CONVERGENCE TO EQUILIBRIUM: ENTROPY PRODUCTION AND HYPOCOERCIVITY

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Abstract. These is the text for my Harold Grad lecture, delivered in the 24th Rarefied Gas Dynamics conference, Bari (July 2004). They describe recent developments about convergence to equilibrium in kinetic theory, related to Boltzmann's H Theorem and entropy production. The style is intentionally informal, at the price of rigor and precision; full details can be found in the research papers quoted within the text. The text is partially based on my earlier contribution to the proceedings of the 14th International Congress of Mathematical Physics, Lisbon (July 2003).

1. 1872: Boltzmann's H Theorem

Boltzmann's equation models the dynamics of a rarefied gas via the (time-dependent) position-velocity density $f(x, v)$; here x is the position variable, varying in a box $\Omega \subset \mathbb{R}^3$, while v is the velocity variable, varying in $\mathbb{R}^3$. In the 1870's, Boltzmann discovered that, under ad hoc boundary condition, the entropy

$$S(f) = -H(f) := -\int_{\Omega \times \mathbb{R}^3_v} f(x, v) \log f(x, v) \, dv \, dx,$$

is **nondecreasing** as time increases if f evolves according to the Boltzmann equation.

More than 100 years later, this theorem is still striking and beautiful:

- Boltzmann managed to recover irreversibility from a model based on reversible mechanics and statistics;

- the H Theorem is a manifestation of the second law of thermodynamics, but it is a **theorem**, as opposed to a postulate;

- although not perfectly rigorous, the proof is beautiful;

- this theorem applies in all generality, even far from equilibrium.

In view of these considerations, it is in some sense a shame for us mathematicians that we are still unable to rigorously prove Boltzmann's theorem in full generality. The difficulty lies in a "slight analytical difficulty" (as Euler said about his own equation): the existence of "smooth" solutions. The regularity theory for the Boltzmann equation is a **huge** work in progress; it is 70 years old (Carleman may be considered as its founder), and has never been so active as now. Yet it is still far from completion, and it is still a riddle whether the Boltzmann equation, starting from a smooth initial datum, admits smooth solutions.

2. A prediction by Boltzmann

Pick up a large number $N \simeq 10^{20}$ of small "billiard balls" of radius $r \simeq 1/\sqrt{N}$, and throw them randomly and independently in a box Ω, according to some nice probability density $f_0(x,v)\,dx\,dv$ in phase space. Of course it is impossible to produce really independent particles, since they have to exclude each other, but let us forget about this issue.

The density of particles, or empirical measure, is given by the formula

$$\widehat{\mu}(dx\,dv) := \frac{1}{N}\sum_{i=1}^{N}\delta_{(X^i,V^i)}$$

where X^i and V^i stand for the position and velocity of particle number i. If N is very large, and the particles are (close to) being independent, some variants of the law of large numbers imply that at time 0, $\widehat{\mu}_0 \simeq f_0(x,v)\,dv\,dx$, in a sense which will not be made precise here.

Now, at positive times the system evolves according to Newton's equations, with *interaction* between the particles, so the balls acquire new positions and velocities. Can one predict a good approximation of the density of particles for large times??

Here is a plausible answer:

(i) For a given time t, if N is large enough, the empirical density $\widehat{\mu}_t$ is (with very high probability) close to the solution f_t at time t of the Boltzmann equation starting from initial datum f_0;

(ii) As time $t \to \infty$, the solution of the Boltzmann equation tries to maximize the entropy $S(f)$ under the constraints given by the conservation laws, which means mass and kinetic energy. Since the maximizer is a **gaussian** distribution, we expect f_t to become nearly gaussian as t becomes large.

So Boltzmann's theory suggests that the empirical measure looks nearly gaussian when t is large. Our familiarity with this statement must not make us forget how striking this prediction is. Of course, gaussian distributions are well-known in classical probability theory, but here we are not looking at such a simple system as sums of independent random variables, we are considering the true, monsterly complicated, deterministic dynamics imposed by Newton's equations!

Now, one has to be very careful about the meaning of statement (i) above. It **cannot** hold true when t is very, very large. Indeed, Poincaré's recurrence theorem implies: *With probability 1, all the particles will come back to (almost) their initial positions, after some time.* There is no contradiction with Boltzmann's theory: it only shows that after a (very, very, very) long time, Boltzmann's equation is not an accurate model.

Keeping this in mind, a theoretical statement about the Boltzmann equation is scientifically satisfactory only if there is a control on the time scales involved. So, in all the discussion above, "large enough", "very high", "very very large" should be quantified in terms of the data of the problem: f_0, interaction, shape of the box, number N of particles. Our seemingly simple problem actually appears to be tremendously complicated!

To this date, **neither** statement (i) nor statement (ii) has received mathematical justification in a quantitative way. Statement (i) is related to Lanford's 1973 famous theorem (a good account of this theorem can be found in Cercignani, Illner and Pulvirenti [4]). This talk is all about statement (ii). So the central question in this lecture is the following: *Can one establish quantitative rates of convergence to equilibrium for solutions of the Boltzmann equation?*

The presentation which follows is quite informal and tries to conceal the extremely technical nature of the subject. More precise information can be obtained in recent papers by the author, some of them in collaboration with Desvillettes [6, 20, 7] (all of them available from `http://www.umpa.ens-lyon.fr/~cvillani`). These references themselves contain pointers to various parts of the mathematical literature.

