Analysis of cross-diffusion systems with entropy structure

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1. Introduction and examples
2. Boundedness-by-entropy method
3. Examples revisited
4. Further topics

Multi-species systems

Examples:

- Animal populations: observing, predicting, harvesting
- Fluid mixtures: heliox (diving, asthma), biofilm reactors, air pollution
- Cell dynamics: tumor growth, ion transport through membranes
- Electrolysis: lithium-ion batteries, production of hydrogen from water

Nature is generally composed of multi-species systems!

Modeling: flux of ith species depends on density gradient of jth species $\rightarrow$ cross-diffusion equations

What are cross-diffusion systems?

$$\partial_t u_i - \operatorname{div}\left(\sum_{j=1}^{n} A_{ij}(u)\nabla u_j\right) = f_i(u) \quad \text{in } \Omega,\ t>0,\ i=1,\ldots,n$$

- Systems of quasilinear parabolic equations
- Initial and (no-flux) boundary conditions

What makes these systems special?

- Adding (cross-) diffusion, constant equilibria may become unstable even if equilibria of associated ODE system linearly stable
- May lead to physically desired pattern formation (Turing 1952)
- Uphill diffusion: diffusion flux in higher concentration area
- Segregation: if $u_i(0)u_j(0)=0$ then $u_i(t)u_j(t)=0$ for $t>0$, $i\neq j$ (Bertsch et al. 1985)
- Blow-up in finite time: $u_i(0)$ Hölder continuous but $\exists\ T^*>0$: $u_i(T^*)$ not Hölder continuous (Stará-John 1995)

Aim: develop mathematical theory only for systems from applications

❶ Multicomponent gas mixtures

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

- Volume fractions of gas components u_1, u_2, $u_3 = 1 - u_1 - u_2$
- Diffusion matrix: $\delta(u) = d_1 d_2(1 - u_1 - u_2) + d_0(d_1 u_1 + d_2 u_2)$

$$A(u) = \frac{1}{\delta(u)} \begin{pmatrix} d_2 + (d_0 - d_2)u_1 & (d_0 - d_1)u_1 \\ (d_0 - d_2)u_2 & d_1 + (d_0 - d_1)u_2 \end{pmatrix}$$

- Application: Patients with airway obstruction inhale Heliox to speed up diffusion
- Proposed by Maxwell 1866/Stefan 1871
- Duncan-Toor 1962: Fick's law ($J_i \sim \nabla u_i$) not sufficient, include cross-diffusion terms
- Derivation: Boudin-Grec-Salvarani 2015
- $A(u)$ not symm., generally not pos. definite

❷ Segregating populations

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

- $u = (u_1, u_2)$ and u_i models population density of ith species
- Diffusion matrix: ($a_{ij} \geq 0$)

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

- Suggested by Shigesada-Kawasaki-Teramoto 1979 to model 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

Difficulties and state of the art

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

Mathematical difficulties:

- Matrix $A(u)$ may be neither symmetric nor positive definite
- Generally no maximum principle: How to prove bounds for u_i?
- Generally no regularity theory

State of the art:

- Ladyženskaya et al. 1968: growth conditions on nonlinearities needed
- Many results for small cross diffusion (Kim 1984, Deuring 1987,...)
- Alt-Luckhaus 1983: global solutions if Onsager matrix unif. pos. def.
- Kawashima-Shizuta 1988: hyperbolic-parabolic systems, entropies
- Amann 1990: parabolic in the sense of Petrovskii $\Rightarrow \exists!$ local classical solution; bounds in $W^{1,p}(\Omega)$, $p > d \Rightarrow \exists$ global weak solution
- Burger et al. 2010: global bounded weak solutions for special model

Novelty of approach: degeneracies allowed, global L^∞ solutions

Gradient-flow or entropy structure

Main assumption

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

$$\partial_t u - \operatorname{div}\left(B\nabla\frac{\delta H(u)}{\delta u}\right) = f(u),$$

where Onsager matrix B is pos. semi-definite, $H(u) = \int_\Omega h(u)dx$ entropy

Equivalent formulation: $\delta H(u)/\delta u \simeq h'(u) =: w$ (entropy variable)

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

Consequences:

1. H is Lyapunov functional if $f = 0$:

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

2. L^∞ bounds for u: Let $h' : D \to \mathbb{R}^n$ ($D \subset \mathbb{R}^n$) be invertible $\Rightarrow$ $u(x,t) = (h')^{-1}(w(x,t)) \in D$ (no maximum principle needed!)

