Entropy dissipation methods for diffusion equations

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Contents

Literature

Main references

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- D. Matthes. Entropy methods and related functional inequalities. Lecture Notes, 2008.
- A. Jüngel and D. Matthes. An algorithmic construction of entropies in higher-order nonlinear PDEs. *Nonlinearity* 19 (2006), 633-659.
- A. Jüngel. The boundedness-by-entropy method for cross-diffusion systems. *Nonlinearity* 28 (2015), 1963-2001.
- L. Evans. Entropy & partial differential equations. Lect. Notes, 2001.

What mathematics skills are needed?

Entropy methods are intradisciplinary!

- Partial differential equations: Fokker-Planck equations, parabolic equations, Sobolev spaces
- Functional analysis: Lemma of Lax-Milgram, fixed-point theorems, compactness
- Stochastics: Markov processes, Markov chain theory
- Numerics: Finite-difference methods, finite-volume methods
- Differential geometry: Geodesic convexity of entropy *(not convered in these lectures)*

Entropy in physics

- Entropy = measure of molecular disorder or energy dispersal
- Introduced by Clausius (1865) in thermodynamics (measure of irreversibility)
- Statistical definition by Boltzmann, Gibbs, Maxwell (1870s)

$$S = -k_B \sum_i p_i \log p_i, \quad p_i: \text{ probability of } i\text{th microstate}$$

- Von Neumann (1927): Quantum mechanical entropy
- Bekenstein, Hawking (1970s): Black hole entropy (to satisfy second law of thermodynamics), entropy $\sim$ radius^2: description of volume encoded on its boundary

Entropy in information theory

- Shannon 1948: Concept of information entropy (measure of information density)
- Information content: $I(p) = -\log_2 p$, p: probability of event
- Rationale: $I(1) = 0$: no information content of sure events, $I(p_1 p_2) = I(p_1) + I(p_2)$: information of independent events additive
- Entropy = expected information content

$$S = \sum_{i \in \Sigma} p_i I(p_i) = -\sum_{i \in \Sigma} p_i \log_2 p_i$$

- Applications: Redundancy in language structure, data compression (entropy coding, idea: minimize entropy)

Entropy in mathematics

- Mathematical entropy is nonincreasing, i.e. negative physical entropy
- Hyperbolic conservation laws (Lax 1971):

$$\partial_t u + \partial_x f(u) = 0, \quad u \in \mathbb{R}^n$$

  h is an entropy if $\exists q : \partial_i q(u) = \sum_j \partial_{u_i} f_j(u) \partial_{u_j} h(u)$ and entropy inequality: $\partial_t h(u) + \partial_x q(u) \leq 0$
- Kinetic equations: entropy $h(f) = \int_{\mathbb{R}^d} f \log f \, dx$ gives a priori estimates for Boltzmann equation (DiPerna/Lions 1989), large-time behavior of solutions (Desvillettes/Villani 1990, Mouhot 2006)
- Large-time behavior for stochastic processes (Bakry/Emery 1985) and parabolic equations (Toscani 1997)
- Regularity for parabolic equations (Nash 1958)
- Relations to gradient flows in metric spaces (Ambrosio, Otto, Savaré...), functional inequalities (Gross, Arnold et al., Dolbeault...)

Entropy and partial differential equations

Generally: Entropy $S(E, X_1, \ldots, X_n)$ is function of internal energy E and state variables X_i (e.g. volume, mole number) such that

$$S \text{ is concave}, \quad \frac{\partial S}{\partial E} > 0, \quad S \text{ homogeneous of order one.}$$

Def. temperature $\frac{1}{\theta} = \frac{\partial S}{\partial E}$, chem. potential $\mu = -\theta \frac{\partial S}{\partial \rho}$ (ρ: mass density)

- Euler equations in thermodynamics:

$$\begin{aligned} &\partial_t \rho + \operatorname{div}(\rho v) = 0, \\ &\partial_t(\rho v) + \operatorname{div}(\rho v \otimes v - T) = 0, \\ &\partial_t(\rho e) + \operatorname{div}(\rho v e + q) = T : \nabla v \end{aligned}$$

  where v: velocity, T: stress tensor, e: internal energy, q: heat flux

- Energy balance: $$\frac{d}{dt} \int_{\mathbb{R}^d} \left(\frac{\rho}{2} |v|^2 + \rho e \right) dx = 0$$
- Monoatomic ideal gas: energy density $\rho e = \frac{3}{2} \rho \theta$, entropy density $\rho s = -\rho \log(\rho / \theta^{3/2}) \Rightarrow \frac{\partial(\rho s)}{\partial(\rho e)} = \frac{1}{\theta} > 0$

Aims of lecture course

- To introduce into several entropy methods for partial differential equations (PDEs) $\to$ Arnold, Jüngel, Schmeiser
- To use entropy methods to prove the qualitative behavior of solutions to PDEs $\to$ Arnold, Jüngel, Schmeiser
- To prove functional inequalities (convex Sobolev inequalities) $\to$ Arnold
- To relate entropy methods to physical principles and the theory of stochastic processes $\to$ Schmeiser
- To introduce into the theory of cross-diffusion systems $\to$ Jüngel

Overview

Example: Heat equation

$$\partial_t u = \Delta u, \quad u(0) = u_0 \geq 0 \quad \text{in } \mathbb{T}^d \text{ (torus)}, \ t > 0$$

- Steady state: $u_\infty = \int_{\mathbb{T}^d} u_0 dx = \int_{\mathbb{T}^d} u(t) dx$, $\text{meas}(\mathbb{T}^d) = 1$
- Question: $u(t) \to u_\infty$ as $t \to \infty$ in which sense and how fast?
- Define the functional $H_2[u] = \int_{\mathbb{T}^d} (u - u_\infty)^2 dx$
- Compute time derivative:

$$\frac{dH_2}{dt}[u] = 2\int_{\mathbb{T}^d} (u - u_\infty)\partial_t u dx = -2 \overbrace{\int_{\mathbb{T}^d} |\nabla u|^2 dx}^{\text{entropy production}} \leq 0$$

- Poincaré inequality: $H_2[u] = \|u - u_\infty\|_{L^2}^2 \leq C_P \|\nabla u\|_{L^2}^2$
- Combining expressions:

$$\frac{dH_2}{dt} = -2\|\nabla u\|_{L^2}^2 \leq -2C_P^{-1} H_2[u]$$

- By Gronwall's inequality, $\|u(t) - u_\infty\|_{L^2}^2 \leq e^{-2C_P^{-1}t} \|u_0 - u_\infty\|_{L^2}^2$

Example: Heat equation

$$\partial_t u = \Delta u, \quad u(0) = u_0 \geq 0 \quad \text{in } \mathbb{T}^d \text{ (torus)}, \ t > 0$$

- Conclusion: $\|u(t) - u_\infty\|_{L^2} \leq e^{-C_P^{-1} t}\|u_0 - u_\infty\|_{L^2}$
- Same result with spectral theory: $C_P^{-1} =$ first eigenvalue of $-\Delta$
- Since spectral analysis gives the same result: What is the benefit?

