Entropy methods and cross-diffusion systems

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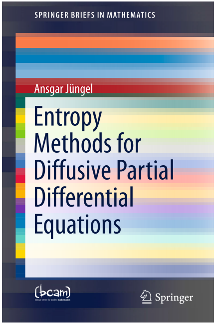
Contents

Literature

Main reference

- A. Jüngel. Entropy methods for diffusive partial differential equations. BCAM Springer Briefs, Springer, 2016.



- A. Jüngel. The boundedness-by-entropy method for cross-diffusion systems. *Nonlinearity* 28 (2015), 1963-2001.
- A. Jüngel. Cross-diffusion systems with entropy structure. *Proceedings of Equadiff 2017*, Bratislava, pp. 181-190.
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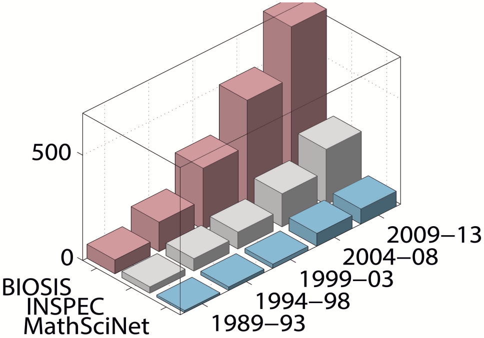
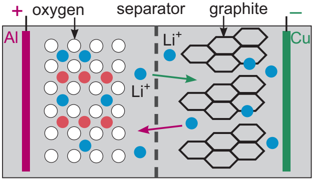
Multi-species systems

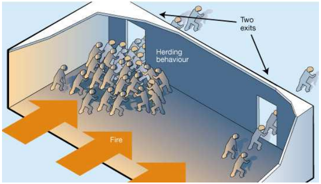
Examples:

- Wildlife populations
- Tumor growth
- Gas mixtures
- Lithium-ion batteries
- Population herding

Nature is composed of multi-species systems



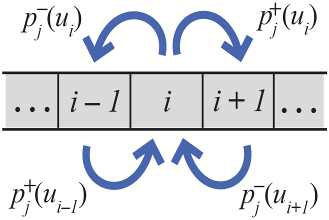




How to model multi-species systems?

Microscopic models:

- Discrete-time Markov chains: matrix-based models
- Continuous-time Markov chains: species move to neighboring cells with transition rate $p_j^{\pm}(u_i)$
- Particle models: Newton's laws with interactions for each individual



Continuum models:

- Stochastic differential equations: Brownian motion represents erratic motion
- Kinetic equations: distribution function depends on phase-space variables (and trait parameters like age, size, maturity)
- Diffusive equations: deterministic dynamics for particle densities $\rightarrow$ considered here

Parabolic partial differential equations

Heat equation:

$$\partial_t u - \Delta u = 0 \quad \text{in } \Omega,\ t > 0,\ \text{initial \& boundary conditions}$$

- Strongly regularizing: $u(0) \in L^2(\Omega) \Rightarrow u(t) \in C^\infty(\Omega)$
- Preserves nonnegativity: $u(0) \geq 0 \Rightarrow u(t) \geq 0$

Reaction-diffusion equations:

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

- Still regularizing and nonnegativity preserving (if $f_i \leq 0$ at $u_i = 0$)
- Global existence of weak solutions if f_i at most quadratic growth
- Global existence of classical solutions not always guaranteed!

Problem:

- Flux $D_i \nabla u_i$ only depends on u_i (Fick's law)
- In multicomponent systems, flux may depend on all ∇u_j
  $\Rightarrow$ cross-diffusion systems

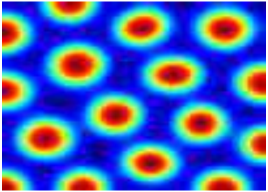
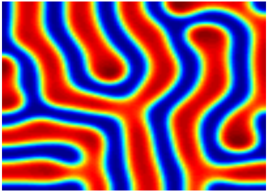
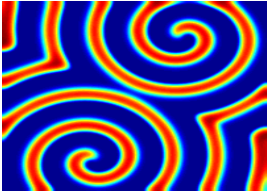
Cross-diffusion systems

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

- Meaning: $\operatorname{div}(A(u)\nabla u)_i = \sum_{j=1}^n \operatorname{div}(A_{ij}(u)\nabla u_j)$, $A \in \mathbb{R}^{n\times n}$, $u \in \mathbb{R}^n$
- 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

Overview

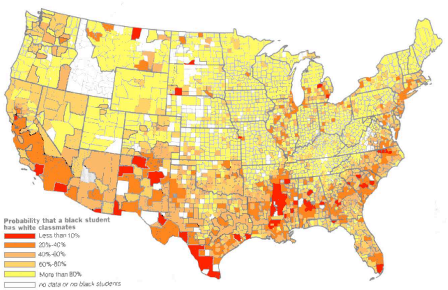
Example ❶: Cross-diffusion population dynamics

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

- $u = (u_1, u_2)$ 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 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



Source: adapted from the New York Times, April 2, 2000, p. A5.

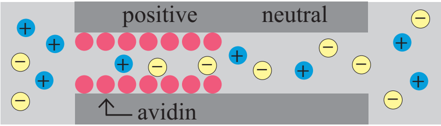
Example ❷: Ion transport through nanopores

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

- Central in biological processes such as neural signal transmission and electrical excitability of muscles
- $(u_1, \ldots, u_N)$ ion volume fractions, $u_N = 1 - \sum_{j=1}^{N-1} u_j$
- 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 $0 \le u_i \le 1$



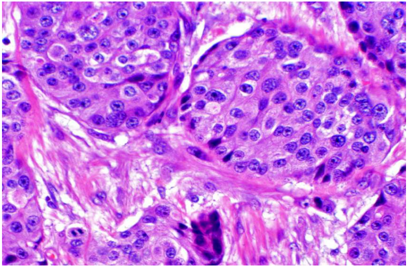
Example ❸: Tumor-growth modeling

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

- Volume fractions of tumor cells u_1, extracellular matrix u_2, nutrients/water $u_3 = 1 - u_1 - u_2$
- Diffusion matrix: (β, θ: pressure parameters)

$$A(u) = \begin{pmatrix} 2u_1(1-u_1) - \beta\theta u_1 u_2^2 & -2\beta u_1 u_2(1+\theta u_1) \\ -2u_1 u_2 + \beta\theta u_2^2(1-u_2) & 2\beta u_2(1-u_2)(1+\theta u_1) \end{pmatrix}$$

- Derived by Jackson-Byrne 2002 from continuum fluid model
- Describes avascular growth of symmetric tumor
- Diffusion matrix generally not positive definite – expect that $0 \le u_i \le 1$



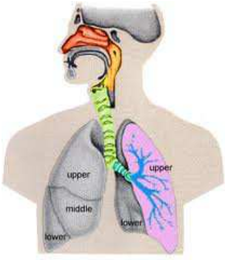
Example ❹: Multicomponent gas mixtures

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

- 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
- Boudin-Grec-Salvarani 2015: Derivation from Boltzmann equation for simple mixtures



Difficulties and objectives

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

Main features:

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

Objectives:

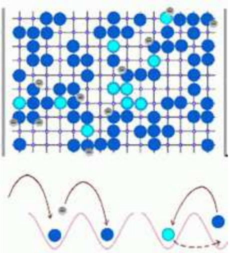
- Derivation of equations (formal or rigorous)
- Global-in-time existence and uniqueness of weak solutions
- Positivity and boundedness of solution (if physically expected)
- Large-time behavior, design of stable numerical schemes

Mathematical difficulties:

- No general theory for diffusion systems
- Generally no maximum principle, no regularity theory
- Lack of positive definiteness $\Rightarrow$ global existence nontrivial

Overview

Derivation of cross-diffusion systems



- From random-walk lattice models: Taylor expansion of transition rates and cell size $h \to 0$
  $\to$ population dynamics & ion transport models
- From fluid models: diffusion scale in balance equations and force proportional to velocity differences
  $\to$ tumor-growth & Maxwell-Stefan models
- From kinetic transport equations for distribution function $f(x, v, t)$: mean-free path limit in moments $\int f(x, v, t)\phi(v)dv$,
  $\to$ Maxwell-Stefan equations
- From stochastic differential equations: large-number limit, Ito formula
  $\to$ cross-diffusion models for multi-species systems