Gradient-flow and thermodynamic structure

$$\partial_t u_i(w) - \operatorname{div}\left(\sum_{j=1}^{n-1} B_{ij}(w)\nabla w_j\right) = f_i(u(w)), \quad i = 1,\ldots,n-1$$

Gradient-flow structure: write equations as

$$\partial_t u_i - \operatorname{div}\left(\sum_{j=1}^{n-1} B_{ij}\nabla \frac{\delta H}{\delta u_j}\right) = 0, \quad w_i = \frac{\delta H}{\delta u_i}$$

- Entropy $H = \int_\Omega h(u)dx$
- Gradient flow: $\partial_t u = -K[u^*]\mathrm{grad} H|_u$ on differential manifold, where $K[u^*]w = -\operatorname{div}(B\nabla w)$ Onsager operator

Thermodynamic structure:

- Mathematical entropy density $h = -s$ physical entropy density
- Entropy variable = chemical potential $w_i = \partial h/\partial u_i$
- Onsager reciprocal relations: B is symmetric
- Entropy production: $-\frac{dH}{dt} = \int_\Omega \nabla w : B\nabla w dx \geq 0$
  $\rightarrow$ expresses second law of thermodynamics

Overview

Boundedness-by-entropy method

$$\partial_t u(w) - \operatorname{div}(B(w)\nabla w) = f(u(w)) \text{ in } \Omega, \qquad u(0) = u^0, \text{ no-flux b.c.}$$

$$\frac{d}{dt}\int_\Omega h(u)dx + \int_\Omega \nabla u : h''(u)A(u)\nabla u dx = \int_\Omega f(u)\cdot h'(u)dx$$

Assumptions:

1. $\exists$ convex entropy $h \in C^2(D;[0,\infty))$, h' invertible on $D \subset \mathbb{R}^n$
2. "Degenerate" positive definiteness: for all $u \in D$,

$$z^\top h''(u)A(u)z \geq c\sum_{i=1}^n u_i^{2m_i-2}z_i^2, \; m_i \geq \frac{1}{2} \quad \Rightarrow \text{ estimate for } |\nabla u_i^{m_i}|^2$$

3. A continuous on D, $\exists C > 0 : \forall u \in D$: $f(u)\cdot h'(u) \leq C(1 + h(u))$

Theorem (A.J. 2015)

Let the above assumptions hold, let $D \subset \mathbb{R}^n$ be bounded, $\int_\Omega h(u^0) < \infty$, $u_i^0(x) \in \overline{D}$. Then $\exists$ global weak solution such that $u(x,t) \in \overline{D}$ and

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

Ideas of proof

Theorem (A.J. 2015)

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

- Regularized equations: given $w^{k-1} \in L^\infty(\Omega)$, set $u^k = (h')^{-1}(w^k)$:

$$\tau^{-1}(u^k - u^{k-1}) - \operatorname{div}(B(w^k)\nabla w^k) + \text{"}\varepsilon((-\Delta)^m w + w)\text{"} = f(u^k)$$

- Uniform estimate from entropy inequality: use test function $h'(u^k)$

$$\int_\Omega h(u^k)dx - \int_\Omega h(u^{k-1})dx + C_1\tau \sum_{i=1}^n \int_\Omega |\nabla u_i^{m_i}|^2 dx + \varepsilon\tau \|w^k\|^2_{H^m(\Omega)} \le C_2\tau \int_\Omega (1 + h(u^k))dx$$

