Multi-species populations: interacting particles, cross diffusion, and entropies

Ansgar Jüngel

Technische Universität Wien, Austria

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Der Wissenschaftsfonds.

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Adobe Firefly: Interacting particles in landscape

Contents

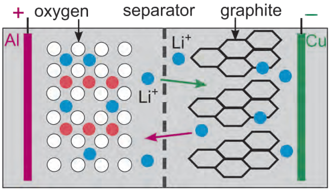
Multi-species systems

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: diffusion equations



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Literature

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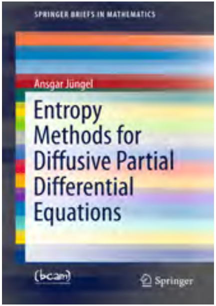

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History of mathematical population dynamics (N. Bacaër)

- Leonardo of Pisa 1202: $P_{n+1} = P_n + P_{n-1} \to$ Fibonacci numbers
- Euler 1748: $P_{n+1} = (1+\kappa)P_n \to$ exponential growth
- Maltus 1798, Verhulst 1838: limit of growth, $dP/dt = \kappa P - P^2$
- Lotka 1925, Volterra 1926: predator–prey differential equations
- McKendrick, Kermack 1926–27: epidemic dynamics (SIR model)
- May 1974: chaotic populations (discrete model)
- Shigesada, Kawasaki, Teramoto 1979: two-species populations
- Busenberg, Travis 1983: segregating populations

Euler

Lotka

Volterra

Modeling of multi-species populations

Microscopic models:

- Discrete-time Markov chain: $u_i(t_{k+1}) = \sum_{j=1}^N u_j(t_k)P_{ji}$
- Time-continuous Markov chain: $du_i/dt = \sum_{j=1}^N (u_j P_{ji} - u_i P_{ij})$
- Particle models: N Newton's equations

Mesoscopic models:

- Kinetic equation: PDEs for distribution functions $f_i(x,a,t)$

Macroscopic models:

- Ordinary differential eqs.: SIR model (Kermack–McKendrick 1927)
- Stochastic differential equations: $du_i = F_i(u)dt + \sigma(u)dW$
- Age-structured model: $\partial_t f + \partial_a f = -\mu f$, $n(0,t) = \int_0^\infty b(a)f(a,t)da$ (McKendrick 1926)
- Diffusive equations: PDEs for density $u_i(x,t)$

Diffusion equations

Reaction-diffusion equation:

$$\partial_t u - \mathrm{div}(D\nabla u) = f(u) \quad \text{in } \Omega,\ t > 0,\ \text{initial \& boundary cond.},\ D > 0$$

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

Reaction-diffusion systems:

$$\partial_t u_i - \mathrm{div}(D_i \nabla u_i) = f_i(u) \quad \text{in } \Omega,\ t > 0,\ D_i > 0,\ i = 1, \ldots, n$$

- f_i quasi-positive: $f_i \leq 0$ at $u_i = 0$
- Global existence if quasi-pos., total mass control, $n = 2$ (Pierre 1987)
- Global existence if quasi-pos., total mass control, f_i at most quadratic

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
  $\Rightarrow$ need for cross-diffusion systems

Fick's law for fluid mixtures

- Mass balance equations: density u_i, diffusion flux J_i

$$\partial_t u_i + \operatorname{div} J_i = 0, \quad i = 1, \ldots, n$$

- Fick's law: flux from high-concentration to low-concentration region

$$J_i = -D_i \nabla u_i, \quad D_i : \text{ diffusion coefficient}$$

- Leads to diffusion equation $\partial_t u_i - \operatorname{div}(D_i \nabla u_i) = 0$

Problem: Uphill diffusion in ternary mixtures (Duncan–Toor 1962)

- Mixture of hydrogen, nitrogen, carbon dioxide in two bulbs
- Flux of nitrogen J_2 significant although $\nabla u_2 \approx 0 \rightarrow$ uphill diffusion
- Fick's law not sufficient $\rightarrow$ $J_i = -\sum_{j=1}^n A_{ij} \nabla u_j$

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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: $\operatorname{supp}(u_i(t)) \cap \operatorname{supp}(u_j(t)) = \emptyset\ \forall\, t$ (Bertsch et al. 1985)
- Blow-up in L^∞ norm in finite time possible (Stará–John 1995)

Aim: Derivation, mathematical analysis, numerical simulations

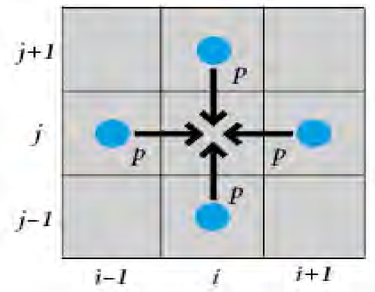
Overview

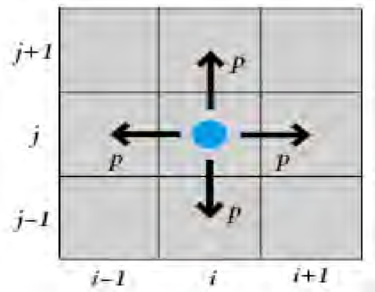
1. Introduction
2. Derivation of population models
   - Derivation from lattice models
   - Derivation from fluid models
   - Derivation from interacting particle systems
3. Analysis of cross-diffusion systems
4. More about the Busenberg–Travis model
5. Numerical approximation

① Derivation from lattice models: single species

- Temporal change of particle number = incoming − outgoing particles
- Lattice with mid points (x_i, y_j), where $x_i = i\eta$, $y_j = j\eta$, $\eta > 0$
- $u_{ij} = u(t, x_i, y_j)$ = population number (i, j) at time t
- p = transition rate (to simplify: constant)

$$\begin{aligned}\frac{d}{dt}u_{ij} &= p(u_{i+1,j} + u_{i-1,j} + u_{i,j-1} + u_{i,j+1}) - 4pu_{ij} \\ &= p(u_{i+1,j} - 2u_{ij} + u_{i-1,j}) + p(u_{i,j+1} - 2u_{ij} + u_{i,j-1})\end{aligned}$$





Taylor approximation

- Abbreviate: $\partial_x u_{ij} = \frac{\partial u}{\partial x}(x_i, y_j)$, $\partial^2_{xx} u_{ij} = \frac{\partial^2 u}{\partial x^2}(x_i, x_j)$ etc.
- Taylor approximation of $u_{i\pm1,j} = u(x_i \pm \eta, y_j)$, y_j fixed

$$
\begin{aligned}
u_{i+1,j} &= u_{ij} + \eta\partial_x u_{ij} + \tfrac{\eta^2}{2}\partial_{xx} u_{ij} + O(\eta^3) \\
u_{i-1,j} &= u_{ij} - \eta\partial_x u_{ij} + \tfrac{\eta^2}{2}\partial_{xx} u_{ij} + O(\eta^3) \\
\hline
\text{sum:} \quad u_{i+1,j} - 2u_{ij} + u_{i-1,j} &= \eta^2\partial_{xx} u_{ij} + O(\eta^3)
\end{aligned}
$$

- Taylor approximation of $u_{i,j\pm1} = u(x_i, y_j \pm \eta)$, x_i fixed

$$u_{i,j+1} - 2u_{ij} + u_{i,j-1} = \eta^2\partial_{yy} u_{ij} + O(\eta^3)$$

- Master equation:

$$
\begin{aligned}
\frac{d}{dt}u_{ij} &= p(u_{i+1,j} - 2u_{ij} + u_{i-1,j}) + p(u_{i,j+1} - 2u_{ij} + u_{i,j-1}) \\
&= \eta^2 p\partial^2_{xx} u_{ij} + \eta^2 p\partial^2_{yy} u_{ij} + 2O(\eta^3) = \eta^2 p\Delta u_{ij} + 2O(\eta^3)
\end{aligned}
$$

