Reaction-Diffusion Equations for chemical networks; Equations de réaction-diffusion pour des réseaux de réactions chimiques

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Quantitative version of La Salle's principle.

We consider the abstract equation (for $f := f(t, ...)$)

$$\partial_t f = A(f)$$

which possesses a Lyapounov functional (entropy) (for $t \mapsto f(t)$ solution of the equation)

$$\frac{d}{dt} H(f(t)) = -D(f(t)) \leq 0,$$

supposed to be strict in the following sense f_∞,

$$A(f) = 0 \iff D(f) = 0 \iff H(f) = H(f_\infty) \iff f = f_\infty.$$

Quantitative entropy method

Entropy equality:

$$\frac{d}{dt} H(f(t)) = -D(f(t)) \leq 0.$$

We look for a **functional inequality** between entropy and entropy dissipation

$$D(f) \geq Cst\,(H(f) - H(f_\infty)).$$

If it exists, all the solutions $t \mapsto f(t)$ of the equation satisfy

$$\frac{d}{dt}\Big(H(f(t)) - H(f_\infty)\Big) \leq -Cst\,\Big(H(f(t)) - H(f_\infty)\Big),$$

so that exponential convergence holds **with explicitly computable parameters** for the entropy

$$0 \leq H(f(t)) - H(f_\infty) \leq Cst\, e^{-Cst\, t}.$$

Quantitative entropy method

The method often allows to show that $f(t) \to f_\infty$ for some norm, with a known rate of convergence

Example of tool: Inequality of Cziszár-Kullback-Pinsker;

Assuming the normalisation

$$\int_{\mathbb{R}^N} f(x)\,dx = \int_{\mathbb{R}^N} g(x)\,dx = 1,$$

one has

$$\int_{\mathbb{R}^N} f(x)\,\ln\left(\frac{f(x)}{g(x)}\right)\,dx \geq \frac{1}{2}\,||f-g||^2_{L^1(\mathbb{R}^N)}.$$

Quantitative entropy method

The method has many useful variants

$$D(f) \geq C(f)\,(H(f) - H(f_\infty)),$$

where $t \mapsto C(f(t)) \geq C_0 > 0$, when $t \mapsto f(t)$ is solution of the equation.

This means that the functional inequality has to be true only on the set of functions satisfying the **uniform in time a priori estimates** of the equation

The convergence towards equilibrium remains then exponential

Quantitative entropy method

In another variant, for some (or all) $\varepsilon > 0$,

$$D(f) \geq C_\varepsilon \, (H(f) - H(f_\infty))^{1+\varepsilon},$$

so that

$$\frac{d}{dt}\Big(H(f(t)) - H(f_\infty)\Big) \leq -C_\varepsilon \, \Big(H(f(t)) - H(f_\infty)\Big)^{1+\varepsilon},$$

and algebraic (power law) convergence holds (with explicitly computable parameters) for the entropy:

$$0 \leq H(f(t)) - H(f_\infty) \leq C_\varepsilon \, t^{-1/\varepsilon}.$$

Example: Boltzmann equation with hard potentials (G. Toscani, C. Villani).

Quantitative entropy method

In another variant

$$D(f) \geq C(f)\,(H(f) - H(f_\infty)),$$

where $t \mapsto C(f(t))$ decays towards when $t \mapsto f(t)$ is a solution of the equation: **Slowly growing a priori bounds**

The convergence towards equilibrium is then usually less quick than exponential

- If $C(f(t)) \geq Cst\, t^{-q}$ with $q \in]0,1[$ then

$$0 \leq H(f(t)) - H(f_\infty) \leq Cst\, e^{-Cst\, t^{1-q}}.$$

- If $C(f(t)) \geq Cst\, t^{-1}$, then

$$0 \leq H(f(t)) - H(f_\infty) \leq \frac{Cst}{t^{Cst}}.$$

Quantitative entropy method

Examples: Boltzmann equation with soft potentials (G. Toscani, C. Villani); Reaction-diffusion systems associated with one reversible chemical reaction with four species in dimension 1 and 2 (J. Canizo, LD, K. Fellner)

Recently used variant

$$D(f) \geq a(t)\,(H(f) - H(f_\infty)) - b(t),$$

where $a(t) \to 0$ slowly $b(t) \to 0$ quickly.