- Existence of regularized system: Lax-Milgram, Leray-Schauder
- Limit $(\varepsilon,\tau) \to 0$: compactness from Aubin-Lions lemma

Aubin-Lions lemmas

Uniform estimates: set $u^{(\tau)}(\cdot,t) = u(w^k)$, $t \in ((k-1)\tau, k\tau]$

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

Lemma (Discrete Aubin-Lions; Simon 1987)

Let $X \hookrightarrow B$ compact and $B \hookrightarrow Y$ continuous, $1 \le p < \infty$, and

$$\|u^{(\tau)}\|_{L^p(0,T;X)} \le C, \quad \sup_{\tau>0}\lim_{h\to 0}\|u^{(\tau)}(t) - u^{(\tau)}(t-h)\|_{L^1(\tau,T;Y)} = 0$$

Then $(u^{(\tau)})$ is relatively compact in $L^p(0,T;B)$.

Problem: nonlinear estimate and time difference involving h

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

Let $(u^{(\tau)})$ be piecewise constant in time, $k \in \mathbb{N}$, $s \ge \frac{1}{2}$, and

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

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

Remark: Alt-Luckhaus 1983: $s = 1$; also see Maître 2003, Moussa 2016

Overview

❶ Maxwell-Stefan models

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

$$A(u) = \frac{1}{\delta(u)} \begin{pmatrix} d_2 + (d_0 - d_2)u_1 & (d_0 - d_1)u_1 \\ (d_0 - d_2)u_2 & d_1 + (d_0 - d_1)u_2 \end{pmatrix}$$

- Entropy: $H(u) = \int_\Omega h(u)dx,\ u \in D = \{u : u_i > 0,\ u_1 + u_2 < 1\} \subset \mathbb{R}^2$

  $h(u) = u_1(\log u_1 - 1) + u_2(\log u_2 - 1) + (1 - u_1 - u_2)(\log(1 - u_1 - u_2) - 1)$

- Entropy production:

$$\frac{dH}{dt} + c\int_\Omega \sum_{i=1}^{2} |\nabla\sqrt{u_i}|^2 dx \le C_f(1 + H)$$

- Entropy variables: $w = h'(u) \in \mathbb{R}^2$ or $u = (h')^{-1}(w)$

$$w_i = \frac{\partial h}{\partial u_i} = \log\frac{u_i}{u_3}, \quad u_i = \frac{e^{w_i}}{1 + e^{w_1} + e^{w_2}} \in D$$

Boundedness-by-entropy theorem: $\exists$ global-in-time weak solution

❷ Population model

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

$$A(u) = \begin{pmatrix} a_{10} + a_{11}u_1 + a_{12}u_2 & a_{12}u_1 \\ a_{21}u_2 & a_{20} + a_{21}u_1 + a_{22}u_2 \end{pmatrix}, \quad a_{ij} \geq 0$$

- Entropy: $h(u) = a_{21}u_1(\log u_1 - 1) + a_{12}u_2(\log u_2 - 1)$, $D = (0,\infty)^2$
- Entropy production:

$$\frac{dH}{dt} + C\sum_{i=1}^{2}\int_\Omega \big(a_{i0}|\nabla\sqrt{u_i}|^2 + a_{ii}|\nabla u_i|^2\big)dx \leq C_f$$

- Entropy variables: $w_i = \partial h/\partial u_i = \log u_i \Rightarrow u_i = \exp(w_i) > 0$

Boundedness-by-entropy method not applicable but technique applies

Theorem (L. Chen-A.J. 2004)

Let $a_{ii} > 0$. Then $\exists$ weak solution u such that $u_i \geq 0$ and

$$u_i \in L^2(0,T;H^1(\Omega)),\ \partial_t u_i \in L^q(0,T;W^{1,q}(\Omega)'), \quad q = 2(d+1)$$