❶ From kinetic models to cross diffusion

- Due to Boudin-Grec-Salvarani 2015
- Boltzmann transport equation for $f_i(x,v,t)$ in diffusion scaling

$$\varepsilon\partial_t f_i + v\cdot\nabla_x f_i = \frac{1}{\varepsilon}Q_i(f_i,f_i) + \frac{1}{\varepsilon}\sum_{j\neq i} Q_{ij}(f_i,f_j), \quad i=1,\ldots,n$$

- Q_i mono-species, Q_{ij} bi-species collision operators
- Collisions are elastic, conserve mass: $\int_{\mathbb{R}^3}(Q_i + \sum_{j\neq i} Q_{ij})dv = 0$
- Particle densities and fluxes:

$$\rho_i(x,t) = \int_{\mathbb{R}^3} f_i(x,v,t)dv, \quad \sum_{i=1}^n \rho_i(x,t) = 1,$$

$$\varepsilon\rho_i(x,t)v_i(x,t) = \int_{\mathbb{R}^3} f_i(x,v,t)vdv$$

- Ansatz: $f_i(x,v,t) = M_i := (2\pi)^{-3/2}\rho_i(x,t)\exp(-|v-\varepsilon v_i(x,t)|^2/2)$ (justification: f_i close to equilibrium M_i, $f_i = M_i + O(\varepsilon)$)

❶ From kinetic models to cross diffusion

$$\varepsilon\partial_t f_i + v\cdot\nabla_x f_i = \varepsilon^{-1}Q_i(f_i,f_i) + \varepsilon^{-1}\sum_{j\neq i}Q_{ij}(f_i,f_j)$$

1. Ansatz: $f_i(x,v,t) = M_i := (2\pi)^{-3/2}\rho_i(x,t)\exp(-|v-v_i(x,t)|^2/2)$
2. Insert into Boltzmann equation, multiply by $(1,v)$, and integrate:

$$\partial_t\rho_i + \operatorname{div}_x(\rho_i v_i) = 0,$$

$$\varepsilon\partial_t(\rho_i v_i) + \operatorname{div}_x\int_{\mathbb{R}^3} f_i v\otimes v dx = \varepsilon^{-1}\sum_{j\neq i}\int_{\mathbb{R}^3}Q_{ij}(f_i,f_j)v dv$$

3. Compute integrals:

$$\varepsilon\partial_t(\rho_i v_i) + \varepsilon\operatorname{div}_x(\rho_i v_i\otimes v_i) + \varepsilon^{-1}\nabla\rho_i = \varepsilon^{-1}\sum_{j\neq i}D_{ij}\rho_i\rho_j(v_j-v_i)$$

4. Limit $\varepsilon\to 0$ gives Maxwell-Stefan system:

$$\partial_t\rho_i + \operatorname{div}(\rho_i v_i) = 0, \quad \nabla\rho_i = \sum_{j\neq i}D_{ij}\rho_i\rho_j(v_j-v_i), \quad i=1,\ldots,n$$

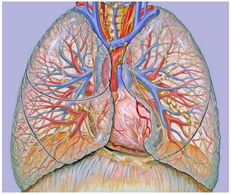
Maxwell-Stefan system

$$\partial_t \rho_i - \operatorname{div} J_i = f_i(\rho), \quad \nabla \rho_i = \sum_{j \neq i} D_{ij}(\rho_j J_i - \rho_i J_j) =: (CJ)_i, \quad i = 1, \ldots, n$$

- Volume fractions of gas components ρ_i, $\sum_{i=1}^n \rho_i = 1$
- Can we write this as $\partial_t \rho_i = \operatorname{div}(\sum_{j=1}^{n-1} A_{ij} \nabla \rho_i)$? Yes!
- Invert $\nabla \rho = CJ$ on $\ker(C)^\perp$, $\ker(C) = \{\mathbf{1}\}$:

$$\partial_t \rho_i - \operatorname{div} J_i = f_i(\rho), \quad J_i = \sum_{j=1}^{n-1} A_{ij} \nabla \rho_j, \quad i = 1, \ldots, n-1$$

- Matrix (A_{ij}) generally not symm. positive definite $\to$ use entropy variables
- Local existence analysis: Bothe 2011, Herberg-Meyries-Prüss-Wilke 2017
- Global existence analysis: Giovangigli 1999, A.J.-Stelzer 2013



❷ From lattice random walk to cross diffusion

Single species: one space dimension to simplify

- Master equation: time variation = incoming − outgoing

$$\partial_t u(x_i) = p(u(x_{i-1}) + u(x_{i+1})) - 2pu(x_i)$$

- Taylor expansion: (h = grid size)

$$u(x_{i\pm1}) - u(x_i) = \pm h\partial_x u(x_i) + \frac{1}{2}h^2\partial_x^2 u(x_i) + O(h^3)$$

- Diffusion scaling: $t \mapsto t/h^2 \Rightarrow \partial_t \rightsquigarrow h^2\partial_t$

$$\begin{aligned} h^2\partial_t u(x_i) &= p(u(x_{i-1}) - u(x_i)) + p(u(x_{i+1}) - u(x_i)) \\ &= ph^2\partial_x^2 u(x_i) + O(h^3) \end{aligned}$$

- Limit $h \to 0$ gives $\partial_t u(x) = p\partial_x^2 u(x)$ (heat equation)
- Rigorous limit: De Masi, Lebowitz, Sinai, Spohn etc. (from 1980s on)

❷ From lattice random walk to cross diffusion

Multiple species:

- Master equation for particle number $u_j(x_i)$ at ith cell:

$$\partial_t u_j(x_i) = p^+_{j,i} u_j(x_{i-1}) + p^-_{j,i+1} u_j(x_{i+1}) - (p^+_{j,i} + p^-_{j,i}) u_j(x_i)$$

- Transition rates: $p^{\pm}_{j,i} = p_i(u(x_j)) q_i(u_n(x_{j\pm1}))$
- Taylor expansion, diffusion scaling and limit $h \to 0$ leads to system of diffusion equations

$$\partial_t u_j = \partial_x \left(\sum_{k=1}^{n} A_{jk}(u) \partial_x u_k \right), \quad j = 1, \ldots, n$$

- Multi-dimensional case analogous

Examples:

- $q_i = 1$: $A_{ij}(u) = \frac{\partial}{\partial u_j}(u_i p_i(u))$ gives population dynamics models
- $p_i = 1$: $A_{ij}(u) = \delta_{ij} q_i(u_n) + u_i \frac{d}{du_n} q(u_n)$ gives volume-filling models

Population dynamics & ion transport models

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

Population dynamics model: $q_i(u) = 1$

- $u = (u_1, \ldots, u_n)$ and u_i models population density of ith species
- Diffusion coefficients for $p_i(u) = a_{i0} + a_{i1}u_1 + \cdots + a_{in}u_n$:

$$A_{ij}(u) = \frac{\partial}{\partial u_j}(u_i pi(u)) = \delta_{ij}a_{i0} + \delta_{ij}\sum_{k=1}^n a_{ik}u_k + a_{ij}u_i$$

- Global existence: Kim 1984, Amann 1989, Chen-A.J. 2004

Ion transport model: $p_i(u) = 1$

- Ion concentration u_i, solvent concentration u_n, $\sum_{j=1}^n u_j = 1$
- Diffusion coefficients for $q_i(u_n) = D_i u_n$:

$$A_{ij}(u) = \delta_{ij}q_i(u_n) + u_i q'(u_n) = \delta_{ij}D_i u_n + D_i u_i$$

- Global existence: Burger et al. 2012, A.J. 2015, Zamponi-A.J. 2015

❸ From fluid models to cross diffusion

- Mass and force balance equations:

$$\partial_t u_i + \operatorname{div}(u_i v_i) = 0, \quad i = 1, \ldots, n$$
$$\varepsilon\big(\partial_t(u_i v_i) + \operatorname{div}(u_i v_i \otimes v_i)\big) - \operatorname{div} T_i - p\nabla u_i = f_i$$

- Force terms: $f_i = \sum_{j=1}^n k_{ij}(v_j - v_i)u_i u_j$
- Properties: $\sum_{i=1}^n u_i = 1$, $\sum_{i=1}^n u_i v_i = 0$, $\sum_{i=1}^n f_i = 0$
- Interphase pressure: $p\nabla u_i$, p: phase pressure (Drew-Segel 1971)
- Assumptions:
  - Inertia approximation: $\varepsilon = 0$
  - Stress tensor: $T_i = -u_i(p\,\mathrm{Id} + P_i)$
  - Pressures: $P_i = P_i(u)$, $P_n = 0$, $k := k_{ij}$