3. Preliminary: the Boltzmann equation

The Boltzmann equation, in its most classical form, can be written

$$\text{(BE)} \qquad \frac{\partial f}{\partial t} + \underbrace{v \cdot \nabla_x f}_{\text{transport}} = \underbrace{Q(f,f)}_{\text{collisions}}$$

$$Q(f,f) = \int_{\mathbb{R}^n} \int_{S^{n-1}} \Big[f(v')f(v'_*) - f(v)f(v_*) \Big] B(v-v_*,\sigma)\, d\sigma\, dv_*.$$

Here I used the somewhat standard notation

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

Moreover, B is the Boltzmann collision kernel, e.g. $B = |v-v_*|$ (hard sphere kernel in dimension 3) or $B = b(\cos\theta)$, where θ is the angle between $v - v_*$ and σ (Maxwellian collision kernel).

To this should be added boundary conditions, for instance specular reflection: $f(x,v) = f(x, R_x v)$ when $x \in \partial\Omega$, where $R_x v := v - 2(n(x)\cdot v)n(x)$ and $n(x)$ is the unit normal at Ω.

In the sequel, I shall write $f(t)$ or $f(t,\cdot)$ or f_t for the solution of the Boltzmann equation at time t.

Recall the connection between kinetic and hydrodynamic description: from a density of particles $f(x,v)$ in phase space, one can cook up hydrodynamic fields by the recipes

$$\rho(t,x) := \int f\, dv \qquad \text{(density)}$$

$$u(t,x) := \frac{1}{\rho}\int f\, v\, dv \qquad \text{(mean velocity)}$$

$$\mathbb{P}(t,x) := \int f\,(v-u)\otimes(v-u)\, dv \qquad \text{(tensor pressure field)}$$

$$T(t,x) := \frac{1}{n\rho}\,\mathrm{tr}\,\mathbb{P} \qquad \text{(temperature)}$$

$$E(t,x) := \int f\frac{|v|^2}{2}\, dv = \rho\frac{|u|^2}{2} + \frac{n}{2}\rho T \qquad \text{(energy)}$$

For the sake of this lecture, it can be assumed that $n = 3$.

4. Reminders about the mathematical theory of the Boltzmann equation

A lot of references and information about the mathematical theory of the Boltzmann equation can be obtained in the author's long survey paper [19]. As said above, the theory is extremely well developed but still far from complete.

Why is it so difficult to deal with the full Boltzmann equation?

- the collision operator Q is quadratic;
- Q is complicated, and fine analysis with it is quite a challenge;
- Q acts only on the velocity-dependence, not on the position, which introduces a fundamental degeneracy;
- $v \cdot \nabla_x$ and Q get along awfully: virtually any trick which works well for one, is a disaster for the other.

The following statement is within reach of present-day techniques:

Under reasonable assumptions on B, and periodic boundary conditions,

IF one has the following a priori estimates:

(i) the density and energy fields are bounded from above;

(ii) the density is bounded below (no vacuum!): $\rho \geq \delta > 0$;

(iii) the pressure tensor is bounded below, in the sense of matrices: $\mathbb{P} \geq \lambda I_n$ $(\lambda > 0)$ [this is a nondegeneracy assumption ensuring that the velocity distribution is not concentrated on a low-dimensional subspace of velocities]

THEN one can construct very nice solutions:

(1) all Sobolev norms (with derivatives in both x and v) of f are bounded;

(2) all v-moments ($\int f|v|^k \, dv \, dx$) are bounded.

5. "Why" is there convergence to equilibrium?

• In Boltzmann's interpretation, the system converges to rest because this is the maximum entropy state (heuristically, increase of entropy means **loss of information**; for instance, the distribution f carries less and less information on the physical system as time evolves).

• In the **linearized** regime, there is another possible explanation, which is the existence of a **spectral gap**. In many situations it can be used to study convergence to equilibrium for the Boltzmann equation. Be careful! There are plenty of traps in the spectral theory of the Boltzmann equation...

• Many other possible explanations are available in the particular case of **spatially homogeneous Maxwellian molecules** (see [19, Chapter 4]):

- other Lyapunov functionals: Fisher information, Tanaka distance, Toscani distance...

- as first noted by Bobylev, the equation lends itself to a study by **Fourier transform**, even though it is nonlinear.

But the entropy production interpretation is the only one which works far from equilibrium in a spatially inhomogeneous context, or for general interactions! This motivated a mathematical program about the entropy production in Boltzmann equation, started in the early nineties by Carlen & Carvalho and Desvillettes, with some impulse by Cercignani:

Question: *Forget about the "slight analytical difficulty", can you put Boltzmann's program on rigorous basis?*

In other words: Let $f(t)$ be a **nice** solution of Boltzmann equation (either because you are in a situation where you know that smooth solutions exist, or just because you assume their existence); can you prove that $f(t,\cdot)$ approaches the global Maxwellian (equilibrium) as $t \to \infty$? (**keeping a control on time scales!!**)

In my opinion, the two main motivations for the program are:

- *Theoretical interest*: Hope to rigorously justify the maximum entropy principle (which is fundamental in so many parts of statistical mechanics) for the Boltzmann equation;

- *Physical interest*: Hope to uncover some interesting qualitative phenomena about the approach to equilibrium.

6. What NOT to do

Let f be a nice solution of Boltzmann equation, with nice bounds, uniform in time. With a bit of functional analysis it is easy to prove that there is **convergence** of f_t to the Maxwellian distribution, as $t \to \infty$. But this is not what we are looking for: we want to get **constructive bounds** on the speed of convergence.

Then, why not linearize close to equilibrium? After all, if we know that the solution will approach equilibrium, then presumably spectral properties of the linearized equation will eventually dictate the final rate of convergence. There are two main reasons why this is a wrong way to start:

- The "natural" estimates of Sobolev and moment bounds are not strong enough to allow the "natural" linearization of the Boltzmann equation in $L^2(M^{-1})$ [$M(v)$ = gaussian in velocity variable];

- *How long do we have to wait until the solution is sufficiently close to equilibrium, that it makes sense to linearize?*

While the first objection is of technical nature, and actually might be about to be answered by recent works of Mouhot, the second objection is intrinsic to linearization. In fact linearization can only be understood as a complement to other "fully nonlinear" techniques. In the end, it will probably yield refined rates of convergence, but cannot replace a study of the equation far from equilibrium.