Diffusion limit

$$\frac{d}{dt}u_{ij} = \eta^2 p\Delta u_{ij} + 2O(\eta^3), \quad \lim_{\eta\to 0}\frac{O(\eta^3)}{\eta^2} = 0$$

- Problem: Limit $\eta \to 0$ leads to trivial dynamics
- Solution: Consider "large" time scale, $t \to t/\eta^2$, $\partial_t \to \eta^2\partial_t$

$$\frac{d}{dt}u_{ij} = p\Delta u_{ij} + \frac{2O(\eta^3)}{\eta^2}, \quad \lim_{\eta\to 0}\frac{O(\eta^3)}{\eta^2} = 0$$

- Diffusion limit $\eta \to 0$:

$$\partial_t u(x,y,t) = \Delta u(x,y,t) := (\partial_{xx}^2 + \partial_{yy}^2)u(x,y,t) \quad \text{in } \mathbb{R}^d,\ t > 0$$

Bounded domains Ω:

- Initial conditions: $u(x,y,0) = u_0(x,y)$ in Ω
- Boundary conditions: $u = u_D$ or $\nabla u \cdot \nu = 0$ on $\partial\Omega$

Nonconstant transition rate

- One-dimensional situation
- Transition rate: $p_j = p(u_j)$, population number u_j at x_j
- Scaled master equation:

$$\eta^2 \partial_t u_j = p_{j-1} u_{j-1} + p_{j+1} u_{j+1} - 2 p_j u_j$$

- Taylor expansion of p:

$$p_{j\pm 1} = p_j \pm \eta \partial_u p_j \partial_x u_j + \frac{\eta^2}{2} \partial_u p_j \partial_x^2 u_j + \frac{\eta^2}{2} \partial_{uu}^2 pj (\partial_x u_j)^2 + O(\eta^3)$$

- Insert in master equation, divide by η^2, and perform $\eta \to 0$:

$$\partial_t u = \partial_x \big((p(u) + u \partial_u p(u)) \partial_x u \big) = \partial_{xx}^2 (up(u))$$

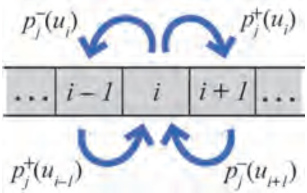
- Multidimensional equation:

$$\partial_t u = \Delta(up(u)) \quad \text{in } \mathbb{R}^d, \ t > 0$$

Derivation from lattice models: multiple species

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

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



- Transition rates: $p^\pm_{j,i} = p_j(u(x_i))$
- One-dimensional case to simplify notation
- Taylor expansion, diffusion scaling, formal limit $\eta \to 0$ leads to system of diffusion eqs. (Zamponi–AJ 2017)

$$\partial_t u_i = \partial_x \left(\sum_{j=1}^n A_{ij}(u) \partial_x u_j \right) = \partial^2_{xx}\big(u_i p_i(u)\big), \quad i = 1, \ldots, n$$

where

$$A_{ij}(u) = \delta_{ij} p_i(u) + u_i \frac{\partial p_i}{\partial u_j}(u), \quad i, j = 1, \ldots, n$$

- Rigorous limit like in Daus–Desvillettes–Dietert 2018
- Multi-dimensional case analogous: $\partial_t u_i = \Delta(u_i p_i(u))$

Derivation from lattice models: size exclusion

- Size exclusion: Species have finite size $\to$ u_i = volume fraction
- Size-exclusion constraint: $\sum_{i=0}^n u_i = 1$ with u_0 = void
- Scaled master equation:

$$\eta^2 \partial_t u_j(x_i) = R^+_{j,i-1} u_j(x_{i-1}) + R^-_{j,i+1} u_j(x_{i+1}) - (R^+_{j,i} + R^-_{j,i}) u_j(x_i)$$

- Transition rate: $R^\pm_{j,i} = p_j(u(x_i)) q_i(u_0(x_{i\pm 1}))$
- Limit $\eta \to 0$ (Zamponi–AJ 2017)

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

- Diffusion matrix $A = (A_{ij})$ with

$$A_{ij}(u) = \delta_{ij} p_i(u) q_i(u_0) + u_i q_i(u) \frac{\partial p_i}{\partial u_j}(u) + u_i p_i(u) \frac{dq_i}{du_0}(u_0)$$

Example 1: Shigesada–Kawasaki–Teramoto (SKT) model

$$A_{ij}(u) = \delta_{ij} p_i(u) + u_i \frac{\partial p_i}{\partial u_j}(u), \quad q_i = 1$$

Example: $p_i(u) = a_{i0} + a_{i1} u_1 + a_{i2} u_2$, $i = 1, 2$ $(a_{ij} \geq 0)$

$$A(u) = \begin{pmatrix} a_{10} + 2a_{11} u_1 + a_{12} u_2 & a_{12} u_1 \\ a_{21} u_2 & a_{20} + a_{21} u_1 + 2a_{22} u_2 \end{pmatrix}$$

- First suggested by Shigesada, Kawasaki, Teramoto 1979
- Diffusion matrix not symmetric, not positive definite
- Eigenvalues of $A(u)$ positive: $\lambda_{1/2} > 0$
- Lotka-Volterra terms: $f_i(u) = (b_{i0} - b_{i1} u_1 - b_{i2} u_2) u_i$

Black residential segregation in Milwaukee (blue dots)
© US Census Bureau 2002

Example 2: Size-exclusion model

$$A_{ij}(u) = \delta_{ij} q_i(u_0) + u_i q_i'(u_0), \quad p_i = 1$$

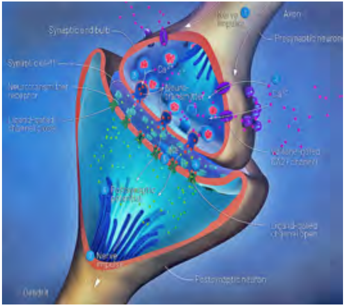
Example: $q_i(u_0) = D_i u_0$, $u_0 = 1 - \sum_{i=1}^n u_i$

$$A_{ii}(u) = D_i(u_i + u_0), \quad A_{ij}(u) = D_i u_i \quad \text{for } i \neq j$$

- Cross-diffusion equations:

$$\partial_t u_i = D_i \operatorname{div}(u_0 \nabla u_i - u_i \nabla u_0)$$

- Ion transport through channels: include drift $D_i \operatorname{div}(u_0 u_i z_i \nabla \Phi)$
- Nernst–Planck equations: $u_0 = 1$
- $A(u)$ not symm., not positive definite
- Volume fractions should satisfy $0 \leq u_i \leq 1$



Ion fractions in synapse channel © Adobe Stock

② Derivation from fluid mixture model

- Mass and momentum balance equations:

$$\partial_t u_i + \operatorname{div}(u_i v_i) = 0, \quad i = 1, \ldots, n$$
$$\varepsilon \partial_t(u_i v_i) + \varepsilon \operatorname{div}(u_i v_i \otimes v_i) + \operatorname{div} S_i = f_i$$

- Mass densities: u_i, velocities: v_i, stress tensor: S_i
- Friction force: $f_i = \sum_{j=1}^n k_{ij} u_i u_j (v_j - v_i)$
- Momentum balance: $\varepsilon \ll 1$ means small inertia effects

