Entropy versus diffusive PDEs

Nicola Zamponi

University of Mannheim
School of Business Informatics and Mathematics
68159 Mannheim, Germany

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Partial Differential Equations and the Universe

"The book of Nature is written in mathematical language."

Galileo Galilei, 1564-1642

Updated version:

"The book of Nature is (mostly) written in the language of **Partial Differential Equations**."

Partial Differential Equations (PDEs) are widely used in the applied sciences to describe a lot of phenomena.

The analysis of PDEs is a very active and challenging field of Mathematics.

Some classes of PDEs that have caught my attention

Evolution equations: describe how relevant physical quantities change with time (transient systems).

Diffusion equations: evolution mainly driven by tendency of particles to move in opposition to concentration gradients ("diffusion").

Reaction-diffusion systems: important role played by "reaction terms", arising from many different physical phenomena, like e.g. chemical reactions.

Cross-diffusion: diffusion of a species influenced by the density gradient of other species.

Nonlocal diffusion: diffusion effect at some point influenced by the values of concentration gradients in the whole spatial domain.

Of course, other types of PDEs exist (hyperbolic conservation laws, stationary elliptic problems . . .)

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Evolution equations: describe how relevant physical quantities change with time (transient systems).

Diffusion equations: evolution mainly driven by tendency of particles to move in opposition to concentration gradients ("diffusion").

Reaction-diffusion systems: important role played by "reaction terms", arising from many different physical phenomena, like e.g. chemical reactions.

$\rightarrow$ **Cross-diffusion:** diffusion of a species influenced by the density gradient of other species.

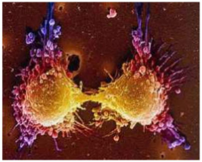
Nonlocal diffusion: diffusion effect at some point influenced by the values of concentration gradients in the whole spatial domain.

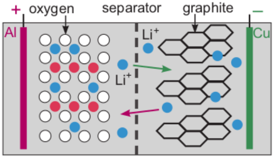
Today I will focus on (reaction-)cross-diffusion PDEs.

Cross-diffusion PDEs in the applied sciences

Some examples of cross-diffusion PDEs from applied sciences:

- the Shigesada-Kawasaki-Teramoto (SKT) model in biology governs the interaction of two competing species in the same environment;
- the Maxwell-Stefan equations in gas dynamics describe diffusion in multicomponent fluids under the assumption of steady state;
- models for ion transport in fluid mixtures describing the time evolution of systems of electrically charged particles;
- models for tumor growth analyzing in a quantitative way the development of cancerous cells conglomerates.





Cross-diffusion systems

Heat equation:

$$\partial_t u = \Delta u, \qquad t > 0, \qquad x \in \Omega \subset \mathbb{R}^d.$$

Reaction-diffusion system with **diagonal diffusion**: for $i = 1, \ldots, n$,

$$\partial_t u_i = \operatorname{div}\left(a_i(u_i)\nabla u_i\right) + f_i(u), \qquad t > 0, \qquad x \in \Omega \subset \mathbb{R}^d.$$

Reaction-cross-diffusion systems: for $i = 1, \ldots, n$,

$$\partial_t u_i = \sum_{j=1}^{n} \operatorname{div}\left(A_{ij}(u)\nabla u_j\right) + f_i(u), \qquad t > 0, \qquad x \in \Omega \subset \mathbb{R}^d,$$

where $u = (u_1, \ldots, u_n) : \Omega \times (0, \infty) \to \mathbb{R}^n$ is the unknown of the system (tipically a vector of densities or concentrations of species), $A = A(u) \in \mathbb{R}^{n\times n}$ is the diffusion matrix, and $f = f(u) \in \mathbb{R}^n$ is the reaction term.

Cross-diffusion systems

Reaction-cross-diffusion systems (compact notation):

$$\partial_t u = \operatorname{div}(A(u)\nabla u) + f(u), \qquad t > 0, \qquad x \in \Omega \subset \mathbb{R}^d, \qquad (1)$$

where $u = (u_1, \ldots, u_n) : \Omega \times (0, \infty) \to \mathbb{R}^n$ is the unknown of the system (tipically a vector of densities or concentrations of species), $A = A(u) \in \mathbb{R}^{n\times n}$ is the diffusion matrix, and $f = f(u) \in \mathbb{R}^n$ is the reaction term.