Example: Landau equation with Coulomb interaction in plasma theory (K. Carrapatoso, LD, L. He).

Use of the quantitative entropy method for specific equations

Kinetic equations:

1. Fokker-Planck: D. Bakry, M. Emery; G. Toscani; A. Arnold, P. Markowich, G. Toscani, A. Unterreiter.
2. Boltzmann (Cercignani's conjecture): E. Carlen, M. Carvalho; G. Toscani, C. Villani; C. Villani
3. Discrete coagulation-fragmentation: P.-E. Jabin, B. Niethammer
4. Continuous coagulation-fragmentation: M. Aizenmann, T. Bak; J. Carrillo, LD, K. Fellner
5. Landau: LD, C. Villani; K. Carrapatoso, LD, L. He

Parabolic equations:

1. Nonlinear diffusion: M. Del Pino, J. Dolbeault
2. Fourth order equations: M. Cáceres, J. Carrillo, G. Toscani
3. Reaction-Drift-Diffusion: A. Glitzky, K. Gröger, R. Hünlich; LD, K. Fellner; LD, K. Fellner, B. Quoc Tang

Large time behavior for a system of equations coming from reversible chemistry; Comportement en temps grand d'un système d'équations provenant de la chimie réversible

Chemical reaction

$$A_1 + A_2 \quad \rightleftharpoons \quad A_3$$

Corresponding reaction-diffusion equations

$$\begin{cases} \partial_t a_1 - d_1 \Delta_x a_1 = a_3 - a_1\, a_2, & x \in \Omega, \quad t > 0, \\ \partial_t a_2 - d_2 \Delta_x a_2 = a_3 - a_1\, a_2, & x \in \Omega, \quad t > 0, \\ \partial_t a_3 - d_3 \Delta_x a_3 = a_1\, a_2 - a_3, & x \in \Omega, \quad t > 0, \\ \\ \nabla_x a_i \cdot n(x) = 0, & x \in \partial\Omega, \quad t > 0, \\ a_i(0,x) = a_{i0}(x), & x \in \Omega. \end{cases}$$

Large time behavior for a system of equations coming from reversible chemistry; Comportement en temps grand d'un système d'équations provenant de la chimie réversible

Theorem (LD, Fellner): Let Ω be a smooth bounded domain of $\mathbb{R}^N$, $d_i > 0$, and $a_{i0} \geq 0$ be smooth. Then the unique smooth solution to the system satisfies

$$\sum_{i=1}^{3} ||a_i(t,\cdot) - a_{i\infty}||_\infty \leq Cst\, e^{-Cst\, t},$$

where Cst can be estimated explicitly, $a_{i\infty} > 0$ is constant, and

$$a_{1\infty}\, a_{2\infty} = a_{3\infty}, \quad a_{1\infty} + a_{3\infty} = |\Omega|^{-1} \int_\Omega [a_{10}(x) + a_{30}(x)]\, dx,$$

$$a_{2\infty} + a_{3\infty} = |\Omega|^{-1} \int_\Omega [a_{20}(x) + a_{30}(x)]\, dx.$$

Large time behavior for a system of equations coming from reversible chemistry; Comportement en temps grand d'un système d'équations provenant de la chimie réversible

Idea: Use the quantitative entropy method with

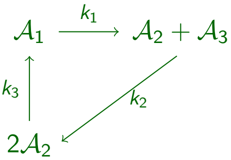
$$H(a_1, a_2, a_3) = \sum_{i=1}^{3} \int_\Omega a_i\,(\ln a_i - 1)\,dx,$$

and

$$D(a_1, a_2, a_3) = \sum_{i=1}^{3} d_i \int_\Omega \frac{|\nabla_x a_i|^2}{a_i}\,dx + \int_\Omega (a_1\,a_2 - a_3)\,(\ln(a_1\,a_2) - \ln a_3)\,dx.$$