Example 1: $S_i = u_i p_i(u)\mathbb{I}$ (no viscous stress, only nonlinear pressure) and $\varepsilon \to 0$. Simplification: $k_{ij} = 1$ gives $\sum_{j=1}^n k_{ij} u_i u_j (v_j - v_i) = -u_i v_i$

$$\partial_t u_i + \operatorname{div}(u_i v_i) = 0, \quad \nabla(u_i p_i(u)) = -u_i v_i$$
$$\Rightarrow \quad \partial_t u_i - \Delta(u_i p_i(u)) = 0 \quad \text{(SKT model)}$$

Derivation from fluid mixture model

$$\partial_t u_i + \operatorname{div}(u_i v_i) = 0, \quad i = 1, \ldots, N$$
$$\varepsilon \partial_t (u_i v_i) + \varepsilon \operatorname{div}(u_i v_i \otimes v_i) + \operatorname{div} S_i = f_i$$

Example 2: $S_i = u_i$ (linear pressure) and $\varepsilon \to 0$

- Barycentric velocity vanishes: $\sum_{i=0}^n u_i v_i = 0$
- Size exclusion: $\sum_{i=0}^n \partial_t u_i = 0 \Rightarrow \sum_{i=0}^n u_i(t) = \sum_{i=0}^n u_i(0) = 1$

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

$\to$ Maxwell-Stefan diffusion system for gas mixtures

- Problem: $\sum_{i=0}^n \nabla u_i = 0$, relation $\nabla u_i \leftrightarrow v_j$ not invertible
- Solution: invert on orthogonal complement of kernel

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

- Gives cross-diffusion system with matrix $(A_{ij}(u))$ which is generally neither symmetric nor positive definite

③ Derivation from interacting particle systems

- Single species: N particles at position $X^k(t)$, $k = 1, \dots, N$

$$dX_\eta^k(t) = \frac{1}{N}\sum_{\ell=1}^{N} \nabla V_\eta(X_\eta^k(t) - X_\eta^\ell(t)) + \sqrt{2\sigma}\,dW^k(t), \quad t > 0$$

$$X_\eta^k(0) = \xi^k \quad \text{in } \mathbb{R}^d, \; k = 1, \dots, N$$

- Brownian motions $W^k(t)$, initial data $\xi^1, \dots, \xi^N$ i.i.d. with common probability density u^0
- Interaction potential: $V_\eta \to \delta_0$ in sense of distributions

$$V_\eta(x) = \frac{1}{\eta^d} V\left(\frac{|x|}{\eta}\right), \quad x \in \mathbb{R}^d, \; \eta > 0$$

- Aim: mean-field limit $N \to \infty$, $\eta \to 0$
- Empirical measure: $\mu_N(t) = N^{-1}\sum_{k=1}^N \delta_{X^k(t)}$

$$dX_\eta^k(t) = \nabla V_\eta * \mu_N(t)dt + \sqrt{2\sigma}\,dW^k(t)$$

Heuristic arguments

$$dX_\eta^k(t) = \nabla V_\eta * \mu_N(t)dt + \sqrt{2\sigma}dW^k(t)$$

- Many-particle limit $N \to \infty$: expect that $\mu_N \to \bar{u}_\eta$, $\bar{u}_\eta = \text{law}(\bar{X}_\eta^k)$

$$d\bar{X}_\eta^k(t) = \nabla V_\eta * \bar{u}_\eta(\bar{X}_\eta^k)dt + \sqrt{2\sigma}dW^k(t)$$

- Determine equation for $\bar{u}_\eta$ from Itô's lemma:

$$d\phi(\bar{X}_\eta^k) = \big\{\nabla\phi(\bar{X}_\eta^k)\cdot\nabla V_\eta * \bar{u}_\eta(\bar{X}_\eta^k) + \sigma\Delta\phi(\bar{X}_\eta^k)\big\}dt + \sqrt{2\sigma}\nabla\phi(\bar{X}_\eta^k)\cdot dW^k$$

Itô's lemma: Let $X(t)$ solve $dX = adt + bdW$, $\phi \in C^2$. Then

$$d\phi(X) = \big(\partial_t\phi(X) + a\partial_x\phi(X) + \tfrac{1}{2}b^2\partial_{xx}^2\phi(X)\big)dt + b\partial_x\phi(X)dW$$

- Integrate over $(0,t)$ and take expectation:

$$\mathbb{E}\phi(\bar{X}_\eta^k(t)) - \mathbb{E}\phi(\bar{X}_\eta^k(0)) = \mathbb{E}\int_0^t \big(\nabla\phi(\bar{X}_\eta^k)\cdot\nabla V_\eta * \bar{u}_\eta(\bar{X}_\eta^k) + \sigma\Delta\phi(\bar{X}_\eta^k)\big)ds$$
$$+ \sqrt{2\sigma}\mathbb{E}\int_0^t \nabla\phi(\bar{X}_\eta^k)\cdot dW^k(s)$$

Heuristic arguments

$$\mathbb{E}\phi(\bar X_\eta^k(t)) - \mathbb{E}\phi(\bar X_\eta^k(0)) = \mathbb{E}\int_0^t \big(\nabla\phi(\bar X_\eta^k)\cdot\nabla V_\eta * \bar u_\eta(\bar X_\eta^k) + \sigma\Delta\phi(\bar X_\eta^k)\big)ds$$
$$+ \sqrt{2\sigma}\,\underbrace{\mathbb{E}\int_0^t \nabla\phi(\bar X_\eta^k)\cdot dW^k(s)}_{=0}$$

- $\bar u_\eta = \mathrm{law}(\bar X_\eta^k)$ implies that $\mathbb{E}\phi(\bar X_\eta^k) = \int_{\mathbb{R}^d}\phi\bar u_\eta dx$
- Gives weak formulation:

$$\int_{\mathbb{R}^d}(\phi\bar u_\eta(t) - \phi\bar u_\eta(0))dx = \int_0^t\int_{\mathbb{R}^d}\big(\nabla\phi(\bar X_\eta^k)\cdot\nabla V_\eta * \bar u_\eta(\bar X_\eta^k) + \sigma\Delta\phi(\bar X_\eta^k)\big)dxds$$

- Strong formulation:

$$\partial_t\bar u_\eta - \sigma\Delta\bar u_\eta = -\operatorname{div}(\bar u_\eta V_\eta * \nabla\bar u_\eta)$$

- Limit $\eta\to 0$:

$$\partial_t u - \sigma\Delta u = -\operatorname{div}(u\delta_0 * \nabla u) = -\operatorname{div}(u\nabla u), \quad t>0$$
$$u(0) = \mathrm{law}(\bar X_\eta^k(0)) = \mathrm{law}(\xi^k) = u^0 \quad \text{in } \mathbb{R}^d$$

Aim: Extend technique to multiple species

Mean-field limit in multi-species system

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

- Species index $i = 1, \ldots, n$, particle index $k = 1, \ldots, N$
- Independent Brownian motions W_i^k, $\xi_i^1, \ldots, \xi_i^N$ i.i.d. with common density u_i^0
- Interaction potential: $V_{ij}^\eta \to a_{ij}\delta_0$ in sense of distributions, $a_{ij} \geq 0$

$$V_{ij}^\eta = \frac{1}{\eta^d} V\left(\frac{|x|}{\eta}\right), \quad x \in \mathbb{R}^d, \ \eta > 0$$

- Limit $N \to \infty$ leads to nonlocal SDE, $\eta \to 0$ leads to local SDE with probability density satisfying PDE (by Itô's lemma)