Consequences:

- $k := k_{ij}$ implies that $f_i = -k u_i v_i$
- Pressure: $-\operatorname{div} T_i - p\nabla u_i = u_i \nabla p + \operatorname{div}(u_i P_i)$

$$\partial_t u_i + \operatorname{div}(u_i v_i) = 0, \quad u_i \nabla p + \operatorname{div}(u_i P_i) = -k u_i v_i$$

From fluid models to cross diffusion

$$\partial_t u_i + \operatorname{div}(u_i v_i) = 0, \quad u_i \nabla p + \operatorname{div}(u_i P_i) = -k u_i v_i$$

- Aim: eliminate p and v_i
- Add all force balance equations:

$$0 = -k \sum_{i=1}^n u_i v_i = \sum_{i=1}^n \big(u_i \nabla p + \operatorname{div}(u_i P_i) \big) = \nabla p + \sum_{i=1}^{n-1} \operatorname{div}(u_i P_i)$$

- Replace ∇p and expand $\operatorname{div} P_i = \sum_{j=1}^{u-1} \frac{\partial P_i}{\partial u_j} \nabla u_j$:

$$\partial_t u_i + \sum_{j=1}^{n-1} \operatorname{div}(A_{ij}(u) \nabla u_j) = 0, \quad i = 1, \ldots, n-1$$

- Diffusion coefficients:

$$A_{ii} = (1 - u_i) \left(P_i + u_i \frac{\partial P_i}{\partial u_i} \right) - u_i \sum_{j \neq i} u_j \frac{\partial P_j}{\partial u_i},$$

$$A_{ij} = u_i (1 - u_i) \frac{\partial P_i}{\partial u_j} - u_i P_j - u_i \sum_{k \neq i} u_k \frac{\partial P_k}{\partial u_j}, \quad j \neq i.$$

Tumor-growth & Maxwell-Stefan models

Tumor-growth model:

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

- Volume fractions of tumor cells u_1, extracellular matrix u_2, nutrients/water $u_3 = 1 - u_1 - u_2$, describes avascular growth of tumor
- Diffusion matrix for $n = 3$, $P_1 = u_1$, $P_2 = \beta u_2(1 + \theta u_1)$:

$$A(u) = \begin{pmatrix} 2u_1(1-u_1) - \beta\theta u_1 u_2^2 & -2\beta u_1 u_2(1+\theta u_1) \\ -2u_1u_2 + \beta\theta u_2^2(1-u_2) & 2\beta u_2(1-u_2)(1+\theta u_1) \end{pmatrix}$$

Maxwell-Stefan systems:

- General limit diffusion model:

$$\partial_t u_i + \operatorname{div}(u_i v_i) = 0, \quad u_i \nabla p + \operatorname{div}(u_i P_i) = -\sum_{j=1}^n k_{ij}(v_j - v_i) u_i u_j$$

- $p = 0$ (no phase pressure), $P_i = 1$

$$\partial_t u_i + \operatorname{div}(u_i v_i) = 0, \quad \nabla u_i = -\sum_{j=1}^n k_{ij}(v_j - v_i) u_i u_j$$

❹ From SDEs to cross diffusion

$$dX_i^k = -\sum_{j=1}^n \frac{1}{N}\sum_{\ell=1}^N \nabla V_{ij}^\eta(X_i^k - X_j^\ell)dt + \sqrt{2\sigma_i}dW_i^k, \quad X_i^k(0) = \xi_i^k$$

- Interacting particles with numbers $N = N_1, \ldots, N = N_n$, trajectories X_i^k ($i = 1, \ldots, n$, $k = 1, \ldots, N$)
- Potential: $V_{ij}^\eta(x) = \eta^{-d}V_{ij}(x/\eta)$, $\eta > 0$,
- Given i.i.d. random variables ξ_i^k and ∇V_{ij}^η bounded Lipschitz $\Rightarrow \exists!$ i.i.d. solution X_i^k with common law μ_i

Aim: limit $N \to \infty$, $\eta \to 0$

Expected result: (L. Chen-Daus-A.J., in progress)

$\mu_i \to \mu_i$ in measure as $N \to \infty$, μ_i with density u_i

$$\partial_t u_i = \operatorname{div}\left(\sigma_i \nabla u_i + \sum_{j=1}^n a_{ij}u_i\nabla u_j\right), \quad a_{ij} = \int_\Omega V_{ij}(|x|)dx$$

Open question: How to derive, e.g., population model?

Overview

Local existence analysis

$$\partial_t u - \mathrm{div}(A(u)\nabla u) = f(u) \text{ in } \Omega \subset \mathbb{R}^d,\ \ t > 0, \quad u(0) = u^0$$

Theorem (Amann 1990)

Let a_{ij}, f_i smooth, $A(u)$ normally elliptic, $u^0 \in W^{1,p}(\Omega;\mathbb{R}^n)$ with $p > d$. Then $\exists$ unique local solution u

$$u \in C^0([0,T^*); W^{1,p}(\Omega)), \quad u \in C^\infty(\overline{\Omega} \times [0,T^*);\mathbb{R}^n), \quad 0 < T^* \le \infty$$

- $A(u)$ normally elliptic = all eigenvalues have positive real parts
- Linear algebra: If $H(u)$ symmetric positive definite such that $H(u)A(u)$ positive definite then $A(u)$ normally elliptic
- Application: Let $h(u)$ convex and set $H(u) := h''(u)$. Then, if $f = 0$,

$$\frac{d}{dt}\int_\Omega h(u)dx = \int_\Omega h'(u)\cdot\partial_t u dx = -\int_\Omega \underbrace{\nabla u : h''(u)A(u)\nabla u}_{\ge 0 \text{ if } h''(u)A(u) \text{ pos. def.}} dx$$

- Aim: find a Lyapunov functional (entropy) $h(u)$

State of the art

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

Global existence if ...

- Growth conditions on nonlinearities (Ladyženskaya ... 1988)
- Control on $W^{1,p}(\Omega)$ norm with $p > d$ (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

Entropy and gradient flows

Entropy: Measure of molecular disorder or energy dispersal

- Introduced by Clausius (1865) in thermodynamics
- Boltzmann, Gibbs, Maxwell: statistical interpretation
- Shannon (1948): concept of information entropy

Entropy in mathematics: $\sim$ convex Lyapunov functional

- Hyperbolic conservation laws (Lax), kinetic theory (Lions)
- Relations to stochastic processes (Bakry, Emery) and optimal transportation (Carrillo, Otto, Villani)

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

- Example: $\mathbb{R}^d$ with Euclidean structure $\Rightarrow \partial_t u = -H'(u)$
  $H(u)$ is Lyapunov functional since $\partial_t H(u) = -|H'(u)|^2$
- Gradient flow of entropy w.r.t. Wasserstein distance (Otto)
- Entropy $H(u) = \int u \log u dx$: $\partial_t u = \mathrm{div}(u \nabla H'(u)) = \Delta u$

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:

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 $\Rightarrow$ $u = (h')^{-1}(w) \in D$ (no maximum principle needed!)

Example: Maxwell-Stefan systems for $n = 3$

Volume fractions of gas components u_1, u_2, $u_3 = 1 - u_1 - u_2$

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

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

Entropy: $H(u) = \int_\Omega h(u)dx$, where

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

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

$$w_i = \frac{\partial h}{\partial u_i} = \log \frac{u_i}{u_3}, \quad u_i = \frac{e^{w_i}}{1 + e^{w_1} + e^{w_2}} \in (0, 1)$$

- Entropy production:

$$\frac{dH}{dt}(u) = -\int_\Omega \left(\sum_{i=1}^{2} d_i \frac{|\nabla u_i|^2}{u_i} + d_0 u_1 u_2 \frac{|\nabla u_3|^2}{u_3} \right) dx \le 0$$

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!

Boundedness-by-entropy method

$\partial_t u(w) - \mathrm{div}(B(w)\nabla w) = f(u(w))$ in Ω, $t > 0$, $u|_{t=0} = u^0$, no-flux b.c.