7. Main difficulties

In dealing with the problem of convergence to equilibrium one encounters difficulties which are reminiscent of the already mentioned difficulties for the Cauchy problem:

- The complexity of Q, again;

- The fact that the entropy production vanishes for hydrodynamical states, which can be seen as a reflection of the degeneracy of the collision operator. In particular, *local Maxwellians* *may be a nuisance here!* This is very different from the problem of hydrodynamical limit,

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\mathrm{Kn}} Q(f,f), \qquad \mathrm{Kn} \to 0.$$

In that limit, on the contrary, one *hopes* (and in some cases proves) that the solution stays very close to be a local Maxwellian at each time.

- One has to understand, and translate into equations, the crucial role of the transport operator $v \cdot \nabla_x$ and the boundary conditions, which help selecting the equilibrium but do not produce any entropy!

8. Short history

The problem of speed of convergence was pioneered by Kac [14] (1954), who tried to treat it in the spatially homogeneous case as the limit of a *many-particle problem.* On this occasion he introduced

– "Kac's problem" about **spectral gap** in large dimension; on this problem there has been a number of recent contributions by Diaconis & Saloff-Coste, Janvresse, Maslin, Carlen & Carvalho & Loss, and others; in particular, it is profitable to consult Carlen, Carvalho & Loss [3];

– the concept of "**propagation of chaos**";

– one of the first continuous mean-field limits;

.... but did not get anywhere about rates of convergence. Then McKean [15] (1966) introduced **information theory** into the game, for an oversimplified one-dimensional model called Kac's caricature.

In the 1990's, Desvillettes, Carlen & Carvalho, Toscani & Villani obtained strong results in the spatially homogeneous case. A review of these results is included in [20].

The result to be presented in the sequel is about explicit rates of convergence in the spatially **in**homogeneous case, for **smooth** solutions; most of it was worked out by the author in collaboration with Desvillettes.

9. Main result to this date

The following theorem is due to Desvillettes and myself [7].

Theorem: *Let $f(t,x,v)$ be a solution of the Boltzmann equation, in a domain Ω_x = smooth bounded domain (specular reflection) or periodic box. Assume that*

(i) f is very regular (uniformly in time): all moments ($\int f|v|^k \, dv \, dx$) are finite and all derivatives (of any order) are bounded;

(ii) f is strictly positive: $f(t,x,v) \geq K e^{-A|v|^q}$.

Then $f(t) \longrightarrow f_\infty$ (global Maxwellian), at least as fast as $O(t^{-k})$ for all $k > 0$.

Remark: From known regularity theory, (i) $\Longrightarrow$ (ii), at least in the case of a periodic box [16].

The theorem stated above is a **conditional** theorem: it assumes from the solution a lot of regularity, which so far are not known to hold true for the Boltzmann equation. These regularity assumptions can be established at least

- in the spatially homogeneous case;
- close to equilibrium (see for instance recent works by Guo [11, 12, 13]).

Further remarks:

- The theorem only shows convergence like $O(t^{-\infty})$, not $O(e^{-\lambda t})$, but it also covers situations where there is no spectral gap.

- In a close-to-equilibrium context, convergence like $O(t^{-\infty})$ was recently recovered by Guo and Strain, using linearization techniques. Our theorem as it stands applies almost verbatim to Guo's solutions, but does **not** need f to be close to equilibrium, and does not rely on linearization.

- Even when the initial datum is not so smooth, one can separate a smooth part from a decaying non-smooth part, under adequate integrability and decay estimates.

- The usual strategy to attack the problem of convergence to equilibrium is to try to show that f looks like a hydrodynamic state in large time, then identify this state. Our proof goes somehow the opposite way, as we shall see.

- The arguments used in the proof can be applied to many other kinetic models, than the Boltzmann equation, as was checked in particular by Schmeiser's team in Vienna (see e.g. [8]).

There are some old and new ingredients in the proof. Let me start by describing the old ones.

10. Old ingredients

(i) **Boltzmann's H Theorem (continued).** Let $(f_t)_{t\geq 0}$ be a nice solution of the Boltzmann equation. Then, as already mentioned, $dH/dt \leq 0$, where $H(t) = \int f_t \log f_t$. But the full H Theorem says more:

- There exists a functional $D \geq 0$, acting on $L^1(\mathbb{R}^n_v)$, such that

$$\frac{d}{dt} H(f_t) \quad = - \underbrace{\int_\Omega D(f_t(x,\cdot))\, dx}_{\textbf{entropy production}} \quad \leq 0.$$

- If $B > 0$ almost everywhere, then $D(f) = 0$ if and only if f is a **Maxwellian**:

$$f(v) = \frac{\rho\, e^{-\frac{|v-u|^2}{2T}}}{(2\pi T)^{n/2}} \equiv M_{\rho\, u\, T}(v).$$

In other words, entropy production can vanish at time t only if f_t is a **local Maxwellian** or "hydrodynamical state":

$$f_t(x,v) = M_{\rho\, u\, T}(v),$$
$$\rho = \rho(x), \quad u = u(x), \quad T = T(x).$$

(ii) **Classification of hydrodynamic solutions.** *Assume appropriate boundary conditions and appropriate geometric conditions on Ω (e.g. specular reflection and the domain is not axisymmetric); then, up to normalization of conservation laws, the unique solution which is* *hydrodynamical (locally Maxwellian) at all times is a global Maxwellian* (Here "global" means that the density, velocity, and temperature are uniform all over the box). In particular, this is the only stationary state.