Mean-field limit: heuristics

- "Microscopic" particle system: $(i = 1, \ldots, n,\ k = 1, \ldots, N)$

$$dX_i^k = -\nabla V_{ij}^\eta * \mu_i^N(t)dt + \sqrt{2\sigma_i}dW_i^k(t),\ X_i^k(0) = \xi_i^k$$

- "$N \to \infty$" $\Rightarrow$ intermediate particle system: u_j^η solves nonlocal PDE

$$d\bar{X}_i^k = -\sum_{j=1}^n (\nabla V_{ij}^\eta * u_j^\eta)(\bar{X}_i^k(t), t)dt + \sqrt{2\sigma_i}dW_i^k(t),\ \bar{X}_i^k(0) = \xi_i^k$$

- $\eta \to 0 \Rightarrow$ "macroscopic" particle system:

$$d\widehat{X}_i^k = -\sum_{j=1}^n a_{ij}\nabla u_j(\widehat{X}_i^k(t), t)dt + \sqrt{2\sigma_i}dW_i^k(t),\ \widehat{X}_i^k(0) = \xi_i^k$$

- Density function $u_i = \mathrm{Law}(\widehat{X}_i^k)$ associated to $\widehat{X}_i^k$ solves

$$\partial_t u_i = \sigma_i \Delta u_i + \operatorname{div}\left(u_i \sum_{j=1}^n a_{ij}\nabla u_j\right), \quad t > 0, \quad u_i(u) = u_i^0 \quad \text{in } \mathbb{R}^d$$

Mean-field limit: rigorous result

$$
\begin{aligned}
dX_i^k &= -\nabla V_{ij}^\eta * \mu_i^N(t)dt + \sqrt{2\sigma_i}dW_i^k(t) \\
d\bar{X}_i^k &= -\sum_{j=1}^n (\nabla V_{ij}^\eta * u_{\eta,j})(\bar{X}_i^k(t),t)dt + \sqrt{2\sigma_i}dW_i^k(t) \\
d\widehat{X}_i^k &= -\sum_{j=1}^n a_{ij}\nabla u_j(\widehat{X}_i^k(t),t)dt + \sqrt{2\sigma_i}dW_i^k(t)
\end{aligned}
$$

Theorem (L. Chen–Daus–AJ 2019)

Let $N \in \mathbb{N}$ and $\eta^{-2d-4} \le c\log N$. Then

$$
\sup_{k=1,\ldots,N} \mathbb{E}\bigg(\sum_{i=1}^n \sup_{0<s<T} \big|X_i^k(s) - \widehat{X}_i^k(s)\big|\bigg) \le C(T)\eta.
$$

Idea of proof: exploit Lipschitz continuity of V_{ij} and estimate

$$
\mathbb{E}\Big(\sup_{0<s<T}\big|X_i^k - \widehat{X}_i^k\big|\Big) \le \mathbb{E}\Big(\sup_{0<s<T}\big|X_i^k - \overline{X}_i^k\big|\Big) + \mathbb{E}\Big(\sup_{0<s<T}\big|\overline{X}_i^k - \widehat{X}_i^k\big|\Big)
$$

Mean-field cross-diffusion system

$$\partial_t u_i = \sigma_i \Delta u_i + \operatorname{div}\Big(u_i \nabla p_i(u)\Big), \quad p_i(u) = \sum_{j=1}^n a_{ij} u_j, \quad j = 1, \ldots, n$$

- Fluiddynamical interpretation if $\sigma_i = 0$:

$$\partial_t u_i + \operatorname{div}(u_i v_i) = 0, \quad v_i = -\nabla p_i(u) \quad \text{(Darcy's law)}$$

- This is not the SKT model, which has stronger diffusion

$$\partial_t u_i = \Delta(u_i p_i(u)) = \operatorname{div}(u_i \nabla p_i(u) + p_i(u) \nabla u_i)$$

- Generalization of Busenberg–Travis system (1983):

$$\partial_t u_i = \operatorname{div}(u_i \nabla p_i(u)), \quad p_i(u) = k_i \sum_{j=1}^n u_j$$

  $\to$ matrix with entries $a_{ij} = k_i$ has rank one only
- Change of unknowns if $k_i = 1$: $v_0 = \sum_{i=1}^n u_i$, $v_i = u_i / v_0$

$$\partial_t v_0 = \operatorname{div}(v_0 \nabla v_0), \quad \partial_t v_i = \nabla v_0 \cdot \nabla v_i$$

  $\to$ mixed hyperbolic–parabolic system

Intermediate summary

- Derivation from lattice models yields SKT model and size-exclusion systems
- Derivation from fluid models yields SKT model and Maxwell–Stefan equations for gas mixtures
- Derivation from interacting particle systems yields generalized Busenberg–Travis equations
- Other derivations:
  - From kinetic models: Maxwell–Stefan equations (Boudin–Grec–Salvarani 2011), population models: open problem (work in progress with Taguchi)
  - From reaction–diffusion equations in fast-reaction limit (Daus–Desvillettes–AJ 2020, Murakawa 2021, ...)
  - Matched asymptotics expansion: Mason–Lack–Bruna 2022

Overview

Mathematical properties

Diffusion equations: $\partial_t u - \Delta u = f$

- Maximum principle: $u \geq 0$ at $t = 0$ and on $\partial\Omega$, $f \geq 0 \Rightarrow u(t) \geq 0$ for all $t \geq 0$
- Regularity: u smooth on $\partial\Omega$, f smooth $\Rightarrow u(t)$ smooth for all $t > 0$

Reaction-diffusion systems: $\partial_t u_i - a_i \Delta u_i = f_i(u)$

- Maximum principle: still holds if f_i appropriate
- Regularity: It may happen that $\exists T^* > 0$: $\lim_{t \to T^*} \sup_x |u(x,t)| = \infty$

Cross-diffusion systems: $\partial_t u - \operatorname{div}(A(u)\nabla u) = f$

- Maximum principle: does not hold generally!
- Regularity: does not hold generally!
- New mathematical ideas necessary, consider only physically motivated systems

State of the art

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

Aim: Develop existence theory (uniqueness, regularity)

- 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: hyperbol.–parabol., need invariance cond.
- Amann 1990: parabolic in the sense of Petrovskii $\Rightarrow \exists!$ local classical solution; bounds in $W^{1,p}(\Omega)$, $p > d$ $\Rightarrow \exists$ global classical solution
- D. Le 2016: BMO bound & condition on $A(u)$ $\Rightarrow$ classical solution (BMO = Bounded Mean Oscillation, $L^\infty \subset \text{BMO} \subset L^p_{\text{loc}}$)
- Burger et al. 2010: global bounded weak solutions for special model

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

Key idea: Exploit entropy structure

Entropy structure: heuristics

Main assumption

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

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

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)

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

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!)

Entropy structure: definition

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

Definition (Entropy structure)

If $\exists\ h \in C^0(D)$ strictly convex such that $B = A(u)h''(u)^{-1}$ or $h''(u)A(u)$ positive definite on D, then cross-diffusion system has an entropy structure.