Some interesting analytical questions:

- existence of solutions (global in time, weak solutions);
- uniform boundedness, nonnegativity, other algebraic constraints;
- the long-time behaviour of solutions (convergence to steady state);
- uniqueness of solutions.

Mathematical challenges of cross-diffusion

The analytical study of cross-diffusion PDEs is **challenging!**

Cross-diffusion $\Rightarrow$ strong coupling between the equations.

Diffusion matrix $A(u)$ in general not positive (semi)definite
$\Rightarrow$ standard coercivity-based approaches ineffective (straightforward monotonicity properties not available).

No general maximum/minimum principle $\Rightarrow$ showing upper/lower bounds for the solution of the system is often a very difficult problem.

The "entropy method"

[Burger-Di Francesco-Pietschmann-Schlake '10, Jüngel '15, Jüngel '16].

If a convex functional $\mathcal{H} = \mathcal{H}[u]$ exists (usually termed **mathematical entropy**) such that (1) can be (formally) restated as

$$\partial_t u = \mathrm{div}\,(B\nabla\mathcal{H}'[u]) + f(u), \qquad t > 0, \qquad x \in \Omega \subset \mathbb{R}^d, \tag{2}$$

with $\mathcal{H}'$ Fréchet derivative of $\mathcal{H}$ and B a **positive semi-definite** matrix, then we say that (1) possesses an **entropy structure**.

$\mathcal{H}[u] = \int_\Omega h(u)dx \quad \Rightarrow \quad \mathcal{H}'[u] = h'(u) \equiv w$ **entropy variable**.

Example (heat equation):

$$\partial_t u = \mathrm{div}\,(u\nabla \log u), \quad \log u = \mathcal{H}'[u], \quad \mathcal{H}[u] = \int_\Omega (u \log u - u)dx.$$

The "entropy method", 2

If (1) admits an entropy structure (and $f \equiv 0$) then

$$\frac{d}{dt}\mathcal{H}[u] = -\sum_{i=1}^{n} \int_\Omega \partial_{x_i} w \cdot B(w) \partial_{x_i} w \, dx \le 0,$$

i.e. $\mathcal{H}$ is nonincreasing along the (smooth) solutions to (1).

- It can be generalized to the case $f \neq 0$ with suitable additional assumptions on f.
- Suitable lower bounds for $-\frac{d}{dt}\mathcal{H}[u] \Rightarrow$ crucial a-priori estimates for the solution u to (1).

Example (heat equation):

$$\frac{d}{dt}\mathcal{H}[u] = -\int_\Omega u |\nabla \log u|^2 dx, \qquad \mathcal{H}[u] = \int_\Omega (u \log u - u) dx.$$

The "entropy method", 3

If $h' : \mathcal{D} \subset \mathbb{R}^n \to \mathbb{R}^n$ is globally invertible:

$$u = u(w) = (h')^{-1}(w) \quad \Rightarrow \quad u \in \mathcal{D} \quad \text{on } \{|w| < \infty\}.$$

$\Rightarrow$ If $\mathcal{D}$ is bounded and w is a.e. finite, then u is bounded with bounds that only depend on $\mathcal{D}$.

Example: "Fermi-Dirac" entropy:

$$\mathcal{H}[u] = \int_\Omega (u \log u + (1-u)\log(1-u))dx.$$

$$w = \mathcal{H}'[u] = \log \frac{u}{1-u} \quad \Rightarrow \quad u = \frac{e^w}{1+e^w} \in \mathcal{D} \equiv (0,1).$$

Existence argument

Three steps in existence argument.

1. Formulation of an approximated problem. Time semi-discretization + regularization. Obtain family $(u^{(\tau)})_{\tau>0}$ of approximated solutions.
2. Entropy inequality for approximated problem $\Rightarrow$ estimates for $u^{(\tau)}$ in Sobolev spaces.
3. Aubin-Lions, Div-Curl lemma $\Rightarrow$ compactness for $u^{(\tau)} \Rightarrow u^{(\tau)} \to u$ as $\tau \to 0$, and u is solution to original PDEs.

Sometimes the bounds for $u^{(\tau)}$ are not sufficient to get compactness. The bounds might become ineffective when $u^{(\tau)}$ approaches some critical value or set $\to$ Degeneracy.

Possible solution to degeneracy: **generalize** Aubin-Lions Lemma to degenerate case. Example: [NZ-Jüngel, Ann. Inst. H. Poinc. (C) 2017].