These two ingredients are found in textbooks and are sufficient to prove convergence to equilibrium, but **without control of time scales**. The problem is to transform them into **quantitative estimates**. Let me describe some sources of inspiration for the solution.

11. Inspiration 1: Conjecture by Carlo Cercignani

Let $f = f(v)$ be a distribution in velocity space. Let ρ, u, T be the associated density, mean velocity, temperature. This defines a Maxwellian distribution $M^f_{\rho u T} = M_{\rho u T}(v)$.

We know: $D(f) = 0$ iff $f = M^f_{\rho u T}$.

Our **goal** is to establish an inequality roughly looking like $D(f) \geq$ "distance $(f,\ M^f_{\rho u T})$". Here D is the functional of entropy production, which appeared in the H Theorem of last section. Its explicit form is

$$D(f) = \frac{1}{4} \int \Big(f(v')f(v'_*) - f(v)f(v_*) \Big) \log \frac{f(v)f(v_*)}{f(v')f(v'_*)}\, B\, d\sigma\, dv\, dv_*$$

In this information-theoretic context, a good notion of "distance" is the Kullback information

$$H(f|M^f_{\rho u T}) = \int f \log \frac{f}{M^f_{\rho u T}}.$$

Strictly speaking, this is not a distance (although often called Kullback-Leibler distance), but it behaves in some respects like the square of a distance.

Cercignani's conjecture (around 1980)**:** *Under suitable positivity assumptions on the collision kernel B, holds the functional inequality*

$$D(f) \geq K\, H(f|M^f_{\rho u T}),$$

where K depends on ρ and T — maybe on other a priori estimates on f as well.

This conjecture is reminiscent of **logarithmic Sobolev inequalities**, which are inequalities about the entropy production for linear diffusion equations, invented several times in Information Theory (e.g. Stam) and in Constructive Quantum Field Theory (Nelson, Gross, Federbush...), and which revolutionized the study of diffusion processes. See [21, Chapter 9] or [1] for introduction and references.

Here is the most basic logarithmic Sobolev inequality. Consider the Fokker-Planck equation

$$\frac{\partial f}{\partial t} = \Delta_v f + \nabla_v \cdot (fv),$$

$$M(v) := \frac{e^{-\frac{|v|^2}{2}}}{(2\pi)^{3/2}},$$

Then

$$\int f \left| \nabla_v \log \frac{f}{M} \right|^2 dv \geq 2 \int f \log \frac{f}{M}\, dv$$

(In other words, the **Fisher information** dominates the entropy).

This suggested a challenging problem: *In spite of the complexity/nonlinearity of the Boltzmann operator, can one prove some similar bound, as suggested by Cercignani?*

12. Inspiration 2: cryptic comments by Harold Grad

Harold Grad was not always a very rigorous mathematician, but this is more than compensated by his brilliant hints and ideas. He is probably one of those who have done most to turn the theory of the Boltzmann equation into a field of mathematics; for that I express my deep gratitude to him, and consider it a great honor to have been selected as a Harold Grad lecturer!

The comments below are extracted from a rather obscure paper of his, entitled *On Boltzmann's H Theorem* (1965), containing some important mistakes but also beautiful intuition. Grad says:

"the H-Theorem gives no indication that there actually will be an approach to absolute equilibrium since it gives no clue to the transition from local to absolute Maxwellian" (...) "the question is whether the deviation from a local Maxwellian, which is fed by molecular streaming in the presence of spatial inhomogeneity, is sufficiently strong to ultimately wipe out the inhomogeneity" (...) "a valid proof of the approach to equilibrium in a spatially varying problem requires just the opposite of the procedure that is followed in a proof of the H-Theorem, viz., to show that the distribution function does not approach too closely to a local Maxwellian."

This calls for a bit of explanation. Here is how I understand Grad's point.

In Boltzmann's point of view, collisions, and the resulting loss of information, are the "driving mechanism" for convergence to equilibrium. But collisions cease to produce entropy as soon as f is **locally** Maxwellian (in this sense the Boltzmann equation is degenerate when seen as a diffusive equation). So why not get stuck around local Maxwellians? The answer is: Because the **streaming** (transport) operator, $v \cdot \nabla_x$, does not allow local Maxwellians to solve the Boltzmann equation! So to prove convergence to equilibrium, one should find a way to express the fact that transport processes are strong enough to destroy the local Maxwellian structure.

Analogy: In regularity theory: a degenerate diffusion (in velocity) operator combined with a drift term, such that both operators satisfy certain relations, may lead to regularization in all variables (this is known as **hypoellipticity**; the most famous hypoelliptic equation is the kinetic Fokker-Planck equation, also called Kramers equation). Similarly, the combination of a degenerately coercive operator (such as the Boltzmann collision operator, in some sense) and a transport term may imply approach to unique equilibrium: this can be called "hypocoercivity". As pointed out to me by Christian Schmeiser and Denis Serre independently, there is also a strong analogy with what is known in hyperbolic systems of conservation laws as Kawashima's condition.

13. Study of Cercignani's conjecture

• Counterexamples by Bobylev, Wennberg, Cercignani, ... show that *Cercignani's conjecture is in general false*

• First positive partial results: Carlen & Carvalho (1992), with subsequent improvement by Toscani & Villani (1999). A recent result by the author [20] establishes that "*Cercignani's conjecture is sometimes true, and always almost true*", in the sense of the theorem below. The paper can be consulted as well for a review of the above-mentioned previous results by Bobylev, Cercignani, Carlen, Carvalho, Toscani, Wennberg and the author.