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

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 $u \in D = (0,\infty)$,
   $u = (h')^{-1}(w) = e^w \in D$
2. "Degenerate" positive definiteness: $h''(u)A(u) \geq \mathrm{diag}(a_i(u_i)^2)$
   $$\nabla w^\top B(w)\nabla w = \nabla u^\top h''(u)A(u)\nabla u \geq \sum_{i=1}^n a_i(u_i)^2|\nabla u_i|^2$$
   Gives estimate for $|\nabla\alpha_i(u_i)|^2$, where $\alpha_i'(u_i) = a_i(u_i) \sim u_i^{m_i-1}$
3. A continuous on D, $\exists C > 0 : \forall u \in D$: $f(u)\cdot h'(u) \leq C(1 + h(u))$
   Needed to control reaction term $f(u)$

Boundedness-by-entropy method

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

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 $u \in D$,
$$z^\top h''(u)A(u)z \geq \sum_{i=1}^n a_i(u)^2 z_i^2, \quad a_i(u) \sim u_i^{m_i-1}$$
3. A continuous on D, $\exists C>0 : \forall u \in D$: $f(u)\cdot h'(u) \leq C(1+h(u))$

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

Boundedness-by-entropy method

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

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

Remarks:

- Result valid for rather general model class
- Yields L^∞ bounds without using a maximum principle
- Boundedness assumption on D is strong but can be weakened in some cases; see examples below
- Main assumptions: existence of entropy h, pos. def. of $h''(u)A(u)$
- How to find entropy functions h? Physical intuition, trial and error
- Yields immediately global existence for Maxwell-Stefan

Proof of existence theorem

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

Key ideas:

- Discretize in time: replace $\partial_t u(w)$ by approximation involving $u(w^k)$
  Benefit: avoid issues with time regularity
- Regularize in space by adding "$\varepsilon(-\Delta)^m w^k$", $\varepsilon > 0$
  Benefit: since $\operatorname{div}(B(w)\nabla w)$ 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 $\to$ solve in w $\to$ limit solves problem in u

Proof of existence theorem

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

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^k: 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

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

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

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

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

Step ❸: uniform estimates

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

$$\|(u_i^{(\tau)})^{m_i}\|_{L^2(0,T;H^1)}+\sqrt{\varepsilon}\|w^{(\tau)}\|_{L^2(0,T;H^m)}\le C$$

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

Lemma (Aubin-Lions 1963/69)

Let $\|u^{(\tau)}\|_{L^2(0,T;H^1)}+\|\partial_t u_i^{(\tau)}\|_{L^2(0,T;H^m(\Omega)')}\le C$.
Then exists subsequence $u^{(\tau)}\to u$ strongly in $L^2(0,T;L^2)$.

Problem: discrete time derivative and nonlinear estimate

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 $L^p(0,T;B)$.

Step ❸: uniform estimates

Lemma (Discrete Aubin-Lions; Dreher-A.J., 2012)

If additionally, $(u^{(\tau)})$ piecewise constant in time, and

$$\|u^{(\tau)}\|_{L^p(0,T;X)} + \tau^{-1}\|u^{(\tau)}(t) - u^{(\tau)}(t-\tau)\|_{L^1(\tau,T;Y)} \le C$$

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

Benefit: study $u^{(\tau)}(t) - u^{(\tau)}(t-\tau)$, not all $u^{(\tau)}(t) - u^{(\tau)}(t-h)$

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

Let $(u^{(\tau)})$ be piecewise constant in time, $k \in \mathbb{N}$, $s \ge \frac{1}{2}$, 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 $L^{2s}(0,T;L^{2s})$

Remark: 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 $(\tau, \varepsilon) \to 0$

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

- Nonlinear Aubin-Lions lemma:

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

- 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 of existence analysis

Theorem (A.J. 2014)

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

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

Strategy of the proof:

- Implicit Euler discretization and $(-\Delta)^m$ 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 Tumor-growth model

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

- Volume fractions of tumor cells u_1, extracellular matrix (ECM) u_2, nutrients/water $u_3 = 1 - u_1 - u_2$, one space dimension
- Diffusion matrix: (β, θ: pressure parameters)

$$A(u) = \begin{pmatrix} 2u_1(1-u_1) - \beta\theta u_1 u_2^2 & -2\beta u_1 u_2(1+\theta u_1) \\ -2u_1u_2 + \beta\theta u_2^2(1-u_2) & 2\beta u_2(1-u_2)(1+\theta u_1) \end{pmatrix}$$

- Entropy: $H(u) = \int_\Omega h(u)dx$, where

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

- Entropy production inequality:

  $$\frac{dH}{dt}[u] + C_\theta \int_\Omega \left((\partial_x u_1)^2 + (\partial_x u_2)^2\right) dx \le C(f)$$

  and $C_\theta > 0$ if $\theta < 4/\sqrt{\beta}$

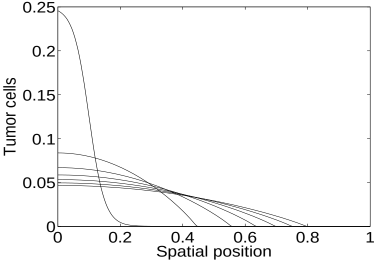
Tumor-growth model

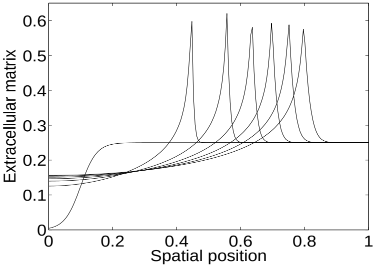
Theorem (A.J./Stelzer, *M3AS* 2012)

Let $\theta < 4/\sqrt{\beta}$, $H(u^0) < \infty \Rightarrow \exists$ *bounded weak solution with* $0 \le u_1, u_2 \le 1$

Question: What happens for $\theta > 4/\sqrt{\beta}$?

Partial answer: Numerical results show "peaks" in ECM fraction





- Tumor front spreads from left to right (production rate $f(u) = 0$)
- Tumor causes increase of ECM (encapsulation of tumor)

❷ Maxwell-Stefan model

$$\partial_t u_i - \operatorname{div} J_i = f_i(u), \quad \nabla u_i = \sum_{j\neq i} c_{ij}(u_j J_i - u_i J_j) =: (CJ)_i$$
$$u_i(0) = u_i^0, \quad i = 1, \ldots, n, \quad \text{no-flux b.c.}$$

- Volume fractions u_i, fluxes J_i
- Problem: need to invert relation $\nabla u_i \leftrightarrow J_i$ but not invertible since $\sum_{i=1}^n u_i = 1 \Rightarrow \sum_{i=1}^n \nabla u_i = 0$
- Solution: solve $\nabla u = CJ$ on $\ker(C)^\perp$ using Perron-Frobenius theorem $\Rightarrow J^* = C_0^{-1}\nabla u^*$, where $u^* = (u_1, \ldots, u_{n-1})$, $J^* = (J_1, \ldots, J_{n-1})$

Entropy structure: $h(u^*) = \sum_{i=1}^n u_i(\log u_i - 1)$, $u_n = 1 - \sum_{i=1}^{n-1} u_i$

- Equations: $\partial_t u^* - \operatorname{div}(B(w)\nabla w) = f^*(u^*(w))$
- Difficulty: show that $B(w) = C_0^{-1} h''(u^*(w))^{-1}$ positive definite
- Boundedness-by-entropy theorem applies with $D = (0,1)^{n-1}$: $\exists$ global weak solution $u_i^{1/2} \in L^2(0,T;H^1)$, $0 \le u_i \le 1$, $\sum_{i=1}^{n-1} u_i \le 1$

❸ Population model of Shigesada-Kawasaki-Teramoto

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

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

- Entropy: $H(u) = \int_\Omega h(u)dx = \int_\Omega \sum_{i=1}^2 u_i(\log u_i - 1)$ defined on unbounded domain $D = (0,\infty)^2$
- Entropy production: for some $C > 0$, if $f(u)$ = Lotka-Volterra term

$$\frac{dH}{dt}[u] \le -C\sum_{i=1}^2 \int_\Omega \big((a_{i0} + a_{ii}u_1)|\nabla\sqrt{u_1}|^2 + |\nabla\sqrt{u_1u_2}|^2\big)dx + C$$

- Main difficulty: 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)

Theorem (Chen-A.J., *SIMA* 2004-2006)

Let $a_{i0} > 0$ or $a_{ii} > 0$. Then $\exists$ nonnegative weak solution (u_1, u_2)

Population model of Shigesada-Kawasaki-Teramoto

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

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

Entropy production: if $f(u)$ = Lotka-Volterra term

$$\frac{dH}{dt} + C\sum_{i=1}^2 \int_\Omega \big((a_{i0}+a_{ii}u_1)|\nabla\sqrt{u_1}|^2 + |\nabla\sqrt{u_1u_2}|^2\big)dx \le C$$

