Logarithmic Sobolev inequality applied to non-linear Cauchy problems

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Reversible chemical reaction (diffusion)

$$\sum_{i=1}^{q} \alpha_i \mathcal{A}_i \rightleftharpoons \sum_{i=1}^{q} \beta_i \mathcal{A}_i,$$

$\mathcal{A}_i$ are species with $\alpha_i \neq \beta_i$.

- Main example : the *two-by-two* case

$$\mathcal{A}_1 + \mathcal{A}_2 \rightleftharpoons \mathcal{B}_1 + \mathcal{B}_2,$$

for instance, *sodium chloride* and *silver nitrate* into *sodium nitrate* and *silver chloride*

$$NaCl + AgNO_3 \rightleftharpoons NaNO_3 + AgCl.$$

• The law of action mass (Waage and Guldberg in 1864) says u_i are concentration

$$\frac{d}{dt}u_i = (\beta_i - \alpha_i)\left(k\prod_{j=1}^{q} u_j^{\alpha_j} - \ell\prod_{j=1}^{q} u_j^{\beta_j}\right),$$

(at the same time than Boltzmann for its equation).
• And the same equation a "diffusion" term

$$\partial_t u_i = L_i u_i + (\beta_i - \alpha_i)\left(k\prod_{j=1}^{q} u_j^{\alpha_j} - \ell\prod_{j=1}^{q} u_j^{\beta_j}\right),$$

L_i is an operator.

General problem : Chemical reversible reaction into an incompressible fluid

• Incompressible Navier-Stokes equation for the fluid v:

$$\partial_t v = \alpha L v + (v \cdot \nabla)(v) + f(T, t, x)$$

with $\nabla^* v = 0$ (or $\nabla v = 0$)

• The temperature T:

$$\partial_t T = \beta L T + (v \cdot \nabla)(T) + H(\vec{u})\Phi(T)$$

The function H describe how the temperature depends on the chemical reaction and $\Phi(T) = \exp(-\gamma/T)$

• The concentration of the species

$$\partial_t u_i = C_i L u_i + (v \cdot \nabla)(u_i) + (\beta_i - \alpha_i)\left(k \prod_{j=1}^{q} u_j^{\alpha_j} - \ell \prod_{j=1}^{q} u_j^{\beta_j}\right)\Phi(T).$$

Our main example (for understanding computations) :
The *two-by-two* case with $L_i = C_i L$

$$\mathcal{A}_1 + \mathcal{A}_2 \rightleftharpoons \mathcal{B}_1 + \mathcal{B}_2,$$

and the equation can by formulated as follow

$$\begin{cases} \partial_t u_1 = C_1 L u_1 - \lambda \left(u_1 u_2 - v_1 v_2 \right) \\ \partial_t u_2 = C_2 L u_2 - \lambda \left(u_1 u_2 - v_1 v_2 \right) \\ \partial_t v_1 = C_3 L v_1 + \lambda \left(u_1 u_2 - v_1 v_2 \right) \\ \partial_t v_2 = C_4 L v_2 + \lambda \left(u_1 u_2 - v_1 v_2 \right) \end{cases}$$

with $u_i(t,x)$, $t \geqslant 0$, $x \in \mathbb{M}$.

Main assumptions :

• L is a **Markov operator** associated to $(P_t)_{t\geqslant 0}$ on $\mathbb{M}$: $P_t f$ is solution of the *parabolic* equation

$$\partial_t u = Lu,$$

with $u(t=0)=f$.

• L **is reversible** with respect to the **probability measure** μ,

$$\forall f, g, \int f\, L\, g d\mu = \int g\, L\, f d\mu.$$

• L **satisfies a logarithmic Sobolev inequality**

$$\mathrm{Ent}_\mu(u^2) \equiv \mu(u^2 \log \frac{u^2}{\mu(u^2)}) \leq C_{LS}\mathcal{E}(u),$$

with

$$\mathcal{E}(u,v) = -\mu(v\, Lu).$$

Examples :

- In $\mathbb{R}^n$, the Ornstein-Uhlenbeck semigroup

$$L = \Delta - x \cdot \nabla$$

with the reversible measure $\mu(dx) = \frac{e^{-||x||^2/2}}{(2\pi)^{n/2}}dx$ then $C_{LS} = 2$.
More generally

$$L = \Delta - \nabla\Psi \cdot \nabla$$

such that $\mathrm{Hess}(\psi) \geqslant \lambda\,\mathrm{Id}$ with $\lambda > 0$, then $C_{LS} = 2/\lambda$.