Best available result for one chemical equation: Exponential convergence in L^1 for systems coming out of one general chemical equations when the equilibrium is interior, convergence when it is a boundary equilibrium. Pierre, Suzuki, Umakoshi

An example of chemical network; Un example de réseau de réactions chimiques



Applying the mass action law leads to the 3×3 reaction-diffusion system ($k_1 = k_2 = k_3 = 1$):

$$\begin{cases} \partial_t a_1 - d_1 \Delta_x a_1 = -a_1 + a_2^2, & x \in \Omega, \quad t > 0, \\ \partial_t a_2 - d_2 \Delta_x a_2 = a_1 + a_2\, a_3 - 2a_2^2, & x \in \Omega, \quad t > 0, \\ \partial_t a_3 - d_3 \Delta_x a_3 = a_1 - a_2\, a_3, & x \in \Omega, \quad t > 0, \\ & \\ \nabla_x a_i \cdot n(x) = 0, & x \in \partial\Omega, \quad t > 0, \\ a_i(0,x) = a_{i0}(x), & x \in \Omega. \end{cases}$$

Conservation law associated to the network

$$\begin{cases} \partial_t a_1 - d_1 \Delta_x a_1 = -a_1 + a_2^2, & x \in \Omega, \quad t > 0, \\ \partial_t a_2 - d_2 \Delta_x a_2 = a_1 + a_2\, a_3 - 2a_2^2, & x \in \Omega, \quad t > 0, \\ \partial_t a_3 - d_3 \Delta_x a_3 = a_1 - a_2\, a_3, & x \in \Omega, \quad t > 0, \\ \\ \nabla_x a_i \cdot n(x) = 0, & x \in \partial\Omega, \quad t > 0, \\ a_i(0,x) = a_{i0}(x), & x \in \Omega. \end{cases}$$

$$\frac{d}{dt} \int_\Omega \Big(2a_1 + a_2 + a_3 \Big)\, dx = 0,$$

$$\int_\Omega \Big(2a_1(t,x) + a_2(t,x) + a_3(t,x) \Big)\, dx = \int_\Omega \Big(2a_{10}(x) + a_{20}(x) + a_{30}(x) \Big)\, dx := M.$$

Existence theory for this model

Proposition: Let Ω be a bounded smooth (C^2) domain of $\mathbb{R}^N$, and $d_1, d_2, d_3 > 0$. Assume nonnegative initial data $a_{i0} \in L^\infty(\Omega)$, and denote

$$\delta := \max\{d_i\} - \min\{d_i\}.$$

Consider either $1 \le N \le 5$ or $N \ge 6$ and $\delta > 0$ sufficiently small (depending on N).
Then, there exists a unique, nonnegative, global classical solution $(a_i)_{i=1,..,3}$ to the system, which satisfies the following L^∞-bound for all $T > 0$

$$\sum_{i=1}^{3} \|a_i\|_{L^\infty(\Omega_T)} \le C(T),$$

where $C(T)$ grows at most polynomially with respect to T.
Moreover the conservation of mass is satisfied:

$$\int_\Omega \Big(2\, a_1(x,t) + a_2(x,t) + a_3(x,t) \Big)\, dx = M \quad \text{for all} \quad t > 0.$$