$a_{ii}>0$: gives $H^1(\Omega)$ estimate for $u_i^{(\tau)}$

$$\nabla u_i^{(\tau)} \overset{L^2}{\rightharpoonup} \nabla u_i, \quad u_j^{(\tau)} \overset{L^2}{\to} u_j \quad \Rightarrow \quad u_j^{(\tau)}\nabla u_i^{(\tau)} \overset{L^1}{\rightharpoonup} u_j\nabla u_i$$

$a_{i0}>0$: gives H^1 estimate for $(u_i^{(\tau)})^{1/2}$ only, exploit L^2 estimate for $\nabla(u_1^{(\tau)}u_2^{(\tau)})^{1/2}$ and L^1 estimate for $(u_i^{(\tau)})^2\log u_i^{(\tau)}$ from source term

Generalization 1: nonlinear coefficients

Macroscopic limit of random-walk on lattice:

$$A(u) = \begin{pmatrix} p_1(u) + u_1 \frac{\partial p_1}{\partial u_1}(u) & u_1 \frac{\partial p_1}{\partial u_2}(u) \\ u_2 \frac{\partial p_2}{\partial u_1}(u) & p_2(u) + u_2 \frac{\partial p_2}{\partial u_2}(u) \end{pmatrix}$$

- p_i linear: Chen-A.J. 2004
- p_i sublinear: Desvillettes-Lepoutre-Moussa 2014
- p_i superlinear: $p_i(u) = a_{i0} + a_{i1} u_1^s + a_{i2} u_2^s$ $(i = 1, 2)$, entropy density: $h(u) = a_{21} u_1^s + a_{12} u_2^s$, $s > 1$

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

Let $1 < s < 4$ *and* $(1 - \frac{1}{s})a_{12}a_{21} \le a_{11}a_{22}$, $H(u^0) < \infty$.
Then $\exists$ *nonnegative weak solution* $u_i^{s/2} \in L^2_{\mathrm{loc}}(0, \infty; H^1(\Omega))$

- p_i superlinear, $s > 1$: Desvillettes-Lepoutre-Moussa-Trescases 2015

Generalization 2: more than two species

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

- 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), $\pi_i > 0$

Why detailed balance?

- Detailed balance $\Leftrightarrow$ (π_i) reversible measure $\Leftrightarrow$ $h''(u)A(u)$ symmetric $\Rightarrow$ entropy $H(u(t))$ decreases $\forall t$
- Detailed balance not satisfied: a_{ii} "large" $\Rightarrow$ $H(u(t))$ decreases, otherwise $\exists$ $u(0)$ such that $H(u(t))$ increases

Theorem (X. Chen-Daus-A.J. 2016)

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

Nonlinear coefficients: Chen-Daus-A.J. 2016, Lepoutre-Moussa 2017

❹ Ion transport model

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

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

- Ion concentrations u_1, u_2, u_3, $u_4 = 1-u_1-u_2-u_3$
- Entropy density: $h(u) = \sum_{i=1}^4 u_i(\log u_i - 1)$, $u_4 = 1 - \sum_{i=1}^3 u_i$
- Entropy production:

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

- L^2 estimate for $\nabla\sqrt{u_4}$ and Aubin-Lions: $u_4^{(\tau)} \to u_4$ strongly in L^1
- Problem: no estimate for $\nabla\sqrt{u_i}$, $i=1,2,3$
- Compensate with L^∞ bounds:

$$u_i = (h')^{-1}(w)_i = \frac{e^{w_i}}{1+e^{w_1}+e^{w_2}+e^{w_3}} \in (0,1)$$

Ion transport model

The limit $(\tau, \varepsilon) \to 0$:

- Goal: show that e.g. $u_i^{(\tau)} \nabla u_4^{(\tau)} \rightharpoonup u_i \nabla u_4$
- Strong convergence of $y^{(\tau)} := (u_4^{(\tau)})^{1/2}$, weak convergence of $u_i^{(\tau)}$:

$$\nabla y^{(\tau)} \rightharpoonup \nabla u_4^{1/2} \quad \text{weakly in } L^2$$
$$u_i^{(\tau)} y^{(\tau)} \rightharpoonup u_i u_4^{1/2} \quad \text{weakly in } L^2$$

- Problem: $u_i^{(\tau)} \nabla u_4^{(\tau)} = 2 u_i^{(\tau)} y^{(\tau)} \nabla y^{(\tau)} \not\rightharpoonup 2 u_i u_4^{1/2} \nabla u_4^{1/2} = u_i \nabla u_4$
- Solution: apply generalized Aubin-Lions lemma

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

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

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

❶ Uniqueness of weak solutions

Uniqueness of strong solutions often holds if we can bound ∇u. The problem are weak solutions. Surprisingly, the entropy concept may help.

Example: $\partial_t u = \operatorname{div}(\nabla u + u\nabla V)$ in Ω, $u(0) = u_0$, no-flux b.c., V given

- Assume that u_1, $u_2 \in L^2(0,T;H^1)$ are nonnegative weak solutions, take difference of corresponding equations
- Use test function $u_1 - u_2$:

$$\frac{1}{2}\frac{d}{dt}\int_\Omega (u_1-u_2)^2 dx = \int_\Omega \partial_t(u_1-u_2)(u_1-u_2)dx$$
$$= -\int_\Omega |\nabla(u_1-u_2)|^2 dx - \int_\Omega \underbrace{(u_1-u_2)\nabla(u_1-u_2)}_{=\frac{1}{2}\nabla((u_1-u_2)^2)}\cdot\nabla V dx$$

- Last integral can be only estimated under additional condition

Example

First idea: Integration by parts

$$\frac{1}{2}\frac{d}{dt}\int_\Omega (u_1-u_2)^2dx+\int_\Omega |\nabla(u_1-u_2)|^2dx=-\int_\Omega (u_1-u_2)\nabla(u_1-u_2)\cdot\nabla V dx$$

$$=-\frac{1}{2}\int_\Omega \nabla((u_1-u_2)^2)\cdot\nabla V dx=\frac{1}{2}\int_\Omega (u_1-u_2)^2\Delta V dx$$

If $\Delta V\in L^\infty$: apply Gronwall $\Rightarrow u_1-u_2=0$, but strong condition on V!

Second idea: Cauchy-Schwarz inequality

$$\frac{1}{2}\frac{d}{dt}\int_\Omega (u_1-u_2)^2dx+\int_\Omega |\nabla(u_1-u_2)|^2dx$$
$$\le\frac{1}{2}\int_\Omega |\nabla(u_1-u_2)|^2dx+\|\nabla V\|_{L^\infty}^2\int_\Omega (u_1-u_2)^2dx$$

If $\nabla V\in L^\infty$: apply Gronwall $\Rightarrow u_1-u_2=0$, but still strong condition!

Third idea: Entropy method (Gajewski 1994)

Example

Third idea: Entropy method, $\phi(s) = s(\log s - 1) + 1 \geq 0$

$$d(u_1, u_2) = \int_\Omega \left(\phi(u_1) + \phi(u_2) - 2\phi\left(\frac{u_1 + u_2}{2}\right)\right) dx$$

- Convexity of ϕ gives $d(u_1, u_2) \geq \frac{1}{8}\|u_1 - u_2\|_{L^2}^2$ if $0 \leq u_i \leq 1$
- Assumption: $u_i \in L^\infty(0, T; L^\infty)$ but only $V \in L^2(0, T; H^1)$
- Differentiate $d(u_1, u_2)$ and insert $\partial_t u_i = \operatorname{div}(\nabla u_i + u_i \nabla V)$

$$\begin{aligned} \frac{d}{dt} d(u_1, u_2) &= \sum_{i=1}^2 \int_\Omega \left(\phi'(u_i) - \phi'\left(\frac{u_1 + u_2}{2}\right)\right) \partial_t u_i dx \\ &= -4 \int_\Omega \left(|\nabla u_1^{1/2}|^2 + |\nabla u_2^{1/2}|^2 - |\nabla (u_1 + u_2)^{1/2}|^2 \right) dx \leq 0 \end{aligned}$$

- Integrate over t:

$$\frac{1}{8}\|u_1 - u_2\|_{L^2}^2 \leq d(u_1(t), u_2(t)) \leq d(u_1(0), u_2(0)) = 0 \;\Rightarrow\; u_1 = u_2$$

- Drawback: Possibly not very robust (see Gajewski-Skrypnik 2004)

A cross-diffusion example

$$\partial_t u - \operatorname{div}(A(u)\nabla u) = 0 \quad \text{in } \Omega, \quad A_{ij}(u) = \delta_{ij} q_i(u_n) + u_i q_i'(u_n)$$