Theorem:

(i) Let $B = 1 + |v - v_*|^2$ *[nonphysical assumption!], then Cercignani's conjecture holds true:* $D(f) \geq K\, H(f|M)$ *with*

$$K(f) = \frac{|S^{n-1}|}{4(2n+1)}\,(n - T^*(f)),$$
$$T^*(f) := \text{max eigenvalue of } \mathbb{P}.$$

(ii) For any reasonable B *(ex:* $|v - v_*|$*), if* f *has all its derivatives bounded, all its moments finite, and satisfies a lower bound* $f \geq K_0 \exp(-A_0|v|^{q_0})$*, then*

$$\forall \varepsilon > 0, \qquad D(f) \geq K_\varepsilon(f)\, H(f|M)^{1+\varepsilon},$$

where K_ε *only depends on smoothness, moments and positivity estimates on* f*.*

Here are some very sketchy elements about the proof of this theorem.

To go from (i) to (ii), the key is to establish the **tricky** non-concentration estimate

$$\int_{|v-v_*|\leq\delta} (f'f'_* - ff_*) \log \frac{f'f'_*}{ff_*}\, d\sigma\, dv\, dv_* = O\Big(\delta^{n-\varepsilon} H(f|M)^{1-\varepsilon}\Big),$$

where δ and ε are arbitrarily small. The fact that the exponent of δ in the right-hand side is close to n is not so important, but it is important that the exponent does not approach 0 as $\varepsilon \to 0$, and that the exponent of $H(f|M)$ be arbitrarily close to 1. This is what ensures that in the end the loss of exponent in the final inequality is arbitrarily small.

Next, here is a vague sketch of proof for (i). The argument involves the **relative Fisher information**, well-known in information theory and statistics:

$$I(f|M) = \int f|\nabla_v \log(f/M)|^2\, dv,$$

and the **Ornstein-Uhlenbeck regularization semigroup** (let's call it $(S_t)_{t\geq 0}$) generated by $\partial_t f = \Delta_v f + \nabla_v \cdot (fv)$. Note that $(d/dt)H(S_t f|M) = -I(S_t f|M)$.

The key identity, partially algebraic, is a commutator identity: let $\mathcal{E}(F,G) := (F-G)\log(F/G)$. Then

$$\frac{d}{dt}\bigg|_{t=0} [S_t, \mathcal{E}] = -\mathcal{J}, \qquad \mathcal{J}(F,G) = |\nabla \log F - \nabla \log G|^2 (F+G).$$

At the end of a quite intricate chain of inequalities, one can derive the following representation formula for a lower bound on D:

$$D(f) \geq K \int_0^{+\infty} e^{-4nt} \int_{\mathbb{R}^{2n}} \mathcal{J}(S_t F, S_t G)\, dv\, dv_*\, dt,$$

where $F(v, v_*) = f(v)f(v_*)$ is a tensor product and $G(v, v_*)$, being the average with respect to σ of $f(v')f(v'_*)$, only depends on $v + v_*$ and $|v|^2 + |v_*|^2$. This **conflict of symmetries** is the key: it implies, after another chain of inequalities,

$$\int_{\mathbb{R}^{2n}} \mathcal{J}(S_t F, S_t G)\, dv\, dv_* \geq K\, I(S_t f|M).$$

To conclude, one uses the inequality

$$e^{-4nt} I(g|M) \geq I(S_{2nt}\, g|M)$$

(a particular case of the **Blachman-Stam inequality** from information theory). The final result is

$$\Longrightarrow D(f) \geq K \int_0^{+\infty} I(S_{(2n+1)t} f|M)\, dt = \frac{K}{2n+1}\, H(f|M).$$

The complete proof is quite tricky and relies on the precise form of the collision operator; but once it is done, *we can forget almost everything about the precise form of the Boltzmann collision operator, and only recall that*

$$-\frac{d}{dt}\, H(f|M) \geq K_\varepsilon\, H(f|M^f_{\rho u T})^{1+\varepsilon}.$$

In the spatially homogeneous case, this would be the end of the game: what we just proved is $-\dfrac{d}{dt}\, H(f|M) \geq K_\varepsilon\, H(f|M)^{1+\varepsilon} \Longrightarrow$ By Gronwall, $H(f|M) = O(t^{-\frac{1}{\varepsilon}})$, and we are done since this implies convergence to equilibrium like $O(t^{-1/2\varepsilon})$.

But now comes another enemy: *spatial inhomogeneity!* Since in general ρ, u, T depend on x, the entropy production does **not** control $H(f|M)$!!! We can only write

$$\frac{d}{dt}[H(f) - H(M_{\rho u T})] = -D(f) \leq -K[H(f) - H(M_{\rho(x)\, u(x)\, T(x)})]^{1+\varepsilon},$$

and then there is no way of applying Gronwall's lemma...

To fight this enemy, we need to leave the world of information theory (collisions) and enter the world of fluid mechanics (streaming). Before, let me list make a brief recap about Cercignani's conjecture and the aftermath of the theorem presented above.

14. Still open problems about Cercignani's conjecture

- Can one get rid of smoothness assumptions when establishing a bound like $D \geq KH^{1+\varepsilon}$?

- Why does the Boltzmann operator fail Cercignani's conjecture by so little?

- Similar problem for Kac's one-dimensional caricature of a Maxwellian gas: in that case it seems that moment bounds are enough to establish a bound like $D \geq KH$! (although this has not been proved). Why then is there a problem with the Boltzmann operator? *Does the problem come from momentum conservation?*

- Can one understand the problem "microscopically" via entropic versions of chaos and Kac's spectral gap conjecture? (works in progress by Carlen, Carvalho, Lieb, Loss, Le Roux, and the author)

All in all, this is a good illustration that **entropic inequalities** are more sensitive to details of dynamics than spectral gap! In some sense, a few "exceptional" particles may affect these inequalities... (after all, entropy is used in large deviation theory for the detection of small probability events).