- In a Riemannian setting (uniform bound on the Ricci curvature).
- In a discret setting (Markov chain).
- In a infinite dimension setting (Gibbs measures).

Two questions :

- **Existence theorem :** find conditions on $\mathbb{M}$, L, C_i and L such that there exists a *positive* solution (weak, strong, mild...) on $\mathbb{R}_+$.
  - On $\Omega \subset \mathbb{R}^n$, bounded, with bounded initial conditions and boundary conditions.

$$\begin{cases} \partial_t u_1 = C_1 L u_1 - \lambda \left(u_1 u_2 - v_1 v_2 \right) \\ \partial_t u_2 = C_2 L u_2 - \lambda \left(u_1 u_2 - v_1 v_2 \right) \\ \partial_t v_1 = C_3 L v_1 + \lambda \left(u_1 u_2 - v_1 v_2 \right) \\ \partial_t v_2 = C_4 L v_2 + \lambda \left(u_1 u_2 - v_1 v_2 \right) \end{cases}$$

    the C_i's could be different. (M. Pierre, L. Desvillettes, Rothe and coauthors...).
  - On $\mathbb{R}^n$ with restriction of the number of species (S. Zelik and coauthors).
- **Asymptotic behaviour :** there exits a unique steady state of the solution (up to conservation mass).

The abstract equation

$$\begin{cases} \frac{\partial}{\partial t}\vec{u}(t) &= \mathfrak{C}L\vec{u}(t) + G(\vec{u}(t))\vec{\lambda}, \quad t > 0 \\ \vec{u}(0) &= \vec{f} \end{cases} \tag{$\mathbb{RDE}$}$$

where

- $\vec{u}(t,x)$ is a function from $[0,\infty) \times \mathbb{M}$ to $\mathbb{R}^4$
- $\vec{\lambda} = \lambda(-1,-1,1,1) \in \mathbb{R}^4$, $\lambda > 0$;
- $G(\vec{u}) = u_1 u_2 - u_3 u_4$.
- $$\mathfrak{C} = \begin{pmatrix} C_1 & 0 & 0 & 0 \\ 0 & C_2 & 0 & 0 \\ 0 & 0 & C_3 & 0 \\ 0 & 0 & 0 & C_4 \end{pmatrix},$$

  we assume that $C_1 = C_3$ and $C_2 = C_4$.
- the initial datum is $\vec{f} = (f_1, f_2, f_3, f_4)$.

Weak solutions :

Let $T > 0$,

$$\vec{u} \in \left(\mathbb{L}^2([0,T],\mathcal{D}) \cap C([0,T],\mathbb{L}^2(\mu)) \cap \mathbb{L}^\infty([0,T],\mathbb{L}^{\Phi_2}(\mu))\right)^4$$

is a weak solution of $(\mathbb{RDE})$ on $[0,T]$ provided, for any $\vec{\varphi} \in C^\infty([0,T],\mathcal{D}^4)$,

$$-\int_0^t \sum_{i=1}^4 \mu(u_i(s)\partial_s\varphi_i(s))\,ds + \left[\sum_{i=1}^4 \mu(u_i(t)\varphi_i(t) - u_i(0)\varphi_i(0))\right]$$

$$= -\int_0^t \sum_{i=1}^4 C_i\mathcal{E}(u_i(s),\varphi_i(s))\,ds + \int_0^t \sum_{i=1}^4 \lambda_i\mu(\varphi_i(s)G(\vec{u}(s)))\,ds.$$

where $\mathbb{L}^{\Phi_2}(\mu) = \{u,\ \exists\gamma > 0,\ s.t.\ \mu(e^{\gamma|u|^2}) < \infty\}$

Theorem

Let (L, μ) be a Markov generator satisfying a log-Sobolev inequality with constant C_{LS} Then $\forall \vec{f}$ s.t. for all $\gamma > 0$

$$\mu(e^{\gamma (f_i)^2}) < \infty \ , i = 1, \dots, 4,$$

there exists a unique weak solution $\vec{u}$ of ($\mathbb{RDE}$) $[0, \infty)$.

$$\frac{\partial}{\partial t}\vec{u}(t) = \mathfrak{C}L\vec{u}(t) + G(\vec{u}(t))\vec{\lambda}, \quad t > 0$$

Moreover, $\vec{u} \geqslant 0$ and satisfies on $\mathbb{R}_+$,

$$\mu(e^{\gamma u_i(t)}) \leq \mu(e^{\gamma f_i}).$$

Recall that $C_1 = C_3$ and $C_2 = C_4$.