- Homogeneous Neumann boundary conditions, initial condition
- $u = (u_1, \ldots, u_n)$: vector of concentrations, $u_n = 1 - \sum_{i=1}^{n-1} u_i$
- Models ion transport with volume filling and transition rate q_i
- Simplification: $q := q_i$ for $i = 1, \ldots, n$, q monotone
- Yields equations in drift-diffusion form:

$$\partial_t u_i = \operatorname{div}(q(u_n)\nabla u_i - u_i \nabla q(u_n)), \quad i = 1, \ldots, n-1$$

Step ❶: Uniqueness for u_n

- Idea: H^{-1} method
- Sum equations for $i = 1, \ldots, n-1$:

$$\partial_t u_n = \operatorname{div}(q(u_n)\nabla u_n + (1-u_n)\nabla q(u_n)) = \Delta Q(u_n),$$
$$Q'(s) = q(s) + (1-s)q'(s) \geq 0$$

- Let u_n, v_n be two weak solutions with same initial data

H^{-1} method for u_n

$$\partial_t u_n = \Delta Q(u_n) \text{ in } \Omega, \quad \nabla u_n \cdot \nu = 0 \text{ on } \partial\Omega, \quad u_n(0) = u_n^0$$

- Use test function ξ solving $-\Delta\xi = u_n - v_n$ and homogeneous b.c.

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_\Omega |\nabla\xi|^2 dx &= \int_\Omega \nabla\partial_t\xi \cdot \nabla\xi dx = -\int_\Omega \partial_t\Delta(\xi)\xi dx \\ &= \int_\Omega \partial_t(u_n - v_n)\xi dx = -\int_\Omega \nabla(Q(u_n) - Q(v_n)) \cdot \nabla\xi dx \\ &= -\int_\Omega (Q(u_n) - Q(v_n))(u_n - v_n) dx \le 0\end{aligned}$$

- Implies that $|\nabla\xi| = \text{const.}$ and $u_n - v_n = -\Delta\xi = 0$

Step ❷: Uniqueness for $u_1, \ldots, u_{n-1}$

$$\partial_t u_i = \operatorname{div}(q(u_n)\nabla u_i - u_i \nabla q(u_n)), \quad i = 1, \ldots, n-1$$

- Idea: entropy method, let $\phi(s) = s(\log s - 1) + 1$

Entropy method for u_i

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

- It holds $d(u,v) \geq \frac{1}{8}\|u-v\|_{L^2}^2$ since $0 \leq u_i \leq 1$ and

$$\frac{d}{dt} d(u,v) = -4 \sum_{i=1}^{n-1} \int_\Omega \left(|\nabla u_i^{1/2}|^2 + |\nabla v_i^{1/2}|^2 - |\nabla (u_i+v_i)^{1/2}|^2 \right) dx \leq 0$$

- $d(u(0),v(0)) = d(u^0,u^0) = 0 \Rightarrow d(u(t),v(t)) = 0 \ \forall \ t \Rightarrow u = v$

Difficulty: As u_i, $v_i \geq 0$, $\log((u_i+v_i)/2)$ may be undefined

Solution: Use $\phi_\varepsilon(s) = (s+\varepsilon)(\log(s+\varepsilon)-1)+1$ and let $\varepsilon \to 0$

Theorem (Zamponi/A.J. 2015)

Let q be nondecreasing. Then there exists at most one weak solution to

$$\partial_t u - \operatorname{div}(A(u)\nabla u) = 0 \quad \text{in } \Omega, \quad A_{ij}(u) = \delta_{ij} q_i(u_n) + u_i q_i'(u_n)$$

with $\nabla u_i \cdot \nu = 0$ on $\partial\Omega$, $u_i(0) = u_i^0$, $i = 1, \ldots, n$.

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: $\langle f(u), H'(u) \rangle \leq 0$ and $\langle A(u), H'(u) \rangle \geq \lambda H$. Then

$$\frac{dH}{dt} + \lambda H \leq 0 \quad \Rightarrow \quad H(u(t)) \leq H(u^0) e^{-\lambda t}$$

- Convex Sobolev inequality: $\langle A(u), H'(u) \rangle \geq \lambda H$

Example: population dynamics model

$$\frac{dH}{dt} + C_1 \sum_{i=1}^n \int_\Omega |\nabla \sqrt{u_i}|^2 dx \leq 0, \quad H(u) = \sum_{i=1}^n \int_\Omega u_i (\log u_i - 1)$$

Use logarithmic Sobolev inequality:

$$\int_\Omega u_i (\log u_i - 1) dx \leq C_S \int_\Omega |\nabla \sqrt{u_i}|^2 dx \;\Rightarrow\; \frac{dH}{dt} + \frac{C_1}{C_S} H \leq 0$$

Large-time asymptotics for reactive mixtures

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

Question: What happens if we do not have $\langle f(u), H'(u)\rangle \le 0$?

Example: Maxwell-Stefan systems and mass action kinetics

$$f_i(u) = \sum_{a=1}^{N} (\beta_i^a - \alpha_i^a)\big(k_f^a u^{\alpha^a} - k_b^a u^{\beta^a}\big), \quad i = 1, \ldots, n$$

- k_f^a: forward reaction rate, k_b^a: backward reaction rate
- α_i^a, β_i^a: stoichiometric coefficients
- Abbreviation: $u^{\alpha^a} := \prod_{j=1}^n u_j^{\alpha_j^a}$
- Conservation of total mass: $\sum_{i=1}^n f_i(u) = 0$
- Entropy inequality: $\frac{dH}{dt} + P[u] \le 0$, we need $P[u] \ge \lambda H[u]$

$$P[u] = \int_\Omega \nabla w : B\nabla w dx + \sum_{a=1}^{a} \int_\Omega \big(k_f^a u^{\alpha^a} - k_b^a u^{\beta^a}\big) \log \frac{k_f^a u^{\alpha^a}}{k_b^a u^{\beta^a}} \ge 0$$

Large-time asymptotics for reactive mixtures

$$P[u] = \int_\Omega \nabla w : B\nabla w dx + \sum_{a=1}^{a} \int_\Omega \left(k_f^a u^{\alpha^a} - k_b^a u^{\beta^a}\right) \log \frac{k_f^a u^{\alpha^a}}{k_b^a u^{\beta^a}} \geq 0$$

- Homogeneous equilibrium: $\nabla w = 0 \Rightarrow u(w)$ constant
- Detailed-balance equilibrium u: $k_f^a u^{\alpha^a} = k_b^a u^{\beta^a}$ (there are many!)
- Wegscheider matrix: $W = (\beta_i^a - \alpha_i^a)_{ia}$, $q_1, \ldots, q_m$ basis of $\ker(W^\top)$, $Q = (q_1, \ldots, q_m)^\top$
- Conservation laws: $\partial_t Q \int_\Omega u(t)dx = \int_\Omega Qf(u)dx = 0$, $t > 0$

Theorem (Daus-A.J.-Tang 2018)

- $\exists$ *unique detailed-balanced equilibrium*
- $\exists\ \lambda > 0$: $P[u^*] \geq \lambda H[u^*]$ *for all detailed-balance equilibria* u^* *satisfying conservation laws*
- *Exponential convergence to equilibrium for* $1 \leq p < \infty$:

$$\|u(t) - u^*\|_{L^p(\Omega)} \leq C(u^0)e^{-\lambda t/(2p)}, \quad t > 0$$

❸ Structure-preserving numerical schemes

$$\partial_t u(w) + \operatorname{div}(B(w)\nabla w) = f(u(w)), \quad t > 0, \quad u = (h')^{-1}(w)$$

Motivation: Numerical scheme should preserve structure of continuous equations: nonnegativity, entropy dissipation, large-time asymptotics

Example: implicit Euler finite-element scheme

$$\frac{1}{\tau}\int_\Omega (u^k - u^{k-1})\cdot v dx + \int_\Omega \nabla v^\top B(w^k)\nabla w^k dx = \int_\Omega f(u^k)\cdot v dx$$

- Finite-dimensional test space $v \in V_h$, $u^k := u(w^k)$
- Test function $v = w^k$: use convexity of $h(u)$

$$\frac{1}{\tau}\int_\Omega \underbrace{(u^k - u^{k-1})\cdot h'(u^k)}_{\geq h(u^k)-h(u^{k-1})} dx + \int_\Omega \underbrace{(\nabla w^k)^\top B(w^k)\nabla w^k}_{\geq |\nabla \alpha_i(u^k)|^2} dx$$

$$= \int_\Omega \underbrace{f(u^k)\cdot w^k}_{\leq C(1+h(u^k))} dx \quad \Rightarrow \quad \text{stability of discrete entropy}$$

Structure-preserving numerical schemes

Implicit Euler scheme:

$$\tau^{-1}(u^k - u^{k-1}) + \mathrm{div}(B(w^k)\nabla w^k) = f(u^k) \quad \text{in } V_h$$

- Entropy estimates:

$$\|h(u^k)\|_{L^\infty(0,T;L^1)} + \sum_{i=1}^n \|\alpha_i(u_i^k)\|_{L^2(0,T;H^1)} \le C$$

- Deduce time-discrete estimates, apply Aubin-Lions, yields convergence of numerical solution to solution of continuous system

Question: what about higher-order schemes?