- Domain D: $u(x,t) \in D$ or $u(x,t) \in \overline{D}$, for instance $D = (0,\infty)^n$
- B is positive definite (possibly nonsymmetric) iff $B + B^T$ is pos. def.
- B may be only positive semi-definite on $\overline{D}$ (degenerate problem)
- $h(u)$ entropy density, $H(u) = \int_\Omega h(u)\mathrm{d}x$ entropy

Relation to thermodynamic structure

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

- Mathematical entropy density h (nonincreasing in time)
- Physical entropy density $s = -h$ (nondecreasing in time)
- Free energy: $F = U - \theta s$, U internal energy density, θ temperature
- Ideal, isothermal mixture: $U =$ const., free energy $=$ math. entropy
- Entropy variable $=$ chemical potential $w_i = \partial h/\partial u_i$
- Onsager reciprocal relations (1931): B is symmetric
- Entropy production: $-\frac{dH}{dt} = \int_\Omega \nabla w : B\nabla w dx \geq 0$
  $\rightarrow$ expresses second law of thermodynamics
- Bothe–Dreyer 2015: Entropy inequality allows to determine constitutive relations for interactions

Relation to hyperbolic conservation laws

$$\partial_t u + \sum_{j=1}^n F_j(u)\partial_j u = 0, \quad F : \mathbb{R}^n \to \mathbb{R}^n,\ \partial_j = \partial/\partial x_j$$

- System symmetric hyperbolic iff $\exists\ A^0(u)$ symmetric positive definite & $A^j(u)$ symmetric such that

$$A^0(u)\partial_t u + \sum_{j=1}^n A^j(u)\partial_j u = 0$$

- Assume: $\exists$ entropy density $h(u)$ & entropy flux $q_j : \mathbb{R}^n \to \mathbb{R}^n$, $\partial_k q_j(u) = h'(u)\cdot\partial_k F_j(u)$. Then $\exists$ entropy equality:

$$\partial_t h(u) + \operatorname{div} q(u) = h'(u)\cdot\big(\partial_t u + \operatorname{div} F(u)\big) = 0$$

- Formulation as symmetric hyperbolic system: $\exists A^j$ symmetric

$$\underbrace{h''(u)^{-1}}_{=A_0(w)}\partial_t w + \sum_{j=1}^n A^j(w)\frac{\partial w}{\partial x_j} = 0$$

$\to$ similar to w-formulation of cross-diffusion systems

Overview

- Entropy structure
- Examples
- Entropy structure revisited
- Boundedness-by-entropy method



Adobe Firefly

① Two-species SKT model

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

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

- Lotka-Volterra terms: $f_i(u) = (b_{i0} - b_{i1}u_1 - b_{i2}u_2)u_i$, $i = 1, 2$
- Entropy: $h(u) = a_{21}u_1(\log u_1 - 1) + a_{12}u_2(\log u_2 - 1)$, $D = (0, \infty)^2$
- Entropy inequality:

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

- Entropy variables: $w_i = \partial h/\partial u_i = \log u_i \Rightarrow u_i = \exp(w_i) > 0$
- Consequences: Estimates for $\nabla\sqrt{u_i}$ if $a_{i0} > 0$ and ∇u_i if $a_{ii} > 0$, nonnegativity for u_i

n-species SKT model

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

$$A_{ij}(u) = \delta_{ij} p_i(u) + u_i \frac{\partial p_i}{\partial u_j}(u), \quad p_i(u) = a_{i0} + \sum_{k=1}^n a_{ik} u_k, \quad a_{ij} \geq 0$$

- Assume: (a_{ij}) positively stable (= real parts of eigenvalues are positive) & detailed-balance condition:

$$\exists \pi_1, \ldots, \pi_n > 0,\ \forall i, j = 1, \ldots, n,\ \pi_i a_{ij} = \pi_j a_{ji}$$

- (π_i) invariant measure of time-cont. Markov chain associated to (a_{ij})
- Assumptions imply that $(\pi_i a_{ij})$ is symmetric positive definite
- Entropy density: $h(u) = \sum_{i=1}^n \pi_i u_i(\log u_i - 1)$, $u \in D = (0, \infty)^n$

$$\frac{d}{dt} \int_\Omega h(u)dx + 4 \sum_{i=1}^n \pi_i p_i(u) |\nabla \sqrt{u_i}|^2 dx + \sum_{i,j=1}^n \int_\Omega \pi_i a_{ij} \nabla u_i \cdot \nabla u_j dx = 0$$

- Gives estimates for $\nabla \sqrt{u_i}$ (if $a_{i0} > 0$) and for ∇u_i

② Generalized Busenberg–Travis model

$$\partial_t u_i = \operatorname{div}(u_i \nabla p_i(u)), \quad p_i(u) = \sum_{j=1}^n a_{ij} u_j, \quad a_{ij} \geq 0$$

- Assume (a_{ij}) pos. stable & detailed-balance condition $\pi_i a_{ij} = \pi_j a_{ji}$
- Change of unknowns $w_i = \pi_i u_i$:

$$\partial_t w_i = \operatorname{div}\left(w_i \sum_{j=1}^n \frac{a_{ij}}{\pi_j} \nabla w_j \right), \quad \frac{a_{ij}}{\pi_j} = \frac{a_{ji}}{\pi_i}$$

If $A = A_1 A_2$ positively stable, A_1 symmetric, A_2 symmetric positive definite $\Rightarrow$ A_1 symmetric positive definite $(A_1 = (a_{ij}/\pi_j),\ A_2 = \operatorname{diag}(\pi_j))$

$\Rightarrow$ a_{ij}/π_j symmetric positive definite $\Rightarrow$ sufficient to assume that (a_{ij}) is symmetric positive definite

- First entropy density: $h_1(u) = \sum_{i=1}^n u_i(\log u_i - 1)$, $u \in D = (0, \infty)^2$

$$\frac{d}{dt} \int_\Omega h_1(u) dx + \sum_{i,j=1}^n \int_\Omega a_{ij} \nabla u_i \cdot \nabla u_j dx = 0 \quad \Rightarrow \text{ estimate for } \nabla u_i$$

Busenberg–Travis model: entropy structure

$$\partial_t u_i = \operatorname{div}(u_i \nabla p_i(u)), \quad p_i(u) = \sum_{j=1}^n a_{ij} u_j$$

- First entropy density: $h_1(u) = \sum_{i=1}^n u_i(\log u_i - 1)$

$$\frac{d}{dt}\int_\Omega h_1(u)dx + \sum_{i,j=1}^n \int_\Omega a_{ij}\nabla u_i \cdot \nabla u_j dx = 0$$

- Second entropy density: $h_2(u) = \frac{1}{2}\sum_{i,j=1}^n a_{ij} u_i u_j$

$$\frac{d}{dt}\int_\Omega h_2(u)dx + \sum_{i=1}^n \int_\Omega u_i |\nabla p_i(u)|^2 = 0$$

$\rightarrow$ gives estimate for u_i in $L^2(\Omega)$

Interpretation:

- $h_1(u)$ = Boltzmann–Shannon entropy density, "fluid entropy"
- $h_2(u)$ = Rao entropy density (measure for functional diversity of species), "fluid energy" with kinetic energy $u_i|v_i|^2 = u_i|\nabla p_i(u)|^2$

③ Ion transport model

$$\partial_t u_i = D_i \operatorname{div}(u_0 \nabla u_i - u_i \nabla u_0 + z_i u_0 u_i \nabla \Phi)$$
$$= D_i \operatorname{div}\big(u_i \nabla(\log u_i - \log u_0 + z_i \Phi)\big), \quad i = 1, \ldots, n$$

- Electric potential Φ (given), volume fractions u_i with $\sum_{i=0}^n u_i = 1$
- Entropy density: $u \in D = \{u \in (0,1)^n : \sum_{i=1}^n u_i < 1\} \subset \mathbb{R}^n$

$$h(u) = \sum_{i=1}^n u_i(\log u_i - 1) + u_0(\log u_0 - 1) + \sum_{i=1}^n z_i u_i \Phi$$