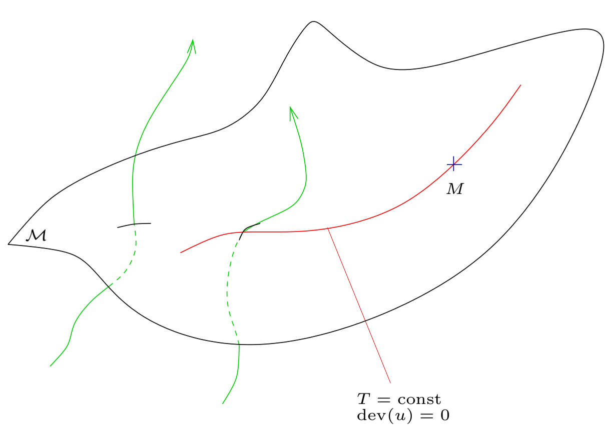
15. Understanding Grad's intuition: instability of hydrodynamical approximation

Here is the **main idea** which we worked out with Desvillettes: *If f approaches a local Maxwellian, not global, then f will depart "transversally" from the space $\mathcal{M}$ of all local Maxwellian distributions.*

This vague statement will be quantified only on the average, and holds true only for generic local Maxwellian. In fact:
– $\nabla T \neq 0$, or $\mathrm{dev}(u) \neq 0 \Longrightarrow$ departure from $\mathcal{M}$;
– symmetrized gradients of $u \Longrightarrow$ departure from the subspace of $\mathcal{M}$ with uniform temperature;
– gradients of $\rho \Longrightarrow$ departure from the subspace of $\mathcal{M}$ with uniform temperature and zero velocity field.

In the above, $\mathrm{dev}(u)$ stands for the *deviatoric part* of the velocity field u, defined as $\dfrac{(\nabla u + (\nabla u)^T)}{2} - \dfrac{\mathrm{div}(u)}{n} I_n$, i.e. the traceless part of the symmetric Reynolds tensor. It is well-known in hydrodynamics and plays an important role here too.

Here is a **schematic picture of the dynamics** summarizing the above statements. The flow is supposed to represent in a fuzzy way the Boltzmann flow; the surface drawn here stands for the infinite-dimensional manifold of locally Maxwellian distributions; this manifold is unstable in some sense, except along a certain sub-manifold (no gradients of temperature, no deviatoric part); this sub-manifold itself is unstable, except for a sub-sub-manifold (not represented here; no gradients of temperature, no gradients of velocity); this sub-sub-manifold is in turn unstable, except for the global equilibrium M.



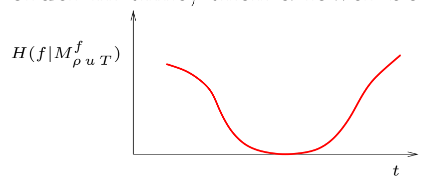
The question is how to turn this picture into **quantitative bounds**. We used the following recipe (adapted from Desvillettes & Villani [5]): compute a lower bound for

$$\frac{d^2}{dt^2}\|f - M^f_{\rho\,u\,T}\|^2_{L^2(\Omega\times\mathbb{R}^n)}.$$

Let me answer some of the most immediate questions about that strategy:

- *Why the second derivative?*

1) to estimate the speed of departure from $\mathcal{M}$; if the Kullback information of f to M^f ever vanishes, one can at best hope that this is at second order in time; then a lower bound on the second derivative will prevent it to vanish too much;



2) by applying the equation twice, **we shall have the transport operator $v \cdot \nabla_x$ enter the equations twice, and this will have the same effect as a** Δ_x; this is the way we recover "ellipticity".

(Cf. the Chapman-Enskog procedure to go from the Boltzmann equation to the compressible Navier-Stokes system: the appearance of the viscosity in that process can be traced back to the repeated appearance of the transport operator)

- *Why a square norm?*

1) for smoothness: the square norm is easier to handle, than, say, the norm itself;

2) because $H(f|g)$ anyway behaves somewhat like a square norm. In fact it is well-known that $H(f|g) \geq \dfrac{\|f-g\|^2_{L^1}}{2}$.

- *Why not look at $(d^2/dt^2)H(f|M^f_{\rho\,u\,T})$?*

Because it is very difficult, if not impossible, to control a Kullback information *from above* by something (almost) quadratic without using stronger estimates, like $L^\infty(M^{-1}\,dv\,dx)$.

Now that the goal is clearer, we can go on: after monster computations, we find

$$\frac{d^2}{dt^2}\|f - M^f_{\rho\,u\,T}\|^2_{L^2} \geq K\int_\Omega \left(|\nabla_x T|^2 + |\mathrm{dev}(u)|^2\right)dx - C_\varepsilon(f)\,\|f - M^f_{\rho\,u\,T}\|^{1-\varepsilon}_{L^2}\,H(f|M)^{\frac{1-\varepsilon}{2}},$$

where $C_\varepsilon(f)$ depends on smoothness/moments of f at high enough order (interpolation...), and a lower bound.

Now there is no gradient of ρ in the right-hand side! This reflects the existence of *quasi-equilibria* (the sub-manifold referred to above), for which the entropy production vanishes at high order in time (typically, order 4 instead of 2), but ρ is not uniform.

To remedy this, we establish two "similar" inequalities with $M^f_{\rho\,u\,T}$ replaced by

$M^f_{\rho\,u\,\langle T\rangle} \longrightarrow$ presence of $\int |\nabla^{\mathrm{sym}} u|^2\,dx$;

$M^f_{\rho\,0\,1} \longrightarrow$ presence of $\int |\nabla \rho|^2\,dx$.

We don't write down these inequalities explicitly here, the reader will find them all in Desvillettes & Villani [7].