First answer: Different "distances" admissible

- Entropy functional $H_1[u] = \int_{\mathbb{T}^d} u \log(u/u_\infty) dx \geq 0$

$$\frac{dH_1}{dt}[u] = \int_{\mathbb{T}^d} \left(\log \frac{u}{u_\infty} + 1\right) \partial_t u dx = -4 \int_{\mathbb{T}^d} |\nabla \sqrt{u}|^2 dx$$

- Logarithmic Sobolev ineq.: $\int_{\mathbb{T}^d} u \log(u/u_\infty) dx \leq C_L \int_{\mathbb{T}^d} |\nabla \sqrt{u}|^2 dx$
- By Gronwall inequality,

$$\frac{dH_1}{dt}[u] \leq -4C_L^{-1} H_1[u] \quad \Rightarrow \quad H_1[u(t)] \leq e^{-4C_L^{-1} t} H_1[u_0], \quad t \geq 0$$

Example: Heat equation

Second answer: Method applicable to nonlinear equations

- Quantum diffusion equation: $\partial_t u = -\operatorname{div}(u\nabla\frac{\Delta\sqrt{u}}{\sqrt{u}})$ in $\mathbb{T}^d$
- Occurs in quantum semiconductor modeling, u: electron density
- Entropy functional: $H_1[u] = \int_{\mathbb{T}^d} u\log(u/u_\infty)dx$
- Entropy production:

$$\frac{dH_1}{dt}[u] = -\int_{\mathbb{T}^d}\operatorname{div}\left(u\nabla\frac{\Delta\sqrt{u}}{\sqrt{u}}\right)\log u dx = -\int_{\mathbb{T}^d}\frac{\Delta\sqrt{u}}{\sqrt{u}}\Delta u dx$$

$$\leq -\kappa\int_{\mathbb{T}^d}(\Delta\sqrt{u})^2dx \leq -\frac{\kappa}{C_P}\int_{\mathbb{T}^d}|\nabla\sqrt{u}|^2dx \leq -\frac{\kappa}{C_P C_L}H_1[u]$$

- Exponential decay of $u(t)$ to u_∞ with explicit rate:

$$H_1[u(t)] \leq e^{-\kappa t/(C_P C_L)}H_1[u_0], \quad t\geq 0$$

Strategy

$$\partial_t u + A(u) = 0, \quad t > 0, \quad u(0) = u_0$$

Strategy:

- Given an entropy $H[u]$, compute entropy production: $-dH/dt = \langle A(u), H'[u] \rangle$
- Find relation between entropy and entropy production: $H[u] \leq C\langle A(u), H'[u] \rangle \Rightarrow dH/dt \leq -CH$
- By Gronwall's inequality, conclude exponential decay: $H[u(t)] \leq e^{-Ct} H[u_0]$

Entropy methods can do much more:

- Self-similar asymptotics
- A priori estimates and global-in-time existence analysis
- Proof of functional inequalities (like logarithmic Sobolev ineq.)
- Positivity of solutions and L^∞ bounds (no maximum principle!)
- Uniqueness of weak solutions
- Stability of numerical discretizations (structure-preservation)

Definitions

Setting:

- $A : D(A) \subset X \to X'$ operator, consider $\partial_t u + A(u) = 0,\ t > 0,$ $u(0) = u_0$
- Steady state: $u_\infty \in D(A)$ solves $A(u_\infty) = 0$

Definitions:

- Lyapunov functional: $H : D(A) \to \mathbb{R}$ such that $\frac{dH}{dt}[u(t)] \le 0,\ t \ge 0$
- Entropy: $H : D(A) \to \mathbb{R}$ convex Lyapunov functional such that
  - $\exists\ \Phi \in C^0(\mathbb{R})$: $\Phi(0) = 0$ and
  - $d(u, u_\infty) \le \Phi(H[u] - H[u_\infty])$ for $u \in D(A)$ and some metric d.
- Entropy production: $EP[u(t)] = -\frac{dH}{dt}[u(t)]$
- Entropy of kth order: contains kth-order partial derivatives

No clear definition of (mathematical) entropy in the literature!

Examples: F_1: Fisher information

$$H_\alpha[u] = \int_\Omega (u^\alpha - u_\infty^\alpha)dx, \quad F_\alpha[u] = \int_\Omega |\nabla u^{\alpha/2}|^2 dx, \quad \alpha \ge 1$$

Heat equation revisited

$$\partial_t u = \Delta u, \quad u(0) = u_0 \geq 0 \quad \text{in } \mathbb{T}^d \text{ (torus)}, \; t > 0$$

Claim: $H_1[u] = \int_{\mathbb{T}^d} u \log(u/u_\infty) dx$ is an *entropy* for the heat equation

Proof:

- Lyapunov functional: $\frac{dH_1}{dt}[u] = -\int_{\mathbb{T}^d} |\nabla \sqrt{u}|^2 dx \leq 0$
- Convexity: $u \mapsto H_1[u]$ is convex
- Csiszár-Kullback inequality for $\Phi(s) = C_\phi \sqrt{s}$, $d(f,g) = \|f-g\|_{L^1}$:
  $d(u, u_\infty) \leq C_\phi (H_1[u] - H_1[u_\infty])^{1/2}$ using $H_1[u_\infty] = 0$

Lemma (Csiszár-Kullback-Pinsker)

Let $\phi \in C^2(\mathbb{R})$ be strictly convex, $\phi(1) = 0$, and $\int_{\mathbb{T}^d} f dx = \int_{\mathbb{T}^d} g dx = 1$. Then, for some $C_\phi > 0$,

$$\|f-g\|_{L^1}^2 \leq C_\phi \int_{\mathbb{T}^d} \phi\left(\frac{f}{g}\right) g dx$$

Proof: Taylor expansion of ϕ around 1

Overview

Systematic integration by parts: Motivation

Second time derivative d^2H/dt^2 requires well chosen integrations by parts.
Aim: Make the integrations by parts systematic.
Motivation: Consider thin-film equation

$$\partial_t u = -(u^\beta u_{xxx})_x \text{ in } \mathbb{T} \text{ (torus)}, \quad t > 0, \quad u(0) = u_0 \geq 0$$

- Models the flow of thin liquid along surface with film height $u(x,t)$
- Entropy $H_\alpha[u] = \frac{1}{\alpha(\alpha-1)}\int_{\mathbb{T}} u^\alpha dx$: For which $\alpha > 1$ is H_α an entropy?

$$\frac{dH_\alpha}{dt}[u] = \frac{1}{\alpha-1}\int_{\mathbb{T}} u^{\alpha-1}\partial_t u dx = \int_{\mathbb{T}} u^{\alpha+\beta-2} u_{xxx} u_x dx$$

$$= -(\alpha+\beta-2)\int_{\mathbb{T}} u^{\alpha+\beta-3} u_x^2 u_{xx} dx - \int_{\mathbb{T}} u^{\alpha+\beta-2} u_{xx}^2 dx, \quad u_x^2 u_{xx} = \frac{1}{3}(u_x^3)_x$$

$$= \frac{1}{3}(\alpha+\beta-2)(\alpha+\beta-3)\int_{\mathbb{T}} u^{\alpha-\beta-4} u_x^4 dx - \int_{\mathbb{T}} u^{\alpha+\beta-2} u_{xx}^2 dx \leq 0$$

if $2 \leq \alpha+\beta \leq 3$ but $\frac{3}{2} \leq \alpha+\beta \leq 3$ is optimal!