- Entropy / free energy inequality:

$$\frac{dt}{dt} \int_\Omega h(u) dx + \sum_{i=1}^n \int_\Omega u_0 u_i \left| \nabla \left(\log \frac{u_i}{u_0} + z_i \Phi \right) \right|^2 dx = 0$$

$\rightarrow$ estimates for $\sqrt{u_0} \nabla \sqrt{u_i}$ and ∇u_0, since

$$u_i \left| \nabla \left(\log \frac{u_i}{u_0} + z_i \Phi \right) \right|^2 = 4 u_0 \sum_{i=1}^n |\nabla \sqrt{u_i}|^2 + |\nabla u_0|^2 + 4 |\nabla \sqrt{u_0}|^2$$

Ion transport model

$$h(u)=\sum_{i=1}^n u_i(\log u_i-1)+u_0(\log u_0-1)+\sum_{i=1}^n z_iu_i\Phi$$

- Estimates for $\sqrt{u_0}\nabla\sqrt{u_i}$ and ∇u_0, but no estimate for $\nabla\sqrt{u_i}$ $\to$ non-standard degeneracy
- Invert entropy variables $w_i=\partial h/\partial u_i=\log(u_i/u_0)$:

$$u_i=\frac{\exp(w_i-z_i\Phi)}{1+\sum_{j=1}^n\exp(w_j-z_j\Phi)},\quad i=1,\ldots,n$$

  $\to$ yields $u\in D=\{u\in(0,1)^n:\sum_{i=1}^n u_i<1\}$ without the use of a maximum principle
- Idea: Solve system in w-variable, transform to u-variable, conclude $L^\infty(\Omega)$ bounds

④ Maxwell–Stefan model

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

- Assume $k_{ij} = k_{ji} > 0$
- Entropy density $h(u) = \sum_{i=0}^n u_i(\log u_i - 1)$, $u \in D = (0,\infty)^{n+1}$

$$\frac{d}{dt}\int_\Omega h(u)dx = \sum_{i=0}^n \int_\Omega \partial_t u_i \log u_i dx = \sum_{i=0}^n \int_\Omega u_i v_i \cdot \nabla \log u_i dx$$

$$= \sum_{i,j=0}^n \int_\Omega k_{ij} u_i u_j v_i \cdot (v_j - v_i) dx = -\sum_{i,j=0}^n \int_\Omega k_{ij} u_i u_j |v_i - v_j|^2 dx$$

$\to \int_\Omega h(u)dx$ Lyapunov functional

- Better estimate if $u \in D = \{u \in (0,1)^n : \sum_{i=1}^n u_i < 1\}$ but need to invert $\nabla u_i \leftrightarrow v_i$:

$$\frac{d}{dt}\int_\Omega h(u)dx + c\sum_{i=1}^n \int_\Omega |\nabla\sqrt{u_i}|^2 dx \le 0$$

Non-logarithmic entropies

Example 1: Keller–Segel system with additional cross-diffusion

$$\partial_t u_1 = \operatorname{div}(\nabla u_1 - u_1 \nabla u_2), \quad \partial_t u_2 - \Delta u_2 - \delta \Delta u_1 = u_1 - u_2$$

- Cell density u_1, chemical substance u_2, $\delta > 0$ (Hittmeir–AJ 2011)
- Entropy density: $h(u) = u_1(\log u_1 - 1) + \frac{1}{2\delta} u_2^2$

$$\frac{d}{dt} \int_\Omega h(u)dx + \int_\Omega \left(2|\nabla \sqrt{u_1}|^2 + \frac{1}{2\delta}|\nabla u_2|^2 + \frac{u_2^2}{2\delta} \right) dx \le 0$$

Example 2: Variant of Busenberg–Travis model

$$\partial_t u_i = \operatorname{div}(u_i \nabla p(u)), \quad p(u) = \left(\sum_{j=1}^n \kappa_j u_j \right)^s, \quad s > 0$$

- Healthy cells u_1, tumor cells u_2 ($s \to \infty$: Debiec–Schmidtchen 2020)
- Entropy density: $h(u) = \frac{1}{s+1}(\sum_{j=1}^n \kappa_j u_j)^{s+1}$

$$\frac{d}{dt} \int_\Omega h(u)dx + \sum_{i=1}^n \int_\Omega \kappa_i u_i |\nabla p(u)|^2 dx = 0$$

Overview

- Entropy structure
- Examples
- Entropy structure revisited
- Boundedness-by-entropy method

Entropy structure and positive stability

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

Definition: $A(u)$ positively stable = eigenvalues of $A(u)$ have positive real parts = $(*)$ parabolic in sense of Petrovskii

Theorem (X. Chen-A.J. 2021)

- *If $(*)$ has entropy structure then $A(u)$ positively stable*
  $\Rightarrow$ local existence of smooth solutions by Amann 1990
- *If $A(u)$ positively stable & $h''(u)A(u)$ symmetric then $(*)$ has an entropy structure and $A(u)$ diagonalizable with positive eigenvalues*
  symmetry of $h''(u)A(u)$ corresponds to Onsager relations
- *If $A = A_0$ constant: A positively stable $\Leftrightarrow$ $(*)$ has entropy structure*
  $A(u) = A_0 +$ nonlinear perturbation $\Rightarrow \exists$ entropy structure

Proof: Use Lyapunov theorem and matrix factorization

How to find an entropy structure?

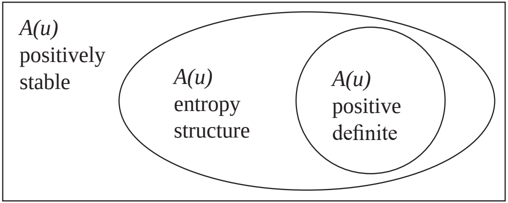
- $A(u)$ has eigenvalues with negative real part $\Rightarrow$ no entropy structure
- Entropy structure often recovered from thermodynamics (free energy)

Example: Population model $\partial_t u_i = \operatorname{div}(u_i \nabla p_i(u))$ with p_i general

Theorem (X. Chen–AJ 2021)

Let $(\partial p_i/\partial u_j)_{ij}$ be symmetric & positively stable. Then $\exists\ h \in C^2$: $h''(u)A(u)$ pos. def. If $h''(u)A(u)$ symm. $\Rightarrow$ h convex $\Rightarrow$ entropy structure.

Proof: Poincaré lemma for closed differential forms: $(\pi_i p_i)$ defines curl-free vector field $\Rightarrow \exists : h \in C^2(D)$: $\partial h/\partial u_i = \pi_i p_i \Rightarrow h''(u)A(u) > 0$



Double entropy structure of Busenberg–Travis system

$$\partial_t u_i = \operatorname{div}(k_i u_i \nabla p(u)), \quad p(u) = \sum_{j=1}^n u_j$$

- Boltzmann–Shannon entropy:

$$\frac{d}{dt}\int_\Omega k_i^{-1} u_i(\log u_i - 1)dx + \int_\Omega |\nabla p(u)|^2 dx = 0$$

- Rao entropy:

$$\frac{d}{dt}\frac{1}{2}\int_\Omega p(u)^2 dx + \sum_{i=1}^n \int_\Omega u_i |\nabla p(u)|^2 dx = 0$$

- Question: Why two entropies?
- Explanation from fluiddynamical approximation (Carrillo–X. Chen–AJ, work in progress 2024)

Fluiddynamical approximation

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

- Mass and momentum balance equations for densities u_i & velocities v_i
- Korteweg regularization $R(u, v)$ needed to derive gradient bounds
- Relaxation term $-u_i v_i$, force term $u_i \nabla p(u)$
- Formal limit $\varepsilon \to 0$ yields $v_i = -\nabla p(u) \Rightarrow$ Busenberg–Travis model