16. Putting both features together

It remains to "glue" together our quantitative H Theorem on one hand, and the instability of hydrodynamical regime on the other. This is not trivial, because these results are expressed in terms of different functionals.

1) *First tool: Additivity of the entropy*

A beautiful property of Boltzmann's entropy is that it can be separated into a "purely kinetic" and a "purely hydrodynamical" parts:

$$H(f|M) = H(f|M^f_{\rho\, u\, T}) + \mathcal{H}(\rho, u, T),$$

where

$$\mathcal{H}(\rho, u, T) = \int_\Omega \rho \log \frac{\rho}{T^{n/2}}\, dx$$

$$= \int (\rho \log \rho - \rho + 1) \quad + \quad \int \rho\, \frac{|u|^2}{2} + \ \frac{n}{2}\, \phi(\langle T \rangle_\rho) \quad + \quad \frac{n}{2}\Big[\langle \phi(T) \rangle_\rho - \phi(\langle T \rangle_\rho)\Big],$$

$$\phi(T) = T - \log T - 1.$$

There are two other "similar" formulas involving $M^f_{\rho\, u\, \langle T \rangle}$, $M^f_{\rho\, 0\, 1}$.

2) *Second tool: "Geometrical" inequalities*

We use two types of inequalities:

Poincaré inequality:

$$\int |\nabla T|^2\, dx \geq K(\Omega)\, \|T - \langle T \rangle_\rho\|^2_{L^2(\rho)}; \qquad \text{etc.}$$

Korn inequality:

$$\int |\nabla^{\mathrm{sym}} u|^2\, dx \geq \mathcal{K}(\Omega) \int |\nabla u|^2\, dx,$$

$\longrightarrow$ For specular reflection (which results in the tangency condition: u tangent to the boundary), the Korn constant $\mathcal{K}(\Omega)$ is positive iff Ω not axisymmetric!

3) *Third tool: Relating entropies and L^2 norms*

For this we use interpolation:

$$H(f|M^f_{\rho\, u\, T}) \geq K_\varepsilon(f) \Big(\|f - M^f_{\rho\, u\, T}\|^2_{L^2}\Big)^{1+\varepsilon}, \qquad \text{etc.}$$

$$\int (\rho \log \rho - \rho + 1) \leq C(f) \|\rho - 1\|^2_{L^2}, \qquad \text{etc.}$$

At the end of the day, we obtain a system of 4 "nonlinear" differential inequalities (first and second-order in t) coupled by identities and inequalities. To deal with this system, we need a replacement for Gronwall's lemma. What will play this role is the following estimate:

Lemma: *Let $h(t) \geq 0$ satisfy*

$$\forall t \in (t_1, t_2), \qquad h''(t) + A h(t)^{1-\varepsilon} \geq \alpha > 0,$$

for some $\varepsilon < 0.1$. Then,

- *either* $t_2 - t_1$ *is small:*

$$t_2 - t_1 \leq 50\, \frac{\alpha^{\frac{\varepsilon}{2(1-\varepsilon)}}}{A^{\frac{1}{2(1-\varepsilon)}}};$$

- *or* h *is large on the average:*

$$\frac{1}{t_2 - t_1} \int_{t_1}^{t_2} h(t)\, dt \geq \frac{\alpha^{\frac{1}{1-\varepsilon}}}{100}\, \inf\left(\frac{1}{A}, \frac{1}{A^2}\right).$$

It is not completely the end: to apply this lemma, we need the differential inequalities to be valid on "not too short" time intervals, and therefore first rule out rapid oscillations of hydrodynamic quantities. Because M is stationary and f is smooth, one can establish inequalities of the style

$$\left|\frac{d}{dt} \int \rho \log \rho\, dx\right| \leq C_\varepsilon(f)\, H(f|M)^{1-\varepsilon}; \qquad \text{etc.}$$

(we obtain three such new differential inequalities).

After putting together all the pieces of the puzzle, we prove: for $\varepsilon < 0.01$, the whole system of differential inequalities implies

$$H(f_t|M) = O(t^{-1/250\varepsilon}).$$

This conclues the proof of the main theorem.

17. What do we learn from the proof?

• An indication of how the shape of the box influences equilibration rates, via the constants in the Korn and Poincaré inequalities. For specular boundary conditions ($u \cdot n = 0$), there is a particularly interesting point: the positivity of the Korn constant $\mathcal{K}(\Omega)$ in

$$\int |\nabla^{\mathrm{sym}} u|^2\, dx \geq \mathcal{K}(\Omega) \int |\nabla u|^2\, dx,$$

quantifies the *departure of* Ω *from axisymmetry.* If Ω is convex, then $\mathcal{K}(\Omega)$ is bounded below in terms of what Desvillettes and myself defined as **Grad's number** (here for $n = 3$):

$$G(\Omega) := \inf_{\sigma \in S^2}\, \inf_u \left\{ \|\nabla^{\mathrm{sym}} u\|^2_{L^2(\Omega)}; \quad \nabla \cdot u \equiv 0, \quad \mathrm{curl}\,(u) \equiv \sigma, \quad u \cdot n = 0. \right\}$$

This quantity appears in Grad [10]! When Desvillettes and myself searched for more quantitative estimates of $G(\Omega)$, it was our great surprise to discover that this could be related to a **Monge-Kantorovich** minimization problem! See [6] and [21, Problem 3, pp. 310–314].

• The proof suggests that $H(f|M^f_{\rho u T})$, which measures *how close* f *is from being hydrodynamic*, may show **strong time-oscillations**.

On some integrable baby models (gaussian diffusion semigroups...), this is true. But for Boltzmann equation??