Idea of method

Example: Thin-film equation $\partial_t u = -(u^\beta u_{xxx})_x$ on torus $\mathbb{T}$

- Entropy production for $H_\alpha[u] = \frac{1}{\alpha(\alpha-1)} \int_{\mathbb{T}} u^\alpha dx$

$$\frac{dH_\alpha}{dt} = \frac{1}{\alpha-1}\int_{\mathbb{T}} u^{\alpha-1}\partial_t u dx = \int_{\mathbb{T}} u^{\alpha+\beta-2} u_x u_{xxx} dx =: -EP[u] \le 0\,?$$

- Standard integration by parts:

$$EP[u] = -\int_{\mathbb{T}} u^{\alpha+\beta-2} u_x u_{xxx} dx = \int_{\mathbb{T}} \frac{u^{\alpha+\beta-1}}{\alpha+\beta-1} u_{xxxx} dx$$

- Formalization of integration by parts:

$$\begin{aligned} I_3 &= \int_{\mathbb{T}} u^{\alpha+\beta}\left((\alpha+\beta-1)\frac{u_x}{u}\frac{u_{xxx}}{u} + \frac{u_{xxxx}}{u}\right)dx \\ &= \int_{\mathbb{T}} (u^{\alpha+\beta-1} u_{xxx})_x dx = 0 \end{aligned}$$

$\Rightarrow EP[u] = EP[u] + cI_3$ with $c = \frac{1}{\alpha+\beta-1}$

Integration-by-parts rules

$$EP[u] = -\int_{\mathbb{T}} u^{\alpha+\beta-2} u_x u_{xxx} dx \geq 0\,?$$

Question: How many independent rules of integration by parts?

$$I_1 = \int_{\mathbb{T}} u^{\alpha+\beta} \left((\alpha+\beta-3)\left(\frac{u_x}{u}\right)^4 + 3\left(\frac{u_x}{u}\right)^2 \frac{u_{xx}}{u} \right) dx = 0$$

$$I_2 = \int_{\mathbb{T}} u^{\alpha+\beta} \left((\alpha+\beta-2)\left(\frac{u_x}{u}\right)^2 \frac{u_{xx}}{u} + \left(\frac{u_{xx}}{u}\right)^2 + \frac{u_x}{u}\frac{u_{xxx}}{u} \right) dx = 0$$

$$I_3 = \int_{\mathbb{T}} u^{\alpha+\beta} \left((\alpha+\beta-1)\frac{u_x}{u}\frac{u_{xxx}}{u} + \frac{u_{xxxx}}{u} \right) dx = 0$$

Aim: Prove that $\exists c_1, c_2, c_3 \in \mathbb{R}$: $EP[u] = EP[u] + c_1 I_1 + c_2 I_2 + c_3 I_3 \geq 0$

New idea: Identify $\xi_1 = \frac{u_x}{u}$, $\xi_2 = \frac{u_{xx}}{u}$ etc. and formulate using polynomials

$EP[u]$	corresponds to	$S(\xi) = -\xi_1\xi_3$
I_1	corresponds to	$T_1(\xi) = (\alpha+\beta-3)\xi_1^4 + 3\xi_1^2\xi_2$
I_2	corresponds to	$T_2(\xi) = (\alpha+\beta-2)\xi_1^2\xi_2 + \xi_1\xi_3 + \xi_2^2$
I_3	corresponds to	$T_3(\xi) = (\alpha+\beta-1)\xi_1\xi_3 + \xi_4$

Integration-by-parts rules

$P[u]$	corresponds to	$S(\xi) = -\xi_1\xi_3$
I_1	corresponds to	$T_1(\xi) = (\alpha+\beta-3)\xi_1^4 + 3\xi_1^2\xi_2$
I_2	corresponds to	$T_2(\xi) = (\alpha+\beta-2)\xi_1^2\xi_2 + \xi_1\xi_3 + \xi_2^2$
I_3	corresponds to	$T_3(\xi) = (\alpha+\beta-1)\xi_1\xi_3 + \xi_4$

$T_i =$ integration-by-parts polynomials $=$ shift polynomials

Nonnegativity of entropy production follows ...

$$\exists c_1, c_2, c_3 \in \mathbb{R}: \; P[u] = P[u] + c_1 I_1 + c_2 I_2 + c_3 I_3 \geq 0$$

... from solution of decision problem:

$$\exists c_1, c_2, c_3 \in \mathbb{R} : \forall \xi : \; (S + c_1 T_1 + c_2 T_2 + c_3 T_3)(\xi) \geq 0$$

- Calculate $EP[u] = -\frac{dH}{dt}$, gives polynomial S
- Determine shift polynomials T_i (depends on differential order of eq.)
- Solve decision problem
- Show that $\exists \kappa > 0 : \; EP[u] - \kappa Q[u] \geq 0, \; Q[u]$ contains $|\nabla^2 u^\gamma|^2$ etc.

Solution of decision problem

$$\exists c_1, c_2, c_3 \in \mathbb{R} : \forall \xi : \ (S + c_1 T_1 + c_2 T_2 + c_3 T_3)(\xi) \geq 0$$

- Tarski 1930: Polynomial decision problems can be reduced to a quantifier-free statement in an algorithmic way
- Problem well known in real algebraic geometry
- Implementations in `Mathematica`, `QEPCAD` (Collins/Hong 1991) available, give complete and exact answer
- Algorithms are doubly exponential in number of c_i, ξ

Reductions:

- Not all integration-by-parts rules are needed: reduces number of c_i
- Write polynomial as sum of squares: many algorithms available, quickly solvable, but only numerical results (relation to Hilbert's 17th problem), and $\exists$ polynomial $P \geq 0$ with $P \neq$ sum of squares
- Several dimensions: symmetry reduction, use scalar variables $|\nabla u|$, Δu, $|\nabla^2 u|$ etc.

Entropies for thin-film equation

$$\partial_t u = -(u^\beta u_{xxx})_x, \quad S(\xi) = -\xi_1\xi_3$$

- Shift polynomials:

$$\begin{aligned} T_1(\xi) &= (\alpha+\beta-3)\xi_1^4 + 3\xi_1^2\xi_2, \\ T_2(\xi) &= (\alpha+\beta-2)\xi_1^2\xi_2 + \xi_2^2 + \xi_1\xi_3 \\ T_3(\xi) &= (\alpha+\beta-1)\xi_1\xi_3 + \xi_4 \end{aligned}$$

- Decision problem:

$$\exists c_1, c_2, c_3 \in \mathbb{R} : \forall \xi \in \mathbb{R}^3 : (S + c_1 T_1 + c_2 T_2 + c_3 T_3)(\xi) \geq 0$$

- Eliminate $\xi_4 \Rightarrow c_3 = 0$; eliminate $\xi_1\xi_3 \Rightarrow c_2 = 1$
- Reduced decision problem: $\exists c_1 \in \mathbb{R} : \forall \xi \in \mathbb{R}^2$:

$$(\alpha+\beta-3)c_1\xi_1^4 + (\alpha+\beta-2+3c_1)\xi_1^2\xi_2 + \xi_2^2 \geq 0$$

- Solution: $9(c_1 + \frac{1}{9}(\alpha+\beta))^2 + \frac{8}{9}(\alpha+\beta-\frac{3}{2})(\alpha+\beta-3) \leq 0$
- Choose $c_1 = -\frac{1}{9}(\alpha+\beta) \Rightarrow$ positive if and only if $\frac{3}{2} \leq \alpha+\beta \leq 3$

Bakry-Emery revisited

$$\partial_t u = \mathrm{div}(\nabla u + u\nabla V) \quad \text{in } \mathbb{R}^d$$

Aim: Show $\frac{d^2 H_\alpha}{dt^2} + \kappa \frac{dH_\alpha}{dt} \geq 0$ with systematic integration by parts

- Assume: $\nabla^2 V \geq \lambda$, one-dimensional case
- Multi-dimensional case: see Matthes/A.J./Toscani 2011
- Entropy:

$$H_\alpha[u] = \frac{\alpha}{4(\alpha-1)}\bigg(\int_{\mathbb{R}}\Big(\frac{u}{u_\infty}\Big)^\alpha u_\infty dx - \Big(\int_{\mathbb{R}} udx\Big)^\alpha\bigg), \ 1 < \alpha \leq 2$$

- Set $w = u^{\alpha/2}$ and compute

$$\frac{d^2 H_\alpha}{dt^2} = \frac{2}{\alpha}\int_{\mathbb{R}} w^2\bigg[\alpha\Big(\frac{w_{xx}}{w}\Big)^2 + (2-\alpha)\Big(\frac{w_x}{w}\Big)^2\frac{w_{xx}}{w} - 2\alpha\frac{w_x}{w}\frac{w_{xx}}{w}V_x - (2-\alpha)\Big(\frac{w_x}{w}\Big)^3 V_x + \alpha\Big(\frac{w_x}{w}\Big)^2 V_x^2\bigg]u_\infty dx$$