Fluid energy and entropy:

$$E = \frac{1}{2} \int_\Omega \left(p_i(u)^2 + \varepsilon \sum_{i=1}^n u_i |v_i|^2 \right) dx, \quad \frac{dE}{dt} + \int_\Omega \sum_{i=1}^n (k_i^{-1} u_i |v_i|^2 + \varepsilon R_E^2) dx = 0$$

$$H = \int_\Omega k_i^{-1} u_i (\log u_i - 1) dx, \quad \frac{dH}{dt} + \int_\Omega |\nabla p(u)|^2 dx = \varepsilon R_H$$

$\to$ In the limit $\varepsilon \to 0$, fluid energy converges to Rao entropy, fluid entropy converges to Boltzmann–Shannon entropy

Intermediate summary

- Entropy structure is inspired from thermodynamics and hyperbolic conservation laws
- Mathematical entropy often equal to Boltzmann–Shannon entropy, but $\exists$ non-logarithmic examples
- Benefits: gradient bounds & nonnegativity / L^∞ bounds
- Question how to determine an entropy structure is widely open

Overview

- Entropy structure
- Examples
- Entropy structure revisited
- Boundedness-by-entropy method

Global existence of solutions

Aim: General existence result for global weak solutions

Literature:

- Alt–Luckhaus 1983: global solutions if matrix $B = A(u)h''(u)^{-1}$ uniformly positive definite $\to$ often not satisfied in applications
- Amann 1990: a priori bounds in $W^{1,p}(\Omega)$ with $p > d \Rightarrow \exists$ global classical solution $\to W^{1,p}(\Omega)$ bounds often too strong

Key idea: Exploit entropy structure

- Introduce entropy variable $w = h'(u)$, $h : D \to \mathbb{R}$
- Solve $\partial_t u(w) - \operatorname{div}(B(w)\nabla w) = f(u(w))$ for w
- Transform back to $u = (h')^{-1}(w)$, conclude pointwise bounds in D

Assumptions:

- Convex entropy $h \in C^2(D)$ such that h' invertible on D
- "Degenerate" positive definiteness of B
- Growth condition for reactions $f(u)$

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 $u \in D$,

$$z^T h''(u)A(u)z \geq c\sum_{i=1}^n u_i^{2s_i-2}z_i^2, \; s_i \geq \frac{1}{2} \Rightarrow \text{ estimate for } |\nabla u_i^{s_i}|^2$$

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

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

Boundedness-by-entropy method

$$z^T h''(u)A(u)z \geq c\sum_{i=1}^n u_i^{2s_i-2}z_i^2,\ s_i \geq \frac{1}{2} \Rightarrow \text{ estimate for } |\nabla u_i^{s_i}|^2$$

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

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

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 SKT model below
- Yields immediately global existence for Maxwell–Stefan model ($s_i = \frac{1}{2}$)

Existence proof: strategy

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

Key ideas:

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

Strategy: problem in u $\to$ solve in w $\to$ limit solves problem in u

Existence proof: details

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

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

- Linearized system: $S : L^\infty(\Omega)\times[0,1] \to L^\infty(\Omega)$, $S(y,\delta) = w^k$ and w^k solves linear problem (by Lax-Milgram)
- Fixed-point argument: show that S compact, entropy estimate for all fixed points $\Rightarrow \exists\, w^k \in H^m(\Omega)$: $S(w^k,1) = w^k$ (by Leray-Schauder)

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

- Limit $(\varepsilon,\tau)\to 0$: Aubin–Lions compactness lemma

Aubin–Lions lemma

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

Aubin–Lions lemma

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

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

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

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–AJ–Liu 2014)

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

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

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

Remark: Alt–Luckhaus 1983: $s = 1$, Maître 2003: nonlinear version of Simon 1987, Moussa 2016: monotone nonlinearities

Example 1: SKT model

- Diffusion matrix: $(a_{ij} \geq 0)$
$$A(u) = \begin{pmatrix} a_{10} + a_{11}u_1 + a_{12}u_2 & a_{12}u_1 \\ a_{21}u_2 & a_{20} + a_{21}u_1 + a_{22}u_2 \end{pmatrix}$$
- Entropy density: $h(u) = \sum_{i=1}^2 \pi_i u_i(\log u_i - 1)$ for $u \in D = (0,\infty)^2$ but no L^∞ bound
- Positivity: $u_i = \exp(w_i) > 0$ and entropy inequality:
$$\frac{d}{dt}\int_\Omega h(u)dx + C_1 \sum_{i=1}^2 \int_\Omega (4a_{i0}|\nabla\sqrt{u_1}|^2 + a_{ii}|\nabla u_i|^2)dx \leq C_2$$
- $a_{ii} > 0$: Gagliardo–Nirenberg $u_i \in L^{2+2/d}_{x,t} \to$ enough to treat $u_i \nabla u_j$
- $a_{i0} > 0$: more sophisticated estimates needed since $u_i \in L^{1+1/d}_{x,t}$ only

Theorem (L. Chen-A.J. 2004/2006)

Let $H(u^0) < \infty$. Then $\exists$ solution (u_1, u_2) with $u_1,\ u_2 \geq 0$ in Ω and

$a_{i0} > 0: \ \sqrt{u_i} \in L^2_{\mathrm{loc}}(0,\infty; H^1(\Omega)), \quad a_{ii} > 0: \ u_i \in L^2_{\mathrm{loc}}(0,\infty; H^1(\Omega))$

Generalization: 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. 2018)

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

Generalization: nonlinear coefficients

Recall: From 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: L. Chen–AJ 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: $h_s(u) = a_{21} u_1^s + a_{12} u_2^s$, $s > 1$

Theorem (AJ 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 $u_i^{s/2} \in L^2_{\mathrm{loc}}(0, \infty; H^1(\Omega))$

Idea of proof: Use entropy $h_s(u) + \varepsilon \sum_i u_i(\log u_i - 1)$

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

Example 2: Generalized Busenberg–Travis system

$$\partial_t u_i = \operatorname{div}(u_i \nabla p_i(u)), \quad p_i(u) = \sum_{j=1}^n a_{ij} u_j \quad \text{in } \Omega_T := \Omega \times (0,T)$$

- Initial and no-flux boundary conditions, (a_{ij}) positive definite
- Entropy densities:

$$h_1(u) = \sum_{i=1}^n u_i(\log u_i - 1), \quad h_2(u) = \frac{1}{2} \sum_{i,j=1}^n a_{ij} u_i u_j$$

- Entropy inequalities: yield $u_i \in L^2(0,T;H^1) \cap L^\infty(0,T;L^2)$

$$\frac{d}{dt} \int_\Omega h_1(u)dx + \sum_{i,j=1}^n \int_\Omega a_{ij} \nabla u_i \cdot \nabla u_j dx = 0$$

$$\frac{d}{dt} \int_\Omega h_2(u)dx + \sum_{i=1}^n \int_\Omega u_i |\nabla p_i(u)|^2 dx = 0$$

- Gagliardo–Nirenberg inequality: $u_i \in L^{2+4/d}(\Omega_T)$
  $\to$ yields compactness in $L^2(\Omega_T)$

Global existence

$$\partial_t u_i = \operatorname{div}(u_i \nabla p_i(u)), \quad p_i(u) = \sum_{j=1}^n a_{ij} u_j$$

Theorem (AJ–Portisch–Zurek 2022)

$\exists$ *global nonnegative weak solution in* $\Omega_T := \Omega \times (0, T)\ \forall\ T > 0$.