About long-time behaviour

Idea: the solution $u(t)$ *should* converge to some "steady state" u^∞ in some norm. Use *relative* entropy $\mathcal{H}[u(t)|u^\infty]$ to measure distance between solution and steady state.

Key tool: relative entropy inequality

$$\frac{d}{dt}\mathcal{H}^{rel}[u|u^\infty] + I[u, \nabla u] \leq 0.$$

Crucial point: relate the entropy dissipation $I[u, \nabla u]$ and the entropy $\mathcal{H}^{rel}[u|u^\infty]$ (remember Fokker-Planck).
Gronwall's lemma $\Rightarrow$ upper bound for $\mathcal{H}[u(t)|u^\infty]$ which decays in time.
$\Rightarrow u(t) \to u^\infty$ in some norm.

Much more difficult for (cross-diffusion) systems than in the scalar case. No log-Sobolev inequality for systems!

Result: in [NZ-Jüngel, Ann. Inst. H. Poinc. (C) 2017] we proved **algebraic** convergence to the steady state for **degenerate** cross-diffusion system.

About uniqueness

[Gajewsky 1994]: take two solutions u, v with the same initial datum and consider the "relative entropy" $H^{rel}[u, v]$ between them:

$$H^{rel}[u, v] = H[u] + H[v] - 2H\left[\frac{u+v}{2}\right].$$

- H convex $\Rightarrow H^{rel}[u, v] \geq 0$ and $H^{rel}[u, v] = 0$ if and only if $u = v$.
- $H^{rel}[u, v]|_{t=0} = 0$ since $u = v$ at initial time.
- So, if one can prove that $\frac{d}{dt}H^{rel}[u(t), v(t)] \leq 0$ for $t > 0$, it follows that $u(t) = v(t)$ for $t > 0$.

Very difficult for cross-diffusion systems!

Idea: argument can be applied to "partially decoupled" systems together with H^{-1} method [NZ-Jüngel, Ann. Inst. H. Poinc. (C) 2017].

A particular cross-diffusion PDEs system

A class of multi-species population models with degenerate cross-diffusion [NZ-Jüngel, Ann. Inst. H. Poinc. (C) 2017]:

$$\partial_t u_i = \sum_{j=1}^{n} \mathrm{div}\left(A_{ij}(u)\nabla u_j\right) \qquad \text{in } \Omega\times(0,T), \quad i=1,\ldots,n,$$

$$A_{ij}(u) = q(u_{n+1})^2 \frac{\partial}{\partial u_j}\left(\frac{u_i p_i(u)}{q(u_{n+1})}\right), \qquad i,j=1,\ldots,n,$$

where

$$u=(u_1,\ldots,u_n):\Omega\times(0,T)\to\mathbb{R}^n \quad \text{proportions of subpopulations},$$

$$u_{n+1} = 1-\sum_{i=1}^{n} u_i = \text{proportion of unoccupied space}.$$

Constraints: $u_i \geq 0$, $i=1,\ldots,n$, and $u_{n+1}\geq 0$ if $q(u_{n+1})\not\equiv 1$.

Employed to model spatial segregation of interacting populations, motility of biological cells, ion transport through nanopores.

The analytical problem

Goal: study existence, uniqueness and long-time behaviour of solutions to the initial-boundary value problem:

find $u : \Omega \times (0, T) \to D = \{u \in (0,1)^n \, : \, \sum_{i=1}^n u_i < 1\}$ such that:

$$\partial_t u = \operatorname{div}(A(u)\nabla u) \qquad \text{in } \Omega \times (0, T), \tag{PB.1}$$

$$\partial_\nu u = 0 \qquad \text{on } \partial\Omega \times (0, T), \tag{PB.2}$$

$$u(\cdot, 0) = u^0 \qquad \text{on } \Omega, \tag{PB.3}$$

with $A(u)$ given by:

$$A_{ij}(u) = q(u_{n+1})^2 \frac{\partial}{\partial u_j}\left(\frac{u_i p_i(u)}{q(u_{n+1})}\right), \qquad u_{n+1} = 1 - \sum_{i=1}^n u_i.$$

Entropy structure with entropy functional: $\mathcal{H}[u] = \int_\Omega h(u)dx$,

$$h(u) = \sum_{i=1}^n (u_i \log u_i - u_i + 1) + \int_a^{u_{n+1}} \log q(s)\, ds + \chi(u) \qquad u \in \mathcal{D}.$$

Hypothesis: $q(0) = 0$ (+ other technical assumptions).