- Integrand formulated as polynomial:
  $S_2(\xi) = \alpha\xi_2^2 + (2-\alpha)\xi_1^2\xi_2 - 2\alpha\xi_1\xi_2 V_x - (2-\alpha)\xi_1^3 V_x + \alpha\xi_1^2 V_x^2$

Shift polynomials

$$S_2(\xi) = \alpha\xi_2^2 + (2-\alpha)\xi_1^2\xi_2 - 2\alpha\xi_1\xi_2 V_x - (2-\alpha)\xi_1^3 V_x + \alpha\xi_1^2 V_x^2$$

- First time derivative: $-\frac{dH_\alpha}{dt} = \int_{\mathbb{R}} w_x^2 u_\infty dx \Rightarrow S_1(\xi) = \xi_1^2$
- Shift polynomials: (recall that $u_{\infty,x} = -u_\infty V_x$)

$$0 = \int_{\mathbb{R}^d} (w_x^2 V_x u_\infty)_x dx = \int_{\mathbb{R}^d} (2w_x w_{xx} V_x + w_x^2 V_{xx} - w_x^2 V_x^2) u_\infty dx$$

$$T_1(\xi) = 2\xi_1\xi_2 V_x + \xi_1^2 V_{xx} - \xi_1^2 V_x^2$$

$$0 = \int_{\mathbb{R}^d} (w^{-1} w_x^3 u_\infty)_x dx = \int_{\mathbb{R}^d} w^{-1}(3w_x^2 w_{xx} - w^{-1} w_x^4 - w_x^3 V_x) u_\infty dx$$

$$T_2(\xi) = 3\xi_1^2\xi_2 - \xi_1^4 - \xi_1^3 V_x$$

- Decision problem: $\exists c_1, c_2 \in \mathbb{R},\ c > 0 : \forall \xi \in \mathbb{R}^3$:

$$S^*(\xi) = (S_2 + c_1 T_1 + c_2 T_2 - cS_1)(\xi) \geq 0$$

Solution of decision problem

$$S^*(\xi) = \alpha\xi_2^2 + (2-\alpha+3c_2)\xi_1^2\xi_2 + 2(-\alpha+c_1)\xi_1\xi_2 V_x - (2-\alpha+c_2)\xi_1^3 V_x + (\alpha-c_1)\xi_1^2 V_x^2 - c_2\xi_1^4 + (c_1 V_{xx} - c)\xi_1^2$$

- Eliminate $\xi_1\xi_2 V_x$: $c_1 = \alpha$, eliminate $\xi_1^3 V_x$: $c_2 = -(2-\alpha)$
- Since $V_{xx} \geq \lambda$: choose $c = \alpha\lambda$
- This gives with $x = \xi_1^2$, $y = \xi_2$:

$$S^*(\xi) \geq \alpha\xi_2^2 - 2(2-\alpha)\xi_1^2\xi_2 + (2-\alpha)\xi_1^4 = \alpha y^2 - 2(2-\alpha)xy + (2-\alpha)x^2$$

- $S^*(\xi) \geq 0$ if and only if $\alpha(2-\alpha) \geq (2-\alpha)^2$ or $2(2-\alpha)(\alpha-1) \geq 0$
  $\Rightarrow 1 \leq \alpha \leq 2$

We have shown: $\frac{d^2 H_\alpha}{dt^2} + \alpha\lambda\frac{dH_\alpha}{dt} \geq 0$ for $1 < \alpha \leq 2$

Theorem

Let $\nabla^2 V \geq \lambda$. Then the solution of $\partial_t u = \operatorname{div}(\nabla u + u\nabla V)$ in $\mathbb{R}^d$ satisfies

$$H_\alpha[u(t)] \leq e^{-\alpha\lambda t} H_\alpha[u(0)], \quad 1 < \alpha \leq 2$$

Overview

Cross-diffusion systems

$$\partial_t u - \mathrm{div}(A(u)\nabla u) = f(u) \text{ in } \Omega,\ t > 0, \quad u(0) = u^0, \quad \text{no-flux b.c.}$$

- Meaning: $\mathrm{div}(A(u)\nabla u)_i = \sum_{j=1}^n \mathrm{div}(A_{ij}(u)\nabla u_j)$, $A \in \mathbb{R}^{n\times n}$, $u \in \mathbb{R}^n$
- Diagonal diffusion matrix: $A_{ij}(u) = 0$ for $i \neq j$
- Cross-diffusion matrix: generally $A_{ij}(u) \neq 0$ for $i \neq j$

Why study cross-diffusion systems?

- They arise in many applications from physics, biology, chemistry...
- Diffusion-induced instabilities may arise
- Cross-diffusion may allow for pattern formation
- They may exhibit an unexpected gradient-flow/entropy structure

Example ❶: Cross-diffusion population dynamics

$$\partial_t u - \mathrm{div}(A(u)\nabla u) = f(u) \text{ in } \Omega,\ t > 0, \quad u(0) = u^0, \quad \text{no-flux b.c.}$$

- $u = (u_1, u_2)$ and u_i models population density of ith species
- Diffusion matrix:

$$A(u) = \begin{pmatrix} a_{10} + a_{11}u_1 + a_{12}u_2 & a_{12}u_1 \\ a_{21}u_2 & a_{20} + a_{21}u_1 + a_{22}u_2 \end{pmatrix}$$

- Suggested by Shigesada- Kawasaki-Teramoto 1979: models population segregation
- Lotka-Volterra functions: $f_i(u) = (b_{i0} - b_{i1}u_1 - b_{i2}u_2)u_i$
- Diffusion matrix is not symmetric, generally not positive definite

Example ❷: Ion transport through nano-pores

$$\partial_t u - \mathrm{div}(A(u)\nabla u) = f(u) \text{ in } \Omega,\ t > 0, \quad u(0) = u^0, \quad \text{no-flux b.c.}$$

- $(u_1, \ldots, u_N)$ ion concentrations, $u_N = 1 - \sum_{j=1}^{N-1} u_j$
- Diffusion matrix for $N = 4$:

$$A(u) = \begin{pmatrix} D_1(1-u_2-u_3) & D_1 u_1 & D_1 u_1 \\ D_2 u_2 & D_2(1-u_1-u_3) & D_2 u_2 \\ D_3 u_3 & D_3 u_3 & D_3(1-u_2-u_3) \end{pmatrix}$$

- Derived by Burger-Schlake-Wolfram 2012 from lattice model
- Electric field neglected to simplify
- Diffusion matrix generally not positive definite – expect that $0 \le u_i \le 1$

Cross-diffusion systems

$$\partial_t u - \operatorname{div}(A(u)\nabla u) = f(u) \text{ in } \Omega,\ t > 0, \quad u(0) = u_0, \quad \text{no-flux b.c.}$$

Main features:

- Diffusion matrix $A(u)$ non-diagonal
- Matrix $A(u)$ may be neither symmetric nor positive definite
- Variables u_i may be bounded from below and/or above

Objectives:

- Global-in-time existence of weak solutions
- Positivity and boundedness of weak solutions
- Large-time asymptotics

Mathematical difficulties:

- No general theory for diffusion systems available
- Generally no maximum principle, no regularity theory
- Lack of positive definiteness → local existence nontrivial

Previous results

$$\partial_t u - \mathrm{div}(A(u)\nabla u) = f(u) \text{ in } \Omega,\ t > 0$$

Global existence if ...