❷ Population model: generalizations

$$A_{ij}(u) = (a_{i0} + a_{i1}u_1 + \cdots + a_{in}u_n)\delta_{ij} + a_{ij}u_i$$

- Entropy: $H(u) = \int_\Omega h(u)dx = \int_\Omega \sum_{i=1}^n \pi_i u_i(\log u_i - 1)$
- Key assumption: $\pi_i a_{ij} = \pi_j a_{ji}$ (detailed balance), $\pi_i > 0$

Detailed balance $\Leftrightarrow$ (π_i) reversible measure of Markov chain for (a_{ij})
$\Leftrightarrow$ $B = A(u)h''(u)^{-1}$ symmetric $\Rightarrow$ entropy $H(u(t))$ decreases $\forall t$

Theorem (X. Chen-Daus-A.J. 2018)

Let $a_{ij} > 0$ and detailed balance hold. Then $\exists$ nonnegative weak solution $\sqrt{u_i} \in L^2(0,T;H^1(\Omega))$, $i = 1,\ldots,n$.

$$A_{ij}(u) = (a_{i0} + a_{i1}u_1^s + \cdots + a_{in}u_n^s)\delta_{ij} + a_{ij}u_i^s, \quad s > 0$$

- Global existence under detailed balance and $a_{ii} > \frac{s-1}{s+1}\sum_{j\neq i} a_{ij}$ (Desvillettes et al. 2015, A.J. 2015, X. Chen-Daus-A.J. 2018)
- Entropy: $H(u) = \frac{1}{s}\int_\Omega \sum_{i=1}^n \pi_i u_i^s dx$, production contains $a_{ii}|\nabla u_i^s|^2$

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❶ Uniqueness of weak solutions

- Alt-Luckhaus 1983: linear elliptic operator, $\partial_t u_i \in L^1$
- Gajewski 1994: elliptic Onsager operator monotone in special sense
- X. Chen-A.J. 2019: renormalized-strong uniqueness for SKT model
- Berendsen et al. 2020: weak-strong uniqueness for special system

$$\partial_t u_i = \operatorname{div}\Big(\sum_{j=1}^n A_{ij}(u)\nabla u_j\Big), \quad A_{ij}(u) = p(u_0)\delta_{ij} + a_j u_i q(u_0)$$

$$u_0 = \sum_{i=1}^n a_i u_i, \quad \text{initial \& no-flux boundary conditions}$$

→ u_i: species' concentrations, u_0: solvent concentration

Theorem (X. Chen-A.J. 2018)

Let $p(s) \geq 0$, $p(s) + sq(s) \geq 0$. Then uniqueness in class of functions $p(u_0)^{1/2}\nabla u_i$, $|q(u_0)|^{1/2}\nabla u_i \in L^2$, $\partial_t u_i \in L^2(0,T;H^1(\Omega)')$.

Idea of proof: ❶ Apply $H^{-1}(\Omega)$ method to $\partial_t u_0 = \Delta Q(u_0)$, where $Q(s) = \int_0^s (p(z) + zq(z))dz$ nondecreasing $\Rightarrow$ u_0 unique

Uniqueness of weak solutions

$$\partial_t u_0 = \Delta Q(u_0), \quad \partial_t u_i = \operatorname{div}(p(u_0)\nabla u_i + u_i q(u_0)\nabla u_0)$$

Idea of proof: ❷ Define Gajewski's semimetric

$$S(u,v) = \sum_{i=1}^n \int_\Omega \left(h(u_i) + h(v_i) - 2h\left(\frac{u_i+v_i}{2}\right)\right)dx, \ \ h(s) = s(\log s - 1)$$

and compute $\frac{d}{dt}S(u(t),v(t)) \le 0 \Rightarrow S(u(t),v(t)) = 0 \Rightarrow u(t) = v(t)$

Comments:

- Test function $\partial h/\partial u_i = \log u_i$ requires to regularize $h(u)$
- Extension: $\partial_t u = \operatorname{div}(A(u)\nabla u + D(u)\nabla\phi)$, $-\Delta\phi = u_0 - f(x)$
- Relation to relative entropies: $S_1(u,v) = H(u|v) + H(v|u)$, where

$$H(u|v) = \int_\Omega \sum_{i=1}^n \left(h_i(u) - h_i(v) - \frac{\partial h_i}{\partial u_i}(v)(u_i - v_i)\right)dx$$