Existence of bounded weak solutions

We proved global-in-time existence of **uniformly bounded** weak solutions $u : \Omega \times (0, T) \to \overline{\mathcal{D}}$ such that $\mathcal{H}[u(t_2)] \leq \mathcal{H}[u(t_1)]$ for $t_1 \leq t_2$.

Key point: a-priori estimates for approximate solution $u^{(\tau)}$:

$$\sum_{i=1}^{n} \|q(u_{n+1}^{(\tau)})^{1/2} \nabla (u_i^{(\tau)})^{1/2}\|_{L^2(\Omega)}^2 + \|\nabla q(u_{n+1}^{(\tau)})^{1/2}\|_{L^2(\Omega)}^2 \leq C.$$

$q(0) = 0$: **Degeneracy!** Compactness?

Novel idea: generalize Aubin-Lions lemma to the degenerate case.

- Bounds for $\nabla q(u_{n+1}^{(\tau)})^{1/2}$ and $\partial_t u_{n+1}^{(\tau)}$ $\Rightarrow$ compactness for $u_{n+1}^{(\tau)}$.
- Strong convergence for $u_{n+1}^{(\tau)}$

  $+$ Bounds for $q(u_{n+1}^{(\tau)})^{1/2} \nabla (u_i^{(\tau)})^{1/2}$ and $\partial_t u_i^{(\tau)}$

  $\Rightarrow$ compactness for $q(u_{n+1}^{(\tau)})^{1/2} f(u^{(\tau)})$ for every f continuous.

This is enough to pass to the limit $\tau \to 0$ in the approximate equations.

Long-time behaviour of solutions

Constant Dirichlet boundary conditions $u = u_D$.
$\Rightarrow u \to u^\infty \equiv u_D$ in $L^1(\Omega)$ with **algebraic rate:**

$$\|u(t) - u^\infty\|_{L^1(\Omega)} \le \frac{C}{\sqrt{1+t}} \qquad \forall t > 0.$$

Key idea: relative entropy inequality:

$$\begin{aligned} \frac{d}{dt}\mathcal{H}[u(t)|u^\infty] &\le -\int_\Omega \sum_{i=1}^{n+1} |\nabla \Phi_i(u)|^2 dx \\ \text{(Poincaré)} &\le -c_P \int_\Omega \sum_{i=1}^{n+1} |\Phi_i(u) - \Phi_i(u^\infty)|^2 dx \\ \text{(Computations)} &\le -c\mathcal{H}[u(t)|u^\infty]^2 \end{aligned}$$

Algebraic decay rate from Gronwall argument.

Uniqueness of solutions

Uniqueness of **weak** solutions. No higher regularity assumptions!

Assume that $p_i(u) \equiv 1$, $i = 1, \ldots, n$. Then the weak solution u with the properties stated in the existence theorem is unique.

Equations become:

$$\partial_t u_i - \mathrm{div}\left(q(u_{n+1})\nabla u_i - u_i \nabla q(u_{n+1})\right) = 0 \qquad (i = 1, \ldots, n).$$

"Partially decoupled equations": summing equations in i yields equation for u_{n+1} **alone.** Two steps:

1. Prove uniqueness for u_{n+1} (H^{-1} method).
2. Prove uniqueness for u_i, $i = 1, \ldots, n$ (relative entropy).

Gajewsky method with "relative entropy between to solutions u, v":

$$\Xi = S[u] + S[v] - 2S\left[\frac{u+v}{2}\right], \quad S[u] = \sum_{i=1}^{n} \int_\Omega u_i \log u_i dx.$$

Convexity of the Fisher information functional $\Rightarrow \Xi(t)$ nonincreasing.

Summary and outlook

Summary.

- We explained a method, based on the idea of mathematical entropy, employed for the analysis of nonlinear PDEs systems.
- We adapted the method to a multi-species population model with degenerate cross-diffusion.
- **Key original ideas:**
  - generalized Aubin-Lions Lemma to cope with degeneracy;
  - algebraic decay rate to steady state for degenerate cross-diffusion system;
  - uniqueness for "partially decoupled" cross-diffusion PDEs.

Outlook.

- Strongly degenerate PDEs systems. Example: model for gang dynamics in a city (coop. with A. Barbaro, N. Rodriguez).
- Hölder regularity for cross-diffusion systems via Campanato iteration employing entropy functional (coop. with C. Raithel, M. Braukhoff).
- Apply entropy method to nonlocal diffusion PDEs systems (coop. with M. Gualdani).

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