Equilibria of the network

The solutions of

$$\begin{cases} a_{1\infty} + a_{2\infty}^2 = 0, \\ a_{1\infty} + a_{2\infty} a_{3\infty} - 2a_{2\infty}^2 = 0, \\ a_{1\infty} - a_{2\infty} a_{3\infty} = 0, \end{cases}$$

with

$$2a_{1\infty} + a_{2\infty} + a_{3\infty} = M > 0$$

are the interior equilibrium

$$a_{1\infty} = a_{2\infty}^2, \;\; a_{2\infty} = \frac{-1 + \sqrt{1 + 2M}}{2}, a_{3\infty} = a_{2\infty},$$

and the boundary equilibrium

$$(a^*, b^*, c^*) = (0, 0, M).$$

Entropy structure

We consider the entropy associated to the so-called complex balance equilibrium structure

$$H(a_1, a_2, a_3) = \sum_{i=1}^{3} \int_\Omega \left(a_i \ln \frac{a_i}{a_{i\infty}} - a_i + a_{i\infty} \right) dx,$$

and its entropy dissipation

$$D(a_1, a_2, a_3) = \sum_{i=1}^{3} d_i \int_\Omega \frac{|\nabla a_i|^2}{a_i} dx + \int_\Omega \Bigg[a_{1\infty} \Psi \left(\frac{a_1}{a_{1\infty}}; \frac{a_2 a_3}{a_{2\infty} a_{3\infty}} \right) + a_{2\infty} a_{3\infty} \Psi \left(\frac{a_2 a_3}{a_{2\infty} a_{3\infty}}; \frac{a_2^2}{a_{2\infty}^2} \right) + a_{2\infty}^2 \Psi \left(\frac{a_2^2}{a_{2\infty}^2}; \frac{a_1}{a_{1\infty}} \right) \Bigg] dx.$$

where

$$\Psi(x; y) = x \log \frac{x}{y} - x + y.$$

Entropy structure: difficulties

Proposition: *When boundary equilibria do not exist* in a chemical reaction network with complex balance equilibrium, an inequality between entropy and entropy dissipation exists for a unique interior equilibrium $(a_{1\infty}, .., a_{N\infty})$:

$$D(a_1, .., a_N) \geq Cst \left(H(a_1, .., a_N) - H(a_{1\infty}, .., a_{N\infty}) \right)$$

(LD, K. Fellner, B. Quoc Tang), leading to exponential equilibration of any renormalised solutions (R. J. DiPerna, P.-L. Lions; LD, K. Fellner, M. Pierre, J. Vovelle; J. Fischer).

$$H(a_1, .., a_N) - H(a_{1\infty}, .., a_{N\infty}) \leq Cst\, e^{-Cst\, t}.$$

Main tools: Logarithmic Sobolev inequalities; Convexification.

Entropy structure: difficulties

Here a_3 always appears multiplied by a_2 in the entropy dissipation, so that when $a_1 = a_2 = 0$, the dissipation is $D = 0$, and there is no hope of getting

$$D(a_1, a_2, a_3) \geq Cst \left(H(a_1, a_2, a_3) - H(a_{1\infty}, a_{2\infty}, a_{3\infty}) \right).$$

Instead we get

$$D(a_1, a_2, a_3) \geq Cst \, \inf(a_2) \left(H(a_1, a_2, a_3) - H(a_{1\infty}, a_{2\infty}, a_{3\infty}) \right).$$

The exponential equilibration towards $(a_{1\infty}, a_{2\infty}, a_{3\infty})$ for all initial data different form $(0, 0, M)$ is not possible. In particular, a whole class of initial data: $(0, 0, a_{30})$, produces solutions which tend to $(0, 0, M)$.

Solution

One computes

$$\partial_t \left(\frac{1}{a_2}\right) - d_2\,\Delta\left(\frac{1}{a_2}\right) = -\frac{a_1}{2a_2^2} - \frac{a_3}{a_2} + 2 - 2d_2\frac{|\nabla a_2|^2}{a_2^3} \leq 2.$$

Thus, using the maximum principle, we obtain

$$\left\|\frac{1}{a_2(t)}\right\|_{L^\infty(\Omega)} \leq \left\|\frac{1}{a_{20}}\right\|_{L^\infty(\Omega)} + 2t, \qquad \text{for all} \quad t.$$