- Growth conditions on nonlinearities (Ladyženskaya ... 1988)
- Control on L^∞ and Hölder norms (Amann 1989)
- Invariance principle holds (Redlinger 1989, Küfner 1996)
- Positivity, mass control, diagonal $A(u)$ (Pierre-Schmitt 1997)

Unexpected behavior:

- Finite-time blow-up of Hölder solutions (Stará-John 1995)
- Weak solutions may exist after L^∞ blow-up (Pierre 2003)
- Cross-diffusion may lead to pattern formation (instability) or may avoid finite-time blow-up (Hittmeir/A.J. 2011)

Special structure needed for global existence theory:
gradient-flow or entropy structure

Abstract gradient flows

Definition: Gradient flow if $\partial_t u = -\operatorname{grad} H|_u$ on differential manifold

- Example: $\mathbb{R}^n$ with Euclidean structure, $\partial_t u = -\nabla H(u)$, $H : \mathbb{R}^n \to \mathbb{R}$

$$\frac{d}{dt}H(u) = \nabla H(u) \cdot \partial_t u = -|\nabla H(u)|^2 \ \Rightarrow \ H \text{ is Lyapunov functional}$$

- Can be generalized to $\partial_t u \in \nabla H(u)$ on Hilbert space (Brézis 1973)
- Heat equation is gradient flow for $H(u) = \frac{1}{2}\int_{\mathbb{R}^d} |\nabla u|^2 dx$ in $L^2(\mathbb{R}^d)$:

$$\operatorname{grad} H(u)\xi = \int_{\mathbb{R}^d} \nabla u \cdot \nabla \xi dx = -\int_{\mathbb{R}^d} \Delta u \xi dx \ \Rightarrow \ \partial_t u = \Delta u$$

- Otto 2001: Heat eq. is gradient flow for $H(u) = \int_{\mathbb{R}^d} u \log u dx$ in Wasserstein space (= probability measures with Wasserstein metric)
- Advantage: allows for geometric interpretation
- Reference for abstract gradient flows: Ambrosio/Gigli/Savaré 2005

Our formal definition: Gradient flow if $\partial_t u = \operatorname{div}(B\nabla \operatorname{grad} H(u))$

Gradient flows: Cross-diffusion systems

Main assumption

$\partial_t u - \operatorname{div}(A(u)\nabla u) = f(u)$ possesses formal gradient-flow structure

$$\partial_t u - \operatorname{div}\big(B\nabla \operatorname{grad} H(u)\big) = f(u),$$

where B is positive semi-definite, $H(u) = \int_\Omega h(u)dx$ entropy

Equivalent formulation: $\operatorname{grad} H(u) \simeq h'(u) =: w$ (entropy variable)

$$\partial_t u - \operatorname{div}(B\nabla w) = f(u), \quad B = A(u)h''(u)^{-1}$$

Consequences:

- H is Lyapunov functional if $f = 0$:

$$\frac{dH}{dt} = \int_\Omega \partial_t u \cdot \underbrace{h'(u)}_{=w} dx = -\int_\Omega \nabla w : B\nabla w dx \le 0$$

- L^∞ bounds for u: Let $h' : D \to \mathbb{R}^n$ ($D \subset \mathbb{R}^n$) be invertible $\Rightarrow$ $u = (h')^{-1}(w) \in D$ (no maximum principle needed!)

Example ❶: Population-dynamics model

$$\partial_t u - \operatorname{div}(A(u)\nabla u) = 0 \text{ in } \Omega,\ t > 0, \quad u(0) = u^0, \quad \text{no-flux b.c.}$$

- $u = (u_1, u_2)$ and u_i models population density of ith species
- Diffusion matrix:

$$A(u) = \begin{pmatrix} a_{10} + a_{11}u_1 + a_{12}u_2 & a_{12}u_1 \\ a_{21}u_2 & a_{20} + a_{21}u_1 + a_{22}u_2 \end{pmatrix}$$

- Entropy:

$$H[u] = \int_\Omega h(u)dx = \int_\Omega \left(\frac{u_1}{a_{12}}(\log u_1 - 1) + \frac{u_2}{a_{21}}(\log u_2 - 1) \right) dx$$

- Entropy production:

$$\begin{aligned} \frac{dH}{dt}[u] &= \int_\Omega \left(\frac{\log u_1}{a_{12}} \partial_t u_1 + \frac{\log u_2}{a_{21}} \partial_t u_2 \right) dx \\ &= -2 \int_\Omega \bigg(\frac{2}{a_{12}}(a_{10} + a_{11}u_1)|\nabla\sqrt{u_1}|^2 + \frac{2}{a_{21}}(a_{20} + a_{22}u_2)|\nabla\sqrt{u_2}|^2 \\ &\quad + |\nabla\sqrt{u_1 u_2}|^2 \bigg) dx \le 0 \end{aligned}$$

Example ❶: Population-dynamics model

$$h(u) = \frac{u_1}{a_{12}}(\log u_1 - 1) + \frac{u_2}{a_{21}}(\log u_2 - 1)$$

Question: Does the model allow for a gradient-flow/entropy structure?

$$\partial_t u - \operatorname{div}(B(w)\nabla w) = 0, \quad B(w) = A(u)h''(u)^{-1}$$

Answer: Yes!

- Entropy variable $w = h'(u)$:

$$w_1 = \frac{\partial h}{\partial u_1} = \frac{\log u_1}{a_{12}}, \quad w_2 = \frac{\partial h}{\partial u_2} = \frac{\log u_2}{a_{21}} \quad \Rightarrow u_2 \sim e^{a_{21} w_2} \text{ positive!}$$

- New diffusion matrix:

$$B(w) = \begin{pmatrix} (a_{10} + a_{11}a_{21}^{-1}e^{w_1} + e^{w_2})e^{w_1} & e^{w_1+w_2} \\ e^{w_1+w_2} & (a_{20} + a_{21}a_{12}^{-1}e^{w_2} + e^{w_1})e^{w_2} \end{pmatrix}$$

$$\det B(w) \ge a_{10}e^{w_1} + a_{20}e^{w_2} > 0$$

- Matrix $B(w)$ is symmetric, positive definite (not uniform in $w \in \mathbb{R}^2$!)

Example ❷: Ion-transport model

$$\partial_t u - \operatorname{div}(A(u)\nabla u) = 0 \text{ in } \Omega,\ t > 0, \quad u(0) = u^0, \quad \text{no-flux b.c.}$$

- $u = (u_1, u_2, u_3)$ and u_i models the ith ion concentration
- Diffusion matrix:

$$A(u) = \begin{pmatrix} D_1(1-u_2-u_3) & D_1 u_1 & D_1 u_1 \\ D_2 u_2 & D_2(1-u_1-u_3) & D_2 u_2 \\ D_3 u_3 & D_3 u_3 & D_3(1-u_2-u_3) \end{pmatrix}$$

- Entropy: $H[u] = \int_\Omega h(u)dx$, $u_4 = 1 - \sum_{i=1}^3 u_i$

$$h(u) = \sum_{i=1}^{3} u_i(\log u_i - 1) + u_4(\log u_4 - 1) + \sum_{i=1}^{3} \log(D_i) u_i$$

- Entropy production:

$$\frac{dH}{dt}[u] = \int_\Omega \left(\sum_{i=1}^{3} \partial_t u_i \log u_i - \sum_{i=1}^{3} \partial_t u_i \log u_4 + \sum_{i=1}^{3} \partial_t u_i \log D_i \right) dx$$

Example ❷: Ion-transport model

$$h(u) = \sum_{i=1}^{3} u_i(\log u_i - 1) + u_4(\log u_4 - 1) + \sum_{i=1}^{3} \log(D_i)u_i$$

- Entropy production:

$$\frac{dH}{dt}[u] = \int_\Omega \sum_{i=1}^{3} \log\left(\frac{D_i u_i}{u_4}\right)\partial_t u_i dx$$
$$\leq -C\int_\Omega \left(u_4^2 \sum_{i=1}^{3} |\nabla\sqrt{u_i}|^2 + |\nabla\sqrt{u_4}|^2\right)dx$$