An iterative procedure :

Let define $(\vec{u}^{(n)})_{n\in\mathbb{N}}$

- for all $n \in \mathbb{N}$, $\vec{u}^{(n)}(t=0) = \vec{f}$;
- for $n = 0$, $\partial_t \vec{u}^{(0)}(t) = \mathfrak{C} L \vec{u}^{(0)}(t)$
- for any $n \geqslant 1$,

$$\partial_t \vec{u}^{(n)} = \mathfrak{C} L \vec{u}^{(n)} + \vec{\lambda}(u_1^{(n)} u_2^{(n-1)} - u_3^{(n)} u_4^{(n-1)}).$$

The sequence is well defined : for $n = 0$, the solution is given by $(P_t)_{t\geqslant 0}$.

Then since $C_1 = C_3$,

$$\begin{cases} \partial_t (u_1^{(n)} + u_3^{(n)}) = C_1 L (u_1^{(n)} + u_3^{(n)}) \\ \partial_t (u_2^{(n)} + u_4^{(n)}) = C_2 L (u_2^{(n)} + u_4^{(n)}) \end{cases}$$

then

$$\partial_t u_1^{(n)} = C_1 L u_1^{(n)} - \lambda u_1^{(n)} (u_2^{(n-1)} + u_3^{(n-1)}) + \lambda P_{C_1 t}(f_1 + f_3) u_4^{(n-1)}.$$

with initial datum f_1

Existence and positivity of the sequence follows from this Lemma, with $A(t) = \lambda(u_2^{(n-1)} + u_3^{(n-1)})$ and $B(t) = \lambda P_{C_1 t}(f_1 + f_3)u_4^{(n-1)}$.

Lemma

Let $T > 0$ and $0 \le A = A(t) \in \mathbb{L}^\infty([0,T], \mathbb{L}^{\Phi_2}(\mu))$ and $0 \le B \in \mathbb{L}^2([0,T], \mathbb{L}^2(\mu))$, then the Cauchy problem

$$\begin{cases} \partial_t u(t) = Lu(t) - A(t)\, u(t) + B(t), \\ u(0) = f, f \in \mathbb{L}^2(\mu) \end{cases}$$

has a unique nonnegative solution in $[0, T)$.

A priori estimates :

Proposition

Let $\vec{u}^{(n)}$ (for any n) be a solution of the sequence then for any $\alpha > 0$ and $t \geqslant 0$,

$$\int e^{\gamma(u_1^{(n)}+u_3^{(n)})^\alpha} d\mu \leq \int e^{\gamma(f_1+f_3)^\alpha} d\mu$$

and similarly for $u_2^{(n)} + u_4^{(n)}$.

Proof : Formally for $\alpha = 1$, since $\partial_t(u_1^{(n)} + u_3^{(n)}) = C_1 L(u_1^{(n)} + u_3^{(n)})$ then

$$\frac{d}{dt} \int e^{\gamma(u_1^{(n)}+u_3^{(n)})} d\mu = \int \gamma C_1 L(u_1^{(n)} + u_3^{(n)}) e^{\gamma(u_1^{(n)}+u_3^{(n)})} d\mu \leq 0,$$

which implies the result.