As a consequence, if $a_{20} \geq Cst > 0$,

$$a_2(t) \geq \frac{Cst}{1 + Cst\, t}, \qquad \text{for all} \quad t.$$

Solution

Entropy-entropy dissipation estimate

$$D(a_1, a_2, a_3) \geq Cst\ \inf(a_2) \Big(H(a_1, a_2, a_3) - H(a_{1\infty}, a_{2\infty}, a_{3\infty}) \Big),$$

so that

$$-\frac{d}{dt}\Big(H(a_1, a_2, a_3) - H(a_{1\infty}, a_{2\infty}, a_{3\infty}) \Big)$$
$$\geq \frac{Cst}{1 + Cst\ t} \Big(H(a_1, a_2, a_3) - H(a_{1\infty}, a_{2\infty}, a_{3\infty}) \Big),$$

and

$$H(a_1(t,\cdot), a_2(t,\cdot), a_3(t,\cdot)) - H(a_{1\infty}, a_{2\infty}, a_{3\infty}) \leq \frac{Cst}{(1 + Cst\ t)^{Cst}}.$$

Solution

Use of a Cziszár-Kullback type inequality

$$||a_2(t) - a_{2\infty}||_{L^1} \leq \frac{1}{2}\, ||a_{2\infty}||_{L^1} \qquad \Rightarrow \qquad ||a_2(t)||_{L^1} \geq Cst > 0,$$

for $t \geq t_0$ (with t_0 computable).

Then we can use again the entropy-entropy dissipation estimate

$$D(a_1, a_2, a_3) \geq Cst\, \inf(a_2) \Big(H(a_1, a_2, a_3) - H(a_{1\infty}, a_{2\infty}, a_{3\infty}) \Big)$$

which leads to the exponential convergence

$$H(a_1(t,\cdot), a_2(t,\cdot), a_3(t,\cdot)) - H(a_{1\infty}, a_{2\infty}, a_{3\infty}) \leq Cst\, e^{-Cst\, t}.$$

Final result

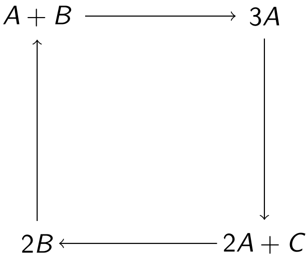
Theorem (LD, K. Fellner, B. Quoc Tang): Let Ω be a bounded smooth (C^2) domain of $\mathbb{R}^n$, and $d_i > 0$. Assume that the initial data $a_{i0} \in (L^\infty(\Omega))^3$ are such that a_{20} is a.e. bounded below by a strictly positive constant, i.e. $\|\frac{1}{a_{20}}\|_{L^\infty(\Omega)} < \infty$

Then, there exist explicit constants $C > 0$ and $\lambda > 0$ such that any classical solutions of the system of equations converge exponentially fast to the unique strictly positive complex balance equilibrium $a_{i\infty}$ with the rate λ, that is

$$\|a_i(t) - a_{i\infty}\|_{L^1(\Omega)} \le C\, e^{-\lambda t}, \qquad \text{for all} \quad t > 0,$$

where the constant C depends only on the initial relative entropy, and λ depends only on Ω, M, d_i, and $\|\frac{1}{a_{20}}\|_{L^\infty(\Omega)}$.

Another example of chemical network



Corresponding equations

$$
\begin{aligned}
\partial_t a - d_1 \Delta a &= 2ab - a^3 - 2a^2 c + b^2, \\
\partial_t b - d_2 \Delta b &= -ab + 2a^2 c - b^2, \\
\partial_t c - d_3 \Delta c &= a^3 - a^2 c,
\end{aligned}
$$

with homogeneous Neumann boundary conditions.

Another example of chemical network

This system has no conservation laws.

It has a unique positive (interior) complex balance equilibrium and a one-dimensional manifold of boundary equilibria
$\mathcal{V} = \{(0, 0, c^*) : c^* \in \mathbb{R}_+\}$.

No proof yet of exponential decay towards the interior complex balance equilibrium

Decay towards the interior complex balance equilibrium known for the corresponding ODE (but hard). Part of a general conjecture on ODEs.