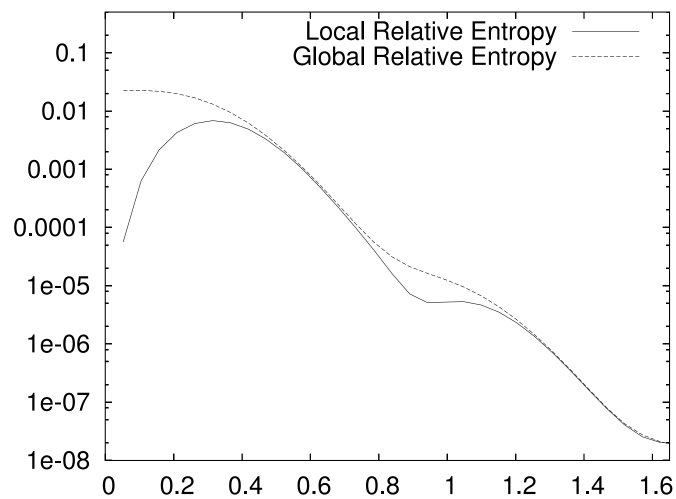


FIGURE 1. Local and global entropy; distance to local equilibrium

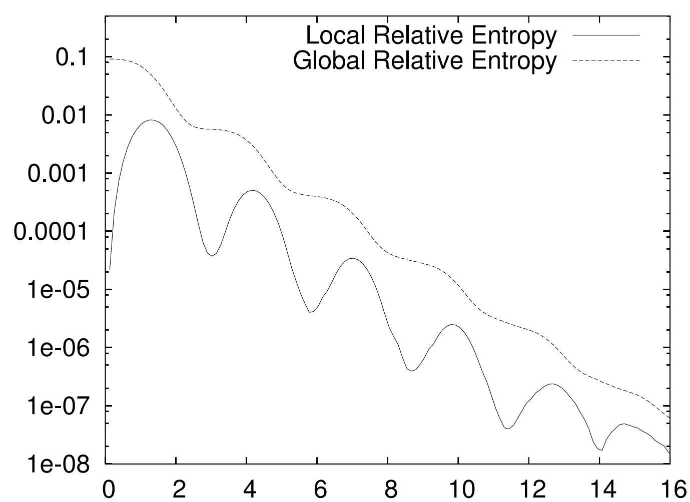


FIGURE 2. The same in a larger box

Let's look at numerical simulations by Filbet on a simplified geometry (periodic, 1 dimension of space, 2 dimensions of velocity) with an accurate spectral code [9] (the length L is the size of the periodic box, the Knudsen number is of order 0.25).

In these experiments, the initial datum was chosen to be in local equilibrium. Since this is a logarithmic plot, the convergence seems to be in fact exponential, as could be expected, and it is faster for a small box. What is much more surprising is the fact that, on Fig. 1, the dynamics behaves almost in a spatially homogeneous way after some time, contrary to the possibly natural guess that the hydrodynamical regime would be attained first. That is left for future understanding!

On Fig. 2 on the contrary, the oscillations in the entropy production are quite well-marked, and definitely suggest that the solution oscillates between states where it is quite close to hydrodynamic, and states where it is not at all.

This kind of behavior in any way is a clear indication that things in the spatially inhomogeneous context can be much, much more subtle than in the spatially homogeneous one. No such "weird" behavior is ever observed in numerical simulations of the spatially homogeneous Boltzmann equation!

Filbet has observed these oscillations for many other kinetic models, linear or not. There often seems to be a well-identified period of oscillation, which varies according to the local conservation laws. Here now is another riddle left for future understanding: in the case of the BGK model, one can choose to impose local conservation of mass, momentum and temperature, or a subset of them. In all the cases, there are oscillations, *except* when only the mass is conserved! This absence of oscillations is not due to the fact that the resulting model is linear: oscillations can be observed for some linear Fokker-Planck equations. So what makes the linear BGK model qualitatively different from the other cases??? Is this related to the high degeneracy of its spectrum?

18. Towards the linearized regime

For certain models of interaction (typically, hard potentials), there is a spectral gap for the Boltzmann operator, so one expects **exponential convergence** and not just convergence in $O(t^{-\infty})$. To prove this, it is natural to first wait until one enters the linearized regime; and then to study the linearized equation. So the question is

How to get exponential convergence in the end!? with an explicit rate?

There are some real difficulties in answering this question. At the time of writing, they seem to be very well under way of being solved.

(i) The spectral gap for the linearized Boltzmann operator is **not computable** (or at least does not seem to be), except in the particular case of Maxwellian kernel

$\longrightarrow$ solved by Baranger-Mouhot [2]: they estimate below the spectral gap for hard potentials by clever reduction to the Maxwellian case;

(ii) Solutions of the nonlinear Boltzmann equation **do not decay fast enough** at infinity to lie in a space where the Boltzmann operator is self-adjoint

$\longrightarrow$ solved by Mouhot [17] in the spatially homogeneous case: the spectral gap for very rapidly decaying solutions determines the rate of exponential convergence, even if the initial datum is not assumed to decay very rapidly, but only to have finite moments;

(iii) **Degeneracy in the x variable** (hypocoercivity problem again)

$\longrightarrow$ related to recent work by Rey-Bellet, Stuart, Hérau, Nier, Lions, Eckmann, Hairer... done on other models. On that issue, recent progress has been made by the author on one hand, by Mouhot and Neumann on the other hand (building on ideas by Guo). Here the need can be felt to develop a new chapter of qualitative study of linear operators, parallel to that of hypoellipticity in regularity theory. Such a theory may have applications to many interesting problems arising in probability theory or partial differential equations.

Let me take this opportunity to conclude by expressing my deep conviction that kinetic theory, being a particularly rich mathematical field, has been, and will be again in the future, a source of inspiration and progress for other fields of applied mathematics.

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