Convergence of the approximation procedure :

- **Idea :** for $\kappa > 0$, let considere

$$\Sigma_n(t) = \mu(|\vec{u}^{(n)} - \vec{u}^{(n-1)}|^2)(t) + \kappa \int_0^t \mathcal{E}(\vec{u}^{(n)} - \vec{u}^{(n-1)})(s)ds,$$

then $\sup_{t\in[0,T]} \Sigma_n(t)$ goes to 0 exponentially fast as $n \to \infty$ if $T > 0$ small enough ; Where

$$|\vec{u}|^2 = \sum_{i=1}^4 u_i^2 \quad \text{and} \quad \mathcal{E}(\vec{u}) = \sum_{i=1}^4 \mathcal{E}(u_i).$$

Estimate of the $\mathbb{L}^2$-norm derivative :

We will focus on the $\mathbb{L}^2$-norm of $u_1^{(n)}$:

$$\frac{1}{2}\frac{d}{dt}\mu((u_1^{(n)} - u_1^{(n-1)})^2) = C_1\mu((u_1^{(n)} - u_1^{(n-1)})L(u_1^{(n)} - u_1^{(n-1)}))$$
$$-\lambda\mu((u_1^{(n)}-u_1^{(n-1)})(u_1^{(n)}u_2^{(n-1)}-u_3^{(n)}u_4^{(n-1)}-u_1^{(n-1)}u_2^{(n-2)}+u_3^{(n-1)}u_4^{(n-2)})),$$

or after natural bilinear handlings,

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\mu((u_1^{(n)}-u_1^{(n-1)})^2) = -C_1\mathcal{E}(u_1^{(n)}-u_1^{(n-1)})-\lambda\mu((u_1^{(n)}-u_1^{(n-1)})^2u_2^{(n-1)}) \\ - \lambda\mu((u_1^{(n)} - u_1^{(n-1)})(u_2^{(n-1)} - u_2^{(n-2)})u_1^{(n-1)}) \\ + \lambda\mu((u_1^{(n)} - u_1^{(n-1)})(u_3^{(n)} - u_3^{(n-1)})u_4^{(n-1)}) \\ + \lambda\mu((u_1^{(n)} - u_1^{(n-1)})(u_4^{(n-1)} - u_4^{(n-2)})u_3^{(n-1)}).\end{aligned}$$

Since $\vec{u}^{(n-1)}$ is nonnegative, and by the quadratic inequality $ab \leq a^2/2 + b^2/2$, one gets

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\mu((u_1^{(n)} - u_1^{(n-1)})^2) \leq -C_1\mathcal{E}(u_1^{(n)} - u_1^{(n-1)})\\+ \frac{\lambda}{2}\mu((u_1^{(n)} - u_1^{(n-1)})^2 u_1^{(n-1)}) + \frac{\lambda}{2}\mu((u_2^{(n-1)} - u_2^{(n-2)})^2 u_1^{(n-1)})\\+ \frac{\lambda}{2}\mu((u_1^{(n)} - u_1^{(n-1)})^2 u_4^{(n-1)}) + \frac{\lambda}{2}\mu((u_3^{(n)} - u_3^{(n-1)})^2 u_4^{(n-1)})\\+ \frac{\lambda}{2}\mu((u_1^{(n)} - u_1^{(n-1)})^2 u_3^{(n-1)}) + \frac{\lambda}{2}\mu((u_4^{(n-1)} - u_4^{(n-2)})^2 u_3^{(n-1)}).\end{aligned}$$

All the similar terms are then estimated thanks to the relative entropy inequality. For instance,

$$\mu((u_1^{(n)} - u_1^{(n-1)})^2 u_1^{(n-1)}) \leq \frac{1}{\gamma}\mathrm{Ent}_\mu\Big((u_1^{(n)} - u_1^{(n-1)})^2\Big) + \frac{1}{\gamma}\mu((u_1^{(n)} - u_1^{(n-1)})^2)\log\mu(e^{\gamma u_1^{(n-1)}})).$$

The logarithmic Sobolev inequality and the a priori bound described in the Proposition give

$$\mu((u_1^{(n)}-u_1^{(n-1)})^2 u_1^{(n-1)}) \leq \frac{C_{LS}}{\gamma}\mathcal{E}(u_1^{(n)}-u_1^{(n-1)})+\frac{D}{\gamma}\mu((u_1^{(n)}-u_1^{(n-1)})^2),$$

where

$$D = \max\Big\{\log\mu(e^{\gamma(f_1+f_3)}), \log\mu(e^{\gamma(f_2+f_4)}))\Big\}.$$