- Difficulty: degeneracy at $u_4 = 0$!
- New diffusion matrix:

$$B(w) = u_4 \,\mathrm{diag}(D_1 u_1, D_2 u_2, D_3 u_3)$$

- Entropy structure: $w_i = \partial h/\partial u_i = \log(u_i/u_4)$, back-transformation:

$$u_i = \frac{e^{w_i}}{1 + e^{w_1} + e^{w_2} + e^{w_3}} \in (0,1) \;\Rightarrow\; L^\infty \text{ bounds!}$$

Relation to nonequilibrium thermodynamics

- Chemical potential: $\mu_i = -\frac{\partial s}{\partial \rho_i}$, s: physical entropy density, ρ_i: mass density of ith species
- Entropy variables: $w_i = \frac{\partial h}{\partial \rho_i}$, $h = -s$: mathematical entropy
- Mixture of ideal gases: $\mu_i = \mu_i^0 + \log \rho_i$, $\mu_i^0 = \text{const.} \Rightarrow$

$$w_i = -\frac{\partial s}{\partial \rho_i} = \mu_i^0 + \log \rho_i \quad \text{or} \quad \rho_i = e^{w_i - \mu_i^0}$$

- Non-ideal gases: $\mu_i = \log a_i$, $a_i = \gamma_i \rho_i$: thermodynamic activity
- Example: volume-filling case, $\gamma_i = 1 + \sum_{j=1}^{n-1} a_j$

$$\rho_i = \frac{a_i}{\gamma_i} = \frac{a_i}{1 + \sum_{j=1}^{n-1} a_i} = \frac{\exp(\mu_i)}{1 + \sum_{j=1}^{n-1} \exp(\mu_i)}$$

$\rightarrow$ exactly the expression for the ion-transport model!

- Open problem: Include nonconstant temperature

Boundedness-by-entropy method

$$\partial_t u - \mathrm{div}(A(u)\nabla u) = f(u) \text{ in } \Omega,\ t>0, \quad u(0)=u_0, \quad \text{no-flux b.c.}$$

Assumptions:

1. $\exists$ entropy density $h \in C^2(D;[0,\infty))$, h' invertible on $D \subset \mathbb{R}^n$
   Example: $h(u) = u\log u$ for $u \in D = (0,\infty)$, $(h')^{-1}(w) = e^w \in D$
2. $h''(u)A(u)$ is positive semidefinite for $u \in D$
   implies $z^\top h''(u)A(u)z = (h''(u)z)^\top B(w)(h''(u)z) \geq 0$ for $z \in \mathbb{R}^N$
3. A continuous on D, $\exists C>0 : \forall u \in D$: $f(u)\cdot h'(u) \leq C(1+h(u))$
   needed to control reaction term $f(u)$

Problem: $h''(u)A(u)$ semidefinite not sufficient, need gradient estimate!
Solution: Assume $D \subset (a,b)^n$, $a_i^* > 0$, $m_i > 0$, and

$$z^\top h''(u)A(u)z \geq \sum_{i=1}^n a_i(u)^2 z_i^2$$

where $a_i(u) = a_i^*(u_i - a)^{m_i-1}$ or $a_i(u) = a_i^*(b-u_i)^{m_i-1}$
$\rightarrow$ Can probably be generalized to arbitrary increasing functions a_i

Boundedness-by-entropy method

$$\partial_t u - \mathrm{div}(A(u)\nabla u) = f(u) \text{ in } \Omega,\ t > 0, \quad u(0) = u_0, \quad \text{no-flux b.c.}$$

Assumptions:

1. $\exists$ convex entropy $h \in C^2(D; [0, \infty))$, h' invertible on $D \subset \mathbb{R}^n$
2. Assume $D \subset (a, b)^n$, $a_i^* > 0$, $m_i > 0$, and
$$z^\top h''(u)A(u)z \geq \sum_{i=1}^n a_i(u)^2 z_i^2, \quad a_i(u) \sim u_i^{m_i-1}$$
3. A continuous on D, $\exists C > 0 : \forall u \in D$: $f(u) \cdot h'(u) \leq C(1 + h(u))$

Consequence of ❷: $\nabla u^\top h''(u)A(u)\nabla u \geq C(|\nabla u_1^{m_1}|^2 + |\nabla u_2^{m_2}|^2)$

Theorem (A.J., *Nonlinearity* 2015)

Let the above assumptions hold, let $D \subset \mathbb{R}^n$ be bounded, $u_0 \in L^1(\Omega) \cap \overline{D}$. Then $\exists$ global weak solution such that $u(x, t) \in \overline{D}$ and

$$u \in L^2_{\mathrm{loc}}(0, \infty; H^1(\Omega)), \quad \partial_t u \in L^2_{\mathrm{loc}}(0, \infty; H^1(\Omega)')$$

Boundedness-by-entropy method

Theorem (A.J., *Nonlinearity* 2015)

Let the above assumptions hold, let $D \subset \mathbb{R}^n$ be bounded, $u_0 \in L^1(\Omega) \cap \overline{D}$. Then $\exists$ global weak solution such that $u(x,t) \in \overline{D}$ and

$$u \in L^2_{\rm loc}(0,\infty; H^1(\Omega)), \quad \partial_t u \in L^2_{\rm loc}(0,\infty; H^1(\Omega)')$$

Remarks:

- Result valid for rather general model class
- Yields L^∞ bounds without using a maximum principle
- Boundedness assumption on D is strong (can be weakened in some cases; see examples below)
- Main assumption: existence of entropy h and invertibility of h' on D
- How to find entropy functions h? Physical intuition, trial-and-error
- Theorem can be generalized for degenerate problems

What's next? Proof of existence result, concrete examples, extensions

Proof of existence theorem

$$\partial_t u - \mathrm{div}(A(u)\nabla u) = f(u) \quad \text{or} \quad \partial_t u(w) - \mathrm{div}(B(w)\nabla w) = f(u(w))$$

Key ideas:

- Discretize in time: replace $\partial_t u(w)$ by $\frac{1}{\tau}(u(w^k) - u(w^{k-1}))$
  Benefit: Avoid issues with time regularity
- Regularize in space by adding "$\varepsilon \Delta^m w^k$"
  Benefit: Since $\mathrm{div}(B(w)\nabla w)$ is not uniformly elliptic; yields solutions $w^k \in H^m(\Omega) \subset L^\infty(\Omega)$ if $m > d/2$
- Solve problem in w^k by fixed-point argument
  Benefit: Problem in w-formulation is elliptic (not true for u-formulation)
- Perform limit $(\varepsilon, \tau) \to 0$, obtain solution $u(t) = \lim u(w^k)$
  Benefit: Compactness comes from entropy estimate; L^∞ bounds coming from $u(w^k) \in D \Rightarrow u \in \overline{D}$

Strategy: Problem in u → Solve in w → Limit gives problem in u

Proof of existence theorem

$$\partial_t u - \mathrm{div}(A(u)\nabla u) = f(u) \quad \text{or} \quad \partial_t u(w) - \mathrm{div}(B(w)\nabla w) = f(u(w))$$

More details:

- Implicit Euler: Replace $\partial_t u(t_k)$ by $\frac{1}{\tau}(u(w^k) - u(w^{k-1}))$, $t_k = k\tau$ to obtain elliptic problems, w: entropy variable
- Regularization: Add $\varepsilon(-1)^m \sum_{|\alpha|=m} D^{2\alpha} w + \varepsilon w$, where $H^m(\Omega) \subset L^\infty(\Omega) \rightsquigarrow$ uniform ellipticity
- Solve approximate problem using Leray-Schauder fixed-point theorem
- Derive estimates uniform in (τ, ε) from entropy production estimate
- Use compactness to perform the limit $(\tau, \varepsilon) \to 0$

