exists \(\varepsilon_0 > 0\) such that for all \(\varepsilon \in ]0, \varepsilon_0[\) :

- there exists a unique global smooth solution to (1)
- the solution belongs to \(H^k\) for all time \(t \geq 0\) and all bounds are uniform with respect to \(t\), and the solution remains \("essentially positive\) uniformly in time,

\[
\forall t \geq 0, \quad \|f^-(t, \cdot)\|_{L^1(D_L)} , \|f^-(t, \cdot)\|_{L^\infty(D_L)} \leq \eta(\varepsilon)
\]

where \(f^-\) représente \(|f| \mathbf{1}_{f \leq 0}\).
- the solution converges in \(H^k\) towards a constant equilibrium state in velocity in \(D_L\), corresponding to the initial mass and the solution is uniformly positive asymptotically in time, that is for all time \(t\) larger than a fixed time.
Some preliminary results

- Using the quadrature structure of the Boltzmann’s operator:

\[
\frac{d}{dt} \|f(t)\|_{L^1} \leq C \|f(t)\|_{L^1}^2
\]

- Then, inequalities about propagation of regularity yield

\[
\frac{d}{dt} \|f(t)\|_{H^k} \leq C(\|f(t)\|_{L^1}) \|f(t)\|_{H^k}
\]

These estimates allow to establish classically there exists a time \(\bar{\tau} > 0\) such that there exists a smooth solution to (1).

- Spreading properties of the gain operator \(Q^+(f, f)\)

**Lemma**: Consider the kernel \(B\) truncated for the velocities \(|v'|, |v'_*| \leq R\). Then, for all \(0 < r < R\), we have

\[
Q^{R,+}(1_{B(v,r)}, 1_{B(v,r)}) \geq C_0 1_{B(v,\mu r)}
\]

for explicit constants \(\mu > 1\) and \(C_0 > 0\).
Proposition: Estimate of the negative part of $f$

Assume that $f_0$ is a nonnegative function such that $f_0 \in H^k_{\text{per}}(D_L)$ with $k \in \mathbb{N}$ and $k > d/2$. Moreover, we set $M = 2 \|f_0\|_{L^1}$ and $f_0,\varepsilon$ an approximation to $f_0$ which has the same mass as $f_0$ but not necessary nonnegative

$$\|f_0 - f_{0,\varepsilon}\|_{H^k} \leq \psi(\varepsilon)$$

and $\psi(\varepsilon) \to 0$ when $\varepsilon \to 0$. We define by $\bar{\tau} > 0$ the time for which there exists a solution satisfying

$$\forall t \in [0, \bar{\tau}], \quad \|f(t)\|_{H^k} \leq C_k(M).$$

Then there exist $\hat{\tau} \in ]0, \bar{\tau}[,$ which only depends on $M$, $R$ and on the collision kernel $B$ and $\hat{\varepsilon} > 0$, which only depends on $\hat{\tau}$, $C_k(M)$ such that for all $\varepsilon \in ]0, \hat{\varepsilon}[,$ and for each solution belonging to $H^k_{\text{per}}(D_L)$ and solution to the perturbed Boltzmann’s equation (1), we have

$$\forall \nu \in D_L, \quad f_\varepsilon(\hat{\tau}, \nu) > 0.$$ 

and there exists $\eta(\varepsilon)$, which is vanishing when $\varepsilon$ goes to zero, such that

$$\|f^{-}(t)\|_{L^\infty} \leq \eta(\varepsilon), \quad t \in [0, \hat{\tau}],$$
Main steps of the proof

The main idea consists to iterate the following steps on time interval in the form $[\tau - \tau/2^j, \tau]$: 

- we split the distribution function as $f = f^+ - f^-$ and using the bilinearity of $Q^R$, we get 

$$Q^R(f, f) = Q^R(f^+, f^+) - 2Q^R(f^+, f^-) + Q^R(f^-, f^-).$$ 

- we show that the terms $Q^R(f^+, f^-)$, $P_\varepsilon(f, f)$ are small and use the monotonicity and spreading properties of $Q^{R,+}(f^+, f^+)$ 

$$Q^{R,+}(f^+, f^+) \geq \alpha^2 Q^{R,+}(1_B(v_0, \delta), 1_B(v_0, \delta)) \geq \frac{C\mu \alpha^2}{2} 1_B(v_0, \mu \delta),$$ 

with $\mu > 1$. 

Therefore, when $\mathcal{D}_L \subset B(v_0, (\mu \delta)^J)$, we have proven that there exist $\hat{\tau}$ and $\hat{\varepsilon}$ small enough such that $\varepsilon \in ]0, \hat{\varepsilon}[$, 

$$f_\varepsilon(\hat{\tau}, v) > 0, \quad v \in \mathcal{D}_L.$$
Boltzmann’s equation, Euler and Navier-Stokes system

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Part I: What’s about stability of such methods? (collab. with C. Mouhot)
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Number of particles goes to $+\infty$

Mesoscopic description: $f(t,x,v)$ solution of the Boltzmann equation.

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\varepsilon} Q(f, f).$$

-$\Rightarrow$ Theoretical works: C. Bardos, F. Golse, D. Levermore, F. Golse & L. Saint-Raymond, P.-L. Lions & N. Masmoudi...
-$\Rightarrow$ Numerical Simulations: initiated by S. Jin with relaxation schemes.
Mathematical Problem

Consider Boltzmann’s equation written in the form

\[
\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\varepsilon} Q(f, f).
\]

The asymptotic study \( \varepsilon \to 0 \) gives that \( f \approx M_{\rho, u, T} \) solution to the compressible Navier-Stokes or Euler equations \( (\varepsilon = 0) \).