Recall

$$\Sigma_n(t) = \mu(|\vec{u}^{(n)} - \vec{u}^{(n-1)}|^2)(t) + \kappa \int_0^t \mathcal{E}(\vec{u}^{(n)} - \vec{u}^{(n-1)})(s)ds,$$

then

$$\begin{aligned}\Sigma_n(t) \leq D\,\frac{4\lambda}{\gamma}\int_0^t \Sigma_n(s)ds \\ + D\,\frac{4\lambda}{\gamma}\Big(\int_0^t \mu(|\vec{u}^{(n-1)} - \vec{u}^{(n-2)}|^2)(s)ds \\ + \frac{C_{LS}}{D}\int_0^t \mathcal{E}(\vec{u}^{(n-1)} - \vec{u}^{(n-2)})(s)ds\Big).\end{aligned}$$

Gronwall argument implies local existence :

$$\sup_{t\in[0,T]} \Sigma_n(t) \leq \eta(T) \sup_{t\in[0,T]} \Sigma_{n-1}(t),$$

where $\eta(T) = \frac{4\lambda}{\gamma} e^{D\,\frac{2\lambda}{\gamma}\,T}(DT + C_{LS}) < 1$ if $T > 0$ small enough.

Existence of the weak solution on $[0,T]$:

Let $T>0$ fixed as before, if $\varphi\in\mathcal{C}^\infty([0,T],\mathcal{D}^4)$,

$$\int_0^t \mu(\varphi\partial_s u_1^{(n)})(s)ds = C_1\int_0^t \mu(\varphi L u_1^{(n)})(s)ds \\ -\lambda\int_0^t \mu(\varphi u_1^{(n)}u_2^{(n-2)})(s)ds + \lambda\int_0^t \mu(\varphi u_3^{(n)}u_4^{(n-1)})(s)ds.$$

Integrate by parts with respect to s :

$$-\int_0^t \mu(u_1^{(n)}\partial_s\varphi)(s)ds + \mu(u_1^{(n)}\partial_t\varphi)(t) - \mu(u_1^{(n)}\partial_t\varphi)(0) = -\int_0^t \mu(\varphi u_1^{(n)}u_2^{(n-2)})(s)ds + \lambda\int_0^t \mu(\varphi u_3^{(n)}u_4^{(n-1)})(s)ds - C_1\int_0^t \mathcal{E}(\varphi,u_1^{(n)})(s)ds$$

- Again the *relative entropy* inequality and *the logarithmic sobolev inequality* imply a weak solution in $[0,T]$.

- The estimates don't depend on $T > 0 \rightarrow$ global solution in $\mathbb{R}_+$.
- Solution are nonnegative since $u_i^{(n)} \geqslant$ are nonnegative.
- Uniqueness is proved in the same way.

The main chemical equation is the following

$$\sum_{i\in I} \alpha_i \mathcal{A}_i \rightleftharpoons \sum_{i\in I} \beta_i \mathcal{A}_i,$$

with $\alpha_i \neq \beta_i$ for any $i \in I$. The main PDE is

$$\partial_t u_i = C_i L u_i + (\beta_i - \alpha_i)\left(\prod_{j=1}^{q} u_j^{\alpha_j} - \prod_{j=1}^{q} u_j^{\beta_j}\right).$$

• Let $I_- = \{i \in I,\ \beta_i - \alpha_i > 0\}$ and $I_+ = \{i \in I,\ \beta_i - \alpha_i < 0\}$.
We assume that $\forall i_- \in I_-$, $\exists j_+ \in I_+$ such that

$$\frac{C_{i_-}}{|\beta_{i_-} - \alpha_{i_-}|} = \frac{C_{i_+}}{|\beta_{i_+} - \alpha_{i_+}|},$$

Iterated procedure :

$$\partial_t u_{i_-}^{(n)} = C_{i_-} L u_{i_-}^{(n)}$$
$$+ (\beta_{i_-} - \alpha_{i_-}) \left(\frac{\prod_{j=1}^q (u_j^{(n-1)})^{\alpha_j}}{(u_i^{(n-1)})^{\alpha_{i_-}-1}} u_{i_-}^{(n)} - \frac{\prod_{j=1}^q (u_j^{(n-1)})^{\beta_j}}{(u_{i_+}^{(n-1)})^{\beta_{i_+}-1}} u_{i_+}^{(n)} \right).$$