Approximate problem: Given $w^{k-1} \in L^\infty(\Omega)$, solve

$$\frac{1}{\tau}\int_\Omega (u(w^k) - u(w^{k-1})) \cdot \phi dx + \int_\Omega \nabla\phi : B(w^k)\nabla w^k dx + \varepsilon \int_\Omega \Big(\sum_{|\alpha|=m} D^\alpha w^k \cdot D^\alpha \phi + w^k \cdot \phi \Big) dx = \int_\Omega f(u(w^k)) \cdot \phi dx$$

Step ❶: Lax-Milgram argument

- Define $S : L^\infty(\Omega) \times [0,1] \to L^\infty(\Omega)$, $S(y,\delta) = w^k$ and w^k solves linear problem:

$$a(w^k,\phi) = \int_\Omega \nabla\phi : B(y)\nabla w^k dx + \varepsilon \int_\Omega \Big(\sum_{|\alpha|=m} D^\alpha w^k \cdot D^\alpha \phi + w^k \cdot \phi \Big) dx$$
$$= -\frac{\delta}{\tau} \int_\Omega (u(y) - u(w^{k-1})) \cdot \phi dx + \delta \int_\Omega f(u(y)) \cdot \phi dx = F(\phi)$$

- Lax-Milgram lemma gives solution $w^k \Rightarrow S$ well defined
- Properties: $S(y,0) = 0$, S compact (since $H^m \hookrightarrow L^\infty$ compact)

Theorem (Leray-Schauder)

Let B Banach space, $S : B \times [0,1] \to B$ compact, $S(y,0) = 0$ for $y \in B$,

$$\exists C > 0 : \forall y \in B,\ \delta \in [0,1] :\ S(y,\delta) = y \ \Rightarrow\ \|y\|_B \le C.$$

Then $S(\cdot,1)$ has a fixed point.

Step ❷: Leray-Schauder argument

- Discrete entropy estimate: choose test fct. w^k, $\tau \ll 1$, use h convex

$$\delta \int_\Omega h(u(w^k))dx + \tau \int_\Omega \nabla w^k : B\nabla w^k dx + \varepsilon\tau C\|w^k\|_{H^m}^2 \\ \le \underbrace{C\tau}_{<1} \delta \int_\Omega (1 + h(u(w^k)))dx + \underbrace{\delta}_{\le 1} \int_\Omega h(u(w^{k-1}))dx$$

- Yields $\|w^k\|_{L^\infty} \le C\|w^k\|_{H^m} \le C(\varepsilon,\tau) \Rightarrow$ estimate uniform in (w^k,δ)
- Leray-Schauder: $\exists$ solution $w^k \in H^m(\Omega)$
- Sum discrete entropy estimate *(slightly simplified)*:

$$\int_\Omega h(u(w^k))dx + C\tau \sum_{j=1}^k \sum_{i=1}^n \int_\Omega |\nabla u_i(w^k)^{m_i}|^2 dx \\ + \varepsilon\tau C \sum_{k=1}^k \|w^j\|_{H^m}^2 \le C$$

- Idea: Derive estimates for $u = u(w)$, not for w

Step ❸: Uniform estimates

- Estimates uniform in (τ,ε): set $u^{(\tau)}(\cdot,t)=u(w^k)$, $t\in((k-1)\tau,k\tau]$

$$\|(u_i^{(\tau)})^{m_i}\|_{L^2(0,T;H^1)}+\sqrt{\varepsilon}\|w^{(\tau)}\|_{L^2(0,T;H^m)}\le C$$
$$\tau^{-1}\|u^{(\tau)}(t)-u^{(\tau)}(t-\tau)\|_{L^2(\tau,T;(H^m)')}\le C$$

Theorem (Nonlinear Aubin-Lions lemma, Chen/A.J./Liu 2014)

Let $(u^{(\tau)})$ be piecewise constant in time, $k\in\mathbb{N}$, $s\ge\frac12$, and

$$\tau^{-1}\|u^{(\tau)}(t)-u^{(\tau)}(t-\tau)\|_{L^1(\tau,T;(H^k)')}+\|(u^{(\tau)})^s\|_{L^2(0,T;H^1)}\le C$$

Then exists subsequence $u^{(\tau)}\to u$ strongly in $L^{2s}(0,T;L^{2s})$

Remarks:

- Generalization of standard Aubin-Lions lemma $(s=1)$
- Result can be generalized to $(u^{(\tau)})^s\in L^p(0,T;W^{1,q})$ and $\phi(u^{(\tau)})\in L^2(0,T;H^1)$ if $(u^{(\tau)})$ bounded in L^∞, ϕ monotone

Step ❹: Limit $(\tau,\varepsilon)\to 0$

$$\frac{1}{\tau}\int_0^T\int_\Omega (u^{(\tau)}(t)-u^{(\tau)}(t-\tau))\cdot\phi dxdt+\int_0^T\int_\Omega \nabla\phi : A(u^{(\tau)})\nabla u^{(\tau)}dxdt$$
$$+\varepsilon\int_0^T\int_\Omega\bigg(\sum_{|\alpha|=m}D^\alpha w^{(\tau)}\cdot D^\alpha\phi+w^{(\tau)}\cdot\phi\bigg)dxdt=\int_0^T\int_\Omega f(u^{(\tau)})\cdot\phi dxdt$$

- Nonlinear Aubin-Lions lemma:

$$\begin{aligned} u^{(\tau)}\to u &\quad \text{strongly in } L^2(0,T;L^2)\\ \varepsilon w^{(\tau)}\to 0 &\quad \text{strongly in } L^2(0,T;H^m)\\ A(u^{(\tau)})\nabla u^{(\tau)}\rightharpoonup A(u)\nabla u &\quad \text{weakly in } L^2(0,T;L^2)\end{aligned}$$

- Limit $(\tau,\varepsilon)\to 0$ in weak formulation $\Rightarrow$ u solves diffusion system
- u satisfies initial datum: Show that linear interpolant of $(u^{(\tau)})$ is bounded in $C^0([0,T];(H^m)')$ $\Rightarrow$ $u(\cdot,0)=u_0$ defined in $H^m(\Omega)'$
- Boundary conditions: Contained in weak formulation

Summary

Theorem (A.J., *Nonlinearity* 2015)

Let the above assumptions hold, let $D \subset \mathbb{R}^n$ be bounded, $u_0 \in L^1(\Omega) \cap \overline{D}$. Then $\exists$ global weak solution such that $u(x,t) \in \overline{D}$ and

$$u \in L^2_{\rm loc}(0,\infty; H^1(\Omega)), \quad \partial_t u \in L^2_{\rm loc}(0,\infty; H^1(\Omega)')$$

Strategy of the proof:

- Implicit Euler discretization and Δ^m regularization
- Entropy formulation gives a priori estimates and L^∞ bounds
- Compactness from nonlinear Aubin-Lions lemma

Benefits:

- General global existence theorem
- Yields bounded weak solutions without a maximum principle

Limitations:

- Boundedness of domain D, how to find entropy density h?
- Particular positive definiteness condition on $h''(u)A(u)$

❶ Population model of Shigesada-Kawasaki-Teramoto

$$\partial_t u - \mathrm{div}(A(u)\nabla u) = 0 \text{ in } \Omega,\ t > 0, \quad u(0) = u_0, \quad \text{no-flux b.c.}$$

- Entropy defined on unbounded domain $D = (0,\infty)^2$
- Entropy-dissipation inequality:

$$\frac{dH}{dt}[u] = -2\int_\Omega \bigg(\frac{2}{a_{12}}(a_{10} + a_{11}u_1)|\nabla\sqrt{u_1}|^2 + \frac{2}{a_{21}}(a_{20} + a_{22}u_2)|\nabla\sqrt{u_2}|^2 + |\nabla\sqrt{u_1u_2}|^2\bigg)dx$$