**Aim**: we want to design a numerical scheme

- which is **stable** with respect to the parameter \( \varepsilon \Rightarrow \) implicit treatment;
- which is **uniformly accurate** with respect to the parameter \( \varepsilon \Rightarrow \) high order and uniform;
- which is systematic for the approximation of **nonlinear** collision operators;
- which has a **reduced computational cost**.
More recently,

- S. Jin, L. Pareschi and G. Toscani for the diffusive limit: from a kinetic model cinétique towards a drift-diffusion equation.
- P. Crispel, P. Degond and M.-H. Vignal for the limit from Euler-Poisson towards quasi-neutral models.
- Then, adaptation for kinetic models R. Belouar, N. Crouseilles, P. Degond, F. Deluzet, E. Sonnendrucker...: the technique is based on a new formulation of the Poisson equation

An important result:

- PhD of M. Bennoune with M. Lemou and L. Mieussens: micro-macroscopic decomposition.

This method can be adapted to any collision nonlinear operator.
From kinetic towards fluid limits

We propose a very simple approach preserving the asymptotic for kinetic equations: it is based on the splitting operator

\[ \frac{\partial f}{\partial t} = \frac{Q(f) - P(f)}{\varepsilon} + \frac{P(f)}{\varepsilon}, \]

where the operator \( P(f) \) satisfies the following properties

- conservation of the structure of the nonlinear operator: steady states \( \mathcal{M} \), differentiel structure, ...
- the linear operator \( P(f) \) is easy to invert

For instance since

\[ Q(f) = Q(\mathcal{M}) + \nabla Q(\mathcal{M}) [f - \mathcal{M}] + O(\|f - \mathcal{M}\|) = 0 \]

one possible choice is \( P(f) := \nabla Q(\mathcal{M}) [f - \mathcal{M}] \). It yields

\[ \frac{f^{n+1} - f^n}{\Delta t} = \frac{Q(f^n, f^n) - P(f^n)}{\varepsilon} + \frac{P(f^{n+1})}{\varepsilon}, \]
Asymptotic Preserving Result

Consider the numerical solution given by the first order IMEX scheme. Then,

(i) If $\varepsilon \rightarrow 0$ and $f^n = M^n + O(\varepsilon)$, then the scheme preserves the asymptotic, that is $f^{n+1} = M^{n+1} + O(\varepsilon)$, and therefore the scheme preserves the asymptotic limit given by Euler equations.

(ii) If $\varepsilon \ll 1$ and $f^n = M^n + O(\varepsilon)$ and there exists a constant $C > 0$ such that

$$
\left\| \frac{f^{n+1} - f^n}{\Delta t} \right\| + \left\| \frac{U^{n+1} - U^n}{\Delta t} \right\| \leq C,
$$

then the IMEX scheme is consistent of order one with the compressible Navier-Stokes system.

(iii) Under a monotonicity assumption of the operator $Q$ and if the solution $(f^n)_n$ is smooth in $(x, v)$, then there exist $1 > \alpha > 0$ and $C > 0$ such that

$$
\|f^n - M^n\| \leq \frac{C}{1 - \alpha} \varepsilon + \alpha^n \|f^0 - M^0\|
$$
Numerical Test I: uniform accuracy with respect to $\varepsilon > 0$

The scheme for the Boltzmann’s equation is given by

\[
\frac{f^{n+1} - f^n}{\Delta t} + v \nabla_x f^n = \frac{Q(f^n) - P(f^n)}{\varepsilon} + \frac{P(f^{n+1})}{\varepsilon},
\]

\[f^0(x, v) = f_0(x, v),\]

\[\varepsilon \log(h)\]

\[
\begin{array}{c|c|c|c|c|c|c|c}
\log(h) & -5 & -4 & -3 & -2 & -1 & 0 \\
\end{array}
\]

\[1.9 x\]

Fig.: Estimate of $L^\infty$ error norm for different values of $\varepsilon = 10^{-5}, \ldots, 1$. 
Numerical Test II: accuracy compared to Euler or CNS

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Numerical Test III: multiscale problem

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Numerical Test IV: Flow around a cylinder ($M = 0.5$),
$\varepsilon = 0.5, 0.1, 0.01, 0.001$

We present the steady state of the local Mach number for different values of Knudsen number:
- (1) $\varepsilon = 0.5$
- (2) $\varepsilon = 0.1$
- (3) $\varepsilon = 0.01$
- (4) $\varepsilon = 0.001$
Numerical Test IV: Flow around a cylinder ($\varepsilon=0.01$, $M=0.1$)

We present the steady state of the density $\rho$ and the temperature $T$ for a Mach number 0.1
Another Application: drift-diffusion problem (porous media)

The distribution function $f$ is solution to
\[ \frac{\partial f}{\partial t} = \nabla_v \cdot (v f + \nabla_v f^m), \]
and converges to the Barenblatt-Pattle distribution
\[ \mathcal{M}(v) = \left( C - \frac{m - 1}{2 m} |v|^2 \right)^{1/(m-1)}, \]
where $C$ is uniquely determined and depends on the initial mass $g_0$ but not on the “details” of the initial data.

We apply the following decomposition
\[ \frac{\partial f}{\partial t} = \Delta_v \underbrace{(f^m - m \mathcal{M}^{m-1} f)}_{\text{non stiff part}} + \nabla_v \cdot \left( v f + m \nabla_v \left( \mathcal{M}^{m-1} f \right) \right). \]
Numerical Test V: convergence to the Barrenblatt

Approach of Kinetic Models

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