Two-step BDF (Backward Differentiation Formula):

$$\tau^{-1}\left(\frac{3}{2}u^k - 2u^{k-1} + \frac{1}{2}u^{k-2}\right) + \mathrm{div}(B(w^k)\nabla w^k) = f(u^k) \quad \text{in } V_h$$

- Assume: $h(u) = \frac{1}{2}\sum_{i=1}^n u_i^2$ is an entropy $\Rightarrow w_i^k = u_i^k$
- Yields entropy stability $\int_\Omega h(u^k)dx \le C$ but not entropy dissipation

Structure-preserving numerical schemes

Two-step BDF scheme:

$$\tau^{-1}\left(\frac{3}{2}u^k - 2u^{k-1} + \frac{1}{2}u^{k-2}\right) + \operatorname{div}(B(w^k)\nabla w^k) = f(u^k) \quad \text{in } V_h$$

- Key inequality:

$$\left(\frac{3}{2}a - 2b + \frac{1}{2}c\right)a \geq \frac{1}{4}\left(a^2 + (2a-b)^2\right) - \frac{1}{4}\left(b^2 + (2b-c)^2\right)$$

- This motivates us to define modify entropy:

$$H(u^k, u^{k-1}) = \int_\Omega \left((u^k)^2 + (2(u^k)^2 - u^{k-1})^2\right)dx$$

- Entropy dissipation:

$$H(u^{k+1}, u^k) + \tau \int_\Omega (\nabla u^{k+1})^\top B(u^{k+1})\nabla u^{k+1} dx \leq H(u^k, u^{k-1})$$

Generalization:

- Entropies $H(u) = \int_\Omega \sum_{i=1}^n u_i^\alpha dx$, $\alpha > 1$, idea: $v_i^2 = u_i^\alpha$ gives quadratic structure
- One-leg multistep schemes: use G-stability theory of Dahlquist

Overview

❶ Van der Waals fluids (A.J.-Mikyška-Zamponi 2016)

- Flow of chemical concentrations u_i in "porous" domain (porosity $= 1$)

$$\partial_t u_i + \operatorname{div}\left(u_i v + \varepsilon \sum_{j=1}^n D_{ij} \nabla \mu_i\right) = 0, \quad i = 1, \ldots, n, \quad u_{\rm tot} = \sum_{i=1}^n u_i$$

$$h(u) = \sum_{i=1}^n u_i(\log u_i - 1) - u_{\rm tot} \log\left(1 - \sum_{j=1}^n b_j u_j\right) - \sum_{i,j=1}^n a_{ij} u_i u_j$$

- Chemical potential:

$$\mu_i = \frac{\partial h}{\partial u_i} = -\log\left(1 - \sum_{j=1}^n b_j u_j\right) + \frac{b_i u_{\rm tot}}{1 - \sum_{j=1}^2 b_j u_j} + \log u_i - 2\sum_{j=1}^n a_{ij} u_j$$

- Darcy's law: $v = -\nabla p$, Gibbs-Duhem relation: $p = \sum_{i=1}^n u_i \mu_i - h(u)$

$$p = \frac{u_{\rm tot}}{1 - \sum_{j=1}^2 b_j u_j} - \sum_{i,j=1}^2 a_{ij} u_i u_j \quad \text{(van der Waals pressure)}$$

- Cross-diffusion system: $\partial_t u_i = \operatorname{div}\left(\sum_{j=1}^n (u_i u_j + \varepsilon D_{ij}) \nabla \mu_j\right)$

Van der Waals fluids

$$\partial_t u_i = \operatorname{div}\left(\sum_{j=1}^n (u_i u_j + \varepsilon D_{ij})\nabla\mu_j\right)$$

- Entropy:
$$H(u) = \int_\Omega \left\{ \sum_{i=1}^n u_i(\log u_i - 1) - u_{\rm tot}\log\left(1 - \sum_{j=1}^n b_j c_j\right) - \sum_{i,j=1}^n a_{ij} u_i u_j \right\} dx$$
- Entropy production:
$$\frac{dH}{dt} + \int_\Omega |\nabla p|^2 dx + \varepsilon \int_\Omega \textstyle\sum_{i,j=1}^n D_{ij}\nabla\mu_i \cdot \nabla\mu_j dx = 0$$

Assumptions:

- Max. eigenvalue of (a_{ij}) “small” $\Rightarrow h''(u)$ pos. def., $u \leftrightarrow \mu$ invertible
- $\varepsilon > 0 \Rightarrow H^1$ estimates, global existence (A.J.-Mikyška-Zamponi 2016)

What about $\varepsilon = 0$?

- System is not parabolic in the sense of Petrovskii
- Lack of parabolicity compensated by conserved quantities: for all ϕ

$$\frac{d}{dt}\int_\Omega u_{\rm tot}\phi\left(\frac{u_1}{u_{\rm tot}}, \ldots, \frac{u_{n-1}}{u_{\rm tot}}\right)dx = 0,$$ open: physical interpretation

❷ Partial averaging in economics (A.J.-Zamponi 2016)

- Reference: talk of P.L. Lions (Vienna 2015)
- Forward Kolmogorov equation with volatility $\sigma = \mathrm{diag}(\sigma_i)$, zero drift

$$\partial_t f = \frac{1}{2}\sum_{j=1}^{n} \frac{\partial^2}{\partial x_j^2}(\sigma_j^2 f), \quad \text{in } \mathbb{R}^n,\ t > 0$$

$f(x_1, \ldots, x_n, t)$ is probability density of Ito process

- Assumption: σ_j is function of partial averages

$$u_i(x,t) = \int_{\mathbb{R}} f(x, x_n, t) e^{\lambda_i x_n} dx_n, \quad x = (x_1, \ldots, x_{n-1})$$

- Interpretation: u_i = average with respect to economic parameter x_n
- Simplify: $i = 1, 2$, $\sigma = \sigma_j$, $\mu_i := \lambda_i^2 \sigma_n / 2$:

$$\partial_t u_i = \frac{1}{2}\Delta\big(\sigma(u)^2 u_i\big) + \mu_i u_i \quad \text{in } \mathbb{R}^{n-1},\ t > 0,\ i = 1, 2$$

- Parabolic in sense of Petrovskii if $\sigma + u_1\partial_1\sigma + u_2\partial_2\sigma \geq 0$
- Fulfilled if e.g. $\sigma(u)^2 = 2a(u_1/u_2)$ for some function a

Partial averaging in economics

$$\partial_t u_i = \Delta\big(a(u_1/u_2)u_i\big) + \mu_i u_i \quad \text{in } \mathbb{T}^d,\ t>0, \quad u_i(0)=u_i^0$$

or $\partial_t u = \operatorname{div}(A(u)\nabla u)$

- Assumptions: $a \in C^1(\mathbb{R})$, $a(r) \geq r|a'(r)|$, $a(r) \geq a_0/(r^p + r^{-p})$, examples: $a(r) = r^p$ for $0 < p \leq 1$, $a(r) = 1/r$
- Nonstandard entropy: $\alpha \geq p + 4$

$$H(u) = \int_{\mathbb{T}^d} h(u)dx,\ h(u) = \left(\frac{u_1}{u_2}\right)^\alpha u_1^2 + \left(\frac{u_2}{u_1}\right)^\alpha u_2^2 + \sum_{i=1}^2 (u_i - \log u_i)$$

- Entropy production:

$$\frac{dH}{dt} + \int_{\mathbb{T}^d}\left(\left(\frac{u_1}{u_2}\right)^{\alpha-p} + \left(\frac{u_2}{u_1}\right)^{\alpha-p}\right)(|\nabla u_1|^2 + |\nabla u_2|^2)dx \leq C(\mu_1,\mu_2)H$$