$\Rightarrow \frac{d}{dt}S_1(u(t),v(t)) \le 0$

❷ Large-time asymptotics

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

- Entropy production:
$$\frac{dH}{dt} + \langle A(u), H'(u) \rangle = \langle f(u), H'(u) \rangle$$
- Assume: $\langle f(u), H'(u) \rangle \le 0$ and $\langle A(u), H'(u) \rangle \ge \lambda H$. Then
$$\frac{dH}{dt} + \lambda H \le 0 \quad \Rightarrow \quad H(u(t)) \le H(u^0)e^{-\lambda t}$$
- Convex Sobolev inequality: $\langle A(u), H'(u) \rangle \ge \lambda H$

Example: population dynamics model (no reactions)

$$\frac{dH}{dt} + c_0 \sum_{i=1}^n \int_\Omega |\nabla\sqrt{u_i}|^2 dx \le 0, \quad H(u) = \sum_{i=1}^n \int_\Omega \pi_i u_i (\log u_i - 1)$$

Use logarithmic Sobolev inequality:

$$\int_\Omega \pi_i u_i (\log u_i - 1) dx \le C_S \int_\Omega |\nabla\sqrt{u_i}|^2 dx \ \Rightarrow \ \frac{dH}{dt} + \frac{c_0}{C_S} H \le 0$$

❸ Maxwell-Stefan-Fourier models

$$\partial_t u_i + \operatorname{div} J_i = r_i, \quad J_i = -\sum_{j=1}^n M_{ij}(u,\theta)\nabla(\mu_i/\theta) - M_i(u,\theta)\nabla(1/\theta)$$

$$\partial_t(u_0\theta) + \operatorname{div} J_e = 0, \quad J_e = -\kappa(\theta)\nabla\theta - \sum_{j=1}^n M_j(u,\theta)\nabla(\mu_j/\theta)$$

no-flux boundary cond., $u_i(0) = u_i^0$

- Variables: u_i densities, θ temperature, $u_0 = \sum_{i=1}^n u_i$ total density
- Chemical potentials: $\mu_i = \theta(\log(u_i/\theta) + 1)$
- Diffusion matrix: (M_{ij}) symm., $\sum_{i=1}^n M_{ij} = 0$, $\sum_{i=1}^n M_i = 0$,

$$\sum_{i,j=1}^n M_{ij} z_i z_j \geq \sum_{i=1}^n u_i (\Pi z)_i^2 \text{ for } z \in \mathbb{R}^n, \quad \Pi z = \text{proj. on } \operatorname{span}(1)^\perp$$

- Entropy density: $h(u) = \sum_{i=1}^n u_i(\log u_i - 1) - u_0 \log\theta$

Theorem (Helmer-A.J. 2020)

Let $\kappa(\theta) \sim c_\theta(1+\theta^2)$, $r_i = 0$. Then $\exists$ weak solution with $u_i \geq 0$, $\theta > 0$

Summary and perspectives

$$\partial_t u - \mathrm{div}(A(u)\nabla u) = f(u)$$

Summary

- Formal gradient-flow or entropy structure yields estimates
- Boundedness-by-entropy: L^∞ solutions, even for degenerate problems
- Uniqueness of weak solutions for special systems
- Large-time asymptotics: relate entropy and entropy production
- Nonstandard degeneracies possible (not of porous-medium type)

Perspectives:

- Stochastic cross-diffusion eqs.: Dhariwal-Huber-AJ-Kuehn-Neamtu 2020
- Maxwell-Stefan-Navier-Stokes-Fourier: Buliček-AJ-Pokorný-Zamponi '20
- Weak-strong uniqueness?
- Regularity? Partial Hölder regularity: Braukhoff-Raithel-Zamponi 2020

Exciting research field due to combination of mathematics, thermodynamics, biology – still many open problems!