- Yields estimate for $(\sqrt{u_i})$ in $H^1(\Omega)$: Previous proof applies
- Main difference: We do not have (u_i) bounded in $L^\infty(\Omega)$ but only $(\sqrt{u_i})$ bounded in $L^6(\Omega)$ (if space dimension ≤ 3)
- Assumption: Transition rates $p_i(u) = a_{i0} + a_{i1}u_1 + a_{i2}u_2$
- Previous technique of proof yield global existence of solutions

❷ Ion-transport model

Entropy production: recall that $u_4 = 1 - u_1 - u_2 - u_3$

$$H[u^{(\tau)}(t)] + C\int_0^t\int_\Omega\Big(u_4^{(\tau)}\sum_{i=1}^3|\nabla(u_i^{(\tau)})^{1/2}|^2 + |\nabla(u_4^{(\tau)})^{1/2}|^2\Big)dxds \le H[u^0]$$

- Problem: degeneracy at $u_4^{(\tau)} = 0$, no estimate for $\nabla(u_i^{(\tau)})^{1/2}$
- Consequence ❶:

$$\Big|\nabla\Big((u_4^{(\tau)})^{1/2}u_i^{(\tau)}\Big)\Big|^2 \le 8u_4^{(\tau)}(u_i^{(\tau)})^{1/2}\Big|\nabla(u_i^{(\tau)})^{1/2}\Big|^2 + 2(u_1^{(\tau)})^2\Big|\nabla(u_4^{(\tau)})^{1/2}\Big|^2 \le C$$

$$\Rightarrow\quad \nabla\Big((u_4^{(\tau)})^{1/2}u_i^{(\tau)}\Big) \rightharpoonup \nabla z \quad \text{weakly in } L^2 \text{ but } z = ?$$

- Consequence ❷: By nonlinear Aubin-Lions lemma,

$$\tau^{-1}\Big\|u_4^{(\tau)}(t) - u_4^{(\tau)}(t-\tau)\Big\|_{L^2(\tau,T;(H^m)')} + \Big\|(u_4^{(\tau)})^{1/2}\Big\|_{L^2(0,T;H^1)} \le C$$

$$\Rightarrow\quad u_4^{(\tau)} \to u \quad \text{strongly in } L^1(0,T;L^1)$$

- Consequence ❸: L^∞ bound: $u_i^{(\tau)} \rightharpoonup u_i$ weakly* in L^∞
- strong × weak = weak: $(u_4^{(\tau)})^{1/2}u_i^{(\tau)} \rightharpoonup u_4^{1/2}u_i = z$ weakly in L^1

❷ Ion-transport model

$$
\begin{aligned}
w_i^{(\tau)} := (u_4^{(\tau)})^{1/2} u_i^{(\tau)} &\rightharpoonup u_4^{1/2} u_i \quad \text{weakly in } L^2(0,T;H^1) \\
y^{(\tau)} := (u_4^{(\tau)})^{1/2} &\to u_4^{1/2} \quad \text{strongly in } L^2(0,T;L^2) \\
\nabla (u_4^{(\tau)})^{1/2} &\rightharpoonup \nabla u_4^{1/2} \quad \text{weakly in } L^2(0,T;L^2)
\end{aligned}
$$

- Aim: Perform limit in

$$
(A(u^{(\tau)})\nabla u^{(\tau)})_i = D_i \underbrace{y^{(\tau)}}_{\text{strong}} \underbrace{\nabla w_i^{(\tau)}}_{\text{weak}} - 3D_i \underbrace{w_i^{(\tau)}}_{\text{weak}} \underbrace{\nabla y^{(\tau)}}_{\text{weak}}
$$

- Problem: weak $\times$ weak $\not\rightharpoonup$ weak. Solution: Use lemma below
- Gives global existence of bounded weak solutions (u_1, u_2, u_3)

Let $(y^{(\tau)})$, $(u^{(\tau)})$ piecewise constant, bounded, $y^{(\tau)} \to y$ in $L^2(0,T;L^2)$,

$$
\|y^{(\tau)}\|_{L^2(0,T;H^1)} \le C
$$

$$
\|y^{(\tau)} u^{(\tau)}\|_{L^2(0,T;H^1)} + \tau^{-1} \|u^{(\tau)}(t) - u^{(\tau)}(t-\tau)\|_{L^2(\tau,T;(H^1)')} \le C
$$

Then $\exists$ subsequence: $w^{(\tau)} = y^{(\tau)} u^{(\tau)} \to yu$ strongly in $L^2(0,T;L^2)$.

Overview

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Exercises

1. Let u be a smooth solution to the heat equation $\partial_t u = \Delta u$ in $\mathbb{T}^d$ and let $H_\alpha[u] = \int_{\mathbb{T}^d} u^\alpha dx$, $\alpha > 1$.
   (a) Show that $d^n H_2/dt^n$ is nonpositive of n is odd and nonnegative if n is even.
   (a) Let $d = 1$. Show that $dH_\alpha/dt \le 0$ for all $\alpha > 1$ and $d^2 H_\alpha/dt^2 \ge 0$ if $2 \le \alpha \le 3$.
2. Let u be a smooth solution to $\partial_t u = (D(x)u_x)_x$ in $\mathbb{T}^d$, where $D(x) \ge 0$, and let $H[u] = \int_{\mathbb{T}^d} u^2 dx$. Assume that $D_{xx} \ge \lambda$, where $\lambda > 0$.
   (a) Show that
   $$\frac{d^2 H}{dt^2} + \lambda \frac{dH}{dt} \ge 0.$$
   (b) Assume that $\lim_{t\to\infty} H[u(t)] = 0$. Deduce from (a) by integration over (t, ∞) that $H[u(t)] \le H[u(0)]e^{-\lambda t}$ for $t > 0$.

3. Let u be a smooth positive solution to the quantum diffusion equation

$$\partial_t u = -(u(\log u)_{xx})_{xx} \quad \text{in } \mathbb{T}^d,$$

and let $H_\alpha[u] = \int_{\mathbb{T}^d} u^\alpha dx/(\alpha(\alpha-1))$ for $\alpha > 0$. Use systematic integration by parts to show that for $0 < \alpha \le 3/2$,

$$\frac{dH_\alpha}{dt}[u(t)] \le 0 \quad \text{for } t > 0.$$

4. Consider the diffusion matrix of the population model

$$A(u) = \begin{pmatrix} a_{10} + a_{11}u_1 + a_{12}u_2 & a_{12}u_1 \\ a_{21}u_2 & a_{20} + a_{21}u_1 + a_{22}u_2 \end{pmatrix},$$

where $a_{ij} > 0$. Let $\sigma(A(u))$ be the spectrum of $A(u)$. Show that $\sigma(A(u)) \subset \{\lambda \in \mathbb{C} : \mathrm{Re}(\lambda) > 0\}$. How large is the distance of $\sigma(A(u))$ to the origin?

5. Let $S : L^\infty(\Omega) \times [0,1] \to L^\infty(\Omega)$ be the fixed-point operator in the proof the the existence theorem of the boundedness-by-entropy method. Show that S is continuous.
6. Let $\Omega \subset \mathbb{R}^d$ be a bounded domain ($d > 1$) and let (u_n) be a sequence with $u_n \geq 0$ and $\exists C > 0$: $\forall n \in \mathbb{N}$:

$$\|\sqrt{u_n}\|_{L^2(0,T;H^1(\Omega))} + \|\partial_t u_n\|_{L^1(0,T;H^m(\Omega)')} \leq C,$$

   where $H^m(\Omega)'$ is the dual of $H^m(\Omega)$, $m > 0$. Show that (u_n) is relatively compact in $L^s(\Omega)$ for $s < d/(d-1)$.
7. Show that the statement of Exercise 5 holds up to $s = d/(d-1)$ if additionally $\|u_n \log u_n\|_{L^\infty(0,T;L^1(\Omega))} \leq C$.