- Properties: h convex, $h''(u)A(u)$ positive definite
- Yields global existence of weak solutions (A.J.-Zamponi 2016)

❸ Biofilm models (Daus-Milisic-Zamponi 2018)

$$\partial_t u_i - \operatorname{div}\left(p(M)^2 \nabla \frac{u_i q(M)}{p(M)} \right) = f_i(u), \quad i = 1, \ldots, n$$

- Plus initial and (mixed Dirichlet-Neumann) boundary conditions
- Biofilm = aggregation of microorganism embedded within slimy ECM (extracellular matrix)
- Models interaction of bacterial species on shared substrate
- u_i: volume fractions of ith biomass species, $M = \sum_{i=1}^n u_i$: total mass
- Formal derivation from lattice model: Rahman-Sudarsan-Eberl 2015
- Nonlinear functions: diffusion system degenerate and singular

$$p(M) \le C_1 \exp(-C_2(1-M)^{-\kappa}), \quad p \text{ decreasing}, \quad p(1) = 0,$$

$$q(M) = \frac{p(M)}{M} \int_0^M \frac{s^\alpha ds}{(1-s)^\beta p(s)^2}, \quad \alpha, \beta > 1, \ \kappa > 0$$

Biofilm models

$$\partial_t u_i - \mathrm{div}\left(p(M)^2 \nabla \frac{u_i q(M)}{p(M)} \right) = f_i(u), \quad i = 1, \ldots, n$$

- Entropy density:

$$h(u) = \sum_{i=1}^n u_i(\log u_i - 1) + \int_0^M \log \frac{q(s)}{p(s)} ds$$

- Entropy inequality: (for suitable reaction terms f_i)

$$\frac{d}{dt} \int_\Omega h(u)dx + 2 \int_\Omega \sum_{i=1}^n p(M)^2 \left| \nabla \left(\frac{u_i q(M)}{p(M)} \right)^{1/2} \right|^2 dx \le C \int_\Omega h(u)dx + C$$

- Lower bound for entropy production:

$$\int_\Omega \frac{M^{\alpha-1}}{(1-M)^{1+\beta+\kappa}} |\nabla M|^2 dx + \int_\Omega \sum_{i=1}^n p(M)q(M)|\nabla u_i^{1/2}|^2 dx \le C$$

- Global existence of bounded weak solutions (Daus-Milisic-Zamponi, draft 2018)

❹ Energy-transport equations for semiconductors

Motivation: All models so far depend on particle densities. What about models including temperature?

- Equations: particle density $\rho(x,t)$, temperature $\theta(x,t)$

$$\partial_t \rho = \Delta(\rho\theta^{1/2-\beta}), \quad \partial_t(\rho\theta) = \kappa\Delta(\rho\theta^{3/2-\beta}) + \frac{\rho}{\tau}(1-\theta) \text{ in } \Omega$$

- Parameters: $-\frac{1}{2} \le \beta \le \frac{1}{2}$, $\kappa = \frac{2}{3}(2-\beta)$
- Dirichlet-Neumann boundary conditions, $\rho(0) = \rho^0$, $\theta(0) = \theta^0$
- Parameter β related to elastic scattering rate, relaxation term: $\frac{\rho}{\tau}(1-\theta)$ with relaxation time $\tau > 0$
- Electric field neglected; to simplify, we ignore boundary conditions

Special case: $\beta = \frac{1}{2}$ leads to uncoupled heat equations
Physical cases: $\beta = 0$ and $\beta = -\frac{1}{2}$

Entropy structure

$$\partial_t \rho = \Delta(\rho\theta^{1/2-\beta}), \quad \partial_t(\rho\theta) = \kappa\Delta(\rho\theta^{3/2-\beta}) + \frac{\rho}{\tau}(1-\theta)$$

Mathematical difficulties:

- Equations are strongly coupled $\to$ a priori estimates?
- Equations are degenerate at $\theta = 0$ $\to$ loss of regularity!

Entropy structure: $H[\rho,\theta] = \int_\Omega \rho\log(\theta^{-3/2}\rho)dx$

- Entropy variables: $w_1 = \log(\theta^{-3/2}\rho)$, $w_2 = -1/\theta$
- New diffusion matrix:

$$B(w) = \theta^{1/2-\beta}\rho \begin{pmatrix} 1 & (2-\beta)\theta \\ (2-\beta)\theta & (3-\beta)(2-\beta)\theta^2 \end{pmatrix} \Rightarrow \text{ pos. semi-def.}$$

- Entropy-dissipation inequality: constants C_1, $C_2 > 0$

$$\frac{dH}{dt} + C_1 \int_\Omega \theta^{1/2-\beta}\big(\rho^{-1}|\nabla\rho|^2 + \theta^{-1}|\nabla\theta|^2\big) \le C_2$$

Problem: Estimate is not helpful near $\theta = 0$

Entropy structure

$$\partial_t \rho = \Delta(\rho\theta^{1/2-\beta}), \quad \partial_t(\rho\theta) = \kappa\Delta(\rho\theta^{3/2-\beta}) + \frac{\rho}{\tau}(1-\theta)$$

Key ideas:

- New variables $u = \rho\theta^{1/2-\beta}$, $v = \rho\theta^{3/2-\beta} \Rightarrow \theta = v/u$:

$$\partial_t \left(\left(\frac{u}{v}\right)^{1/2-\beta} u \right) = \Delta u, \quad \partial_t \left(\left(\frac{v}{u}\right)^{1/2+\beta} u \right) = \Delta v + R(u,v)$$

- Nonlogarithmic entropies:

$$\frac{d}{dt}\int_\Omega \rho^2\theta^b dx + C_1 \int_\Omega \left|\nabla\left(\rho\theta^{(2b+1-2\beta)/4}\right)\right|^2 dx \le C_2$$

- Special choices of $b \in \mathbb{R}$ yields estimates

$$\int_\Omega \left(|\nabla\rho|^2 + |\nabla u|^2 + |\nabla v|^2\right) dx \le C_3$$

- Implicit Euler scheme (u^k, v^k): apply maximum principle

$$u^k \ge m(u^{k-1}, v^{k-1}) > 0, \quad v^k \ge m(u^{k-1}, v^{k-1}) > 0$$

Global existence

$$\partial_t \rho = \Delta(\rho\theta^{1/2-\beta}), \quad \partial_t(\rho\theta) = \kappa\Delta(\rho\theta^{3/2-\beta}) + \frac{\rho}{\tau}(1-\theta)$$

Theorem (Zamponi/A.J. 2015)

Let $d \le 3$, $-\frac{1}{2} \le \beta < \frac{1}{2}$. *Then* $\exists$ *weak solution* $\rho > 0$, $\rho\theta > 0$ *in* Ω, $t > 0$

$$\rho,\ \rho\theta^b \in L^2_{\rm loc}(0,\infty; H^1), \quad b \in \{1, \tfrac{1}{2}-\beta, \tfrac{3}{2}-\beta\}$$

- Proof highly technical: truncate $\theta^k = v^k/u^k$, show that $\theta^k \ge m(\theta^{k-1}) > 0$, include boundary cond., use different entropies
- Open problem: Existence with electric field term

$$\partial_t \rho = \operatorname{div}\left(\nabla(\rho\theta^{1/2-\beta}) + \rho\theta^{-1/2-\beta}\nabla V\right)$$

- Equilibration to constant steady state (ρ_D, θ_D):

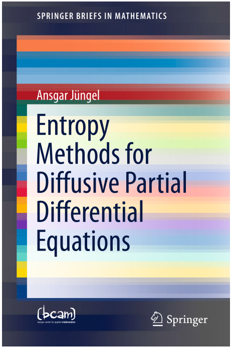
$$\|n(t) - n_D\|_{L^2} + \|\theta(t) - \theta_D\|_{L^2} \le \frac{C_1}{(1 + C_2 t)^{1/2}}$$

- Open problem: Prove exponential decay rate (numerical evidence)

Summary

Cross-diffusion systems:

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



Boundedness-by-entropy method:

- Main ingredient: entropy density $h(u)$ such that $h''(u)A(u)$ is positive definite
- Yields global existence of weak solutions and lower/upper bounds
- Applicable to large class of systems

Open problems:

- Do global weak solutions to n-species population model exist without detailed balance, for all $a_{ij} > 0$?
- How large is class of diffusion systems having an entropy structure?
- Are the weak solutions unique?
- How to translate technique to numerical discretizations?