Proof:

- Define $B = A(u)h_1''(u)^{-1}$ and entropy variable $w = h_1'(u)$

$$\partial_t u(w) = \operatorname{div}(B \nabla w), \quad u(w) = (h_1')^{-1}(w)$$

- Explicitly: $u_i(w) = e^{w_i}$, $B_{ij} = a_{ij} u_i u_j$ symm. pos. def. on $\{u_i > 0\}$
- Solve approximate problem for u_i^ε by using Leray–Schauder theorem
- Uniform estimates for u_i in $L^2(0, T; H^1)$, $\partial_t u_i$ in $L^q(0, T; W^{-1,q})$, $q = (d+2)/(d+1) > 1 \Rightarrow \nabla u_i^\varepsilon \rightharpoonup \nabla u_i$, $\partial_t u_i^\varepsilon \rightharpoonup \partial_t u_i$
- Aubin–Lions compactness: $u_i^\varepsilon \to u_i$ strongly in $L^2(\Omega_T)$

Regularity of solutions

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

Negative result:

- Stará–John 1995: $\exists\ A \in L^\infty$: $u(t)$ Hölder blows up at $t = 1$ in L^∞

Full regularity:

- Amann 1990: $u(t)$ bounded in $W^{1,p}(\Omega)$, $p > d \Rightarrow u$ classical solution
- D. Le 2017: $A(u)$ has polynomial growth of order ≤ 5, $u(t) \in \mathrm{BMO}$ $\Rightarrow u$ class. solution (BMO = Bounded Mean Oscillation, $L^\infty \subset \mathrm{BMO} \subset L^p_{\mathrm{loc}}$)

Partial regularity:

- Giaquinta–Struwe 1982 ($A(u)$ pos. def.): u is Hölder continuous in $\Omega_T \setminus S$, where $\mathcal{H}_{d-\varepsilon}(S) = 0$ for some $\varepsilon > 0$ (Hausdorff measure)
- Braukhoff–Raithel–Zamponi 2020 ($h''(u)A(u)$ pos. def.): u bounded $\Rightarrow u$ is Hölder continuous in $\Omega_T \setminus S$, $\mathcal{H}_{d-\varepsilon}(S) = 0$

  Idea: Use relative entropy $h(u|v) = h(u) - h(v) - h'(v) \cdot (u - v)$ and $h(u|v) \sim |u - v|^2$ for u_i far from zero, $A_{ij}(u)$ diagonal for $u_i \to 0$

Uniqueness of solutions

Uniqueness of weak solutions: u, v weak solutions $\Rightarrow u = v$

- Alt–Luckhaus 1983: linear elliptic operator, $\partial_t u_i \in L^1$
- Gajewski 1994: operator $w \mapsto \operatorname{div}(B(w)\nabla w)$ strictly monotone
- X. Chen–AJ 2018: population system if $p_i = p$, $q_i = q$, and $p(s) + sq(s) \geq 0$

Weak–strong uniqueness: u weak solution, v strong solution $\Rightarrow u = v$

- Fischer 2017: diagonal diffusion systems
- X. Chen–AJ 2019: SKT model (u: renormalized solution)
- Berendsen et al. 2020: ion transport system ($d = 1$, $D_i = 1$)
- Huo–AJ–Tzavaras 2022: Maxwell–Stefan system
- AJ–Portisch–Zurek 2022: nonlocal Busenberg–Travis system
- Laurençot–Matioc 2023: two-species Busenberg–Travis system

$\rightarrow$ Details later!

Overview

Boundedness

$$\partial_t u_1 = \operatorname{div}(u_1 \nabla(a_{11}u_1 + a_{12}u_2)), \quad \partial_t u_2 = \operatorname{div}(u_2 \nabla(a_{21}u_1 + a_{22}u_2))$$

- Initial and no-flux boundary conditions, (a_{ij}) positive definite
- Entropies: $h_n(u) = \sum_{j=0}^n b_{jn} u_1^j u_2^{n-j}$

$$b_{jn} = \binom{n}{j} \prod_{k=0}^{j-1} \frac{a_{11}k + a_{21}(n-k-1)}{a_{12}k + a_{22}(n-k-1)}, \quad b_{0n} = 1$$

- Entropy $h_2(u) = b_{02}u_2^2 + b_{12}u_1u_2 + b_{22}u_1^2$ similar to Rao entropy

Theorem (Laurençot–Matioc 2022)

$$\frac{d}{dt}\int_\Omega h_n(u)dx \le 0, \quad \|(u_1+u_2)(t)\|_{L^\infty} \le \frac{a_{22}\max\{a_{11},a_{12}\}}{a_{12}\min\{a_{21},a_{22}\}}\|(u_1+u_2)(0)\|_{L^\infty}$$

Proof: Show that $h_n''(u)A(u)$ is positive semidefinite

$\rightarrow$ Generalization to $n>2$ species not (easily) possible

Uniqueness of solutions

$$\partial_t u_i = \operatorname{div}(u_i \nabla p_i(u)), \quad p_i(u) = \sum_{j=1}^n a_{ij} u_j$$

Uniqueness of weak solutions u and v:

- Use $u_i - v_i$ as test function in difference of equations:

$$\frac{1}{2} \sum_{i,j=1}^n \int_\Omega (u_i - v_i)^2 + \sum_{i,j=1}^n \int_\Omega a_{ij} u_i \nabla(u_i - v_i) \cdot \nabla(u_j - v_j) dx$$
$$= - \sum_{i,j=1}^n \int_\Omega a_{ij}(u_i - v_i) \nabla(u_i - v_i) \cdot \nabla v_j dx$$

- Problem: factor u_i prevents to exploit positive definiteness of (a_{ij}) $\to$ L^2-type estimate not possible
- Solution: Use "nonlinear distance" (relative entropy)

$$h(u|v) = h_1(u) - h_1(v) - h_1'(v) \cdot (u - v) = \sum_{i=1}^n u_i \log \frac{u_i}{v_i}$$

Weak–strong uniqueness

$$\partial_t u_i = \operatorname{div}(u_i \nabla p_i(u)), \quad p_i(u) = \sum_{j=1}^n a_{ij} u_j$$

- Relative entropy:
$$h(u|v) = \sum_{i=1}^n u_i \log \frac{u_i}{v_i}$$
- Relative entropy inequality:
$$\begin{aligned}\frac{d}{dt}\int_\Omega h(u|v)dx &= \sum_{i=1}^n \int_\Omega \Big(\partial_t u_i \log \frac{u_i}{v_i} - \partial_t v_i \frac{u_i}{v_i}\Big) dx \\ &= \sum_{i=1}^n \int_\Omega \nabla(p_i(u) - p_i(v)) \cdot \nabla \log \frac{u_i}{v_i} dx \\ &\le \int_\Omega \Big(-\alpha \sum_{i=1}^n |\nabla(u_i - v_i)|^2 + \sum_{i,j=1}^n a_{ij}(u_i - v_i)\nabla \log v_i \cdot \nabla(u_j - v_j)\Big) dx\end{aligned}$$
- Assume that $|\nabla \log v_i|$ bounded, use Young's inequality:
$$\frac{d}{dt}\int_\Omega h(u|v)dx + \frac{\alpha}{2}\int_\Omega |\nabla(u-v)|^2 dx \le C(\alpha, v_i) \int_\Omega |u-v|^2$$

Weak–strong uniqueness

$$\frac{d}{dt}\int_\Omega h(u|v)dx + \frac{\alpha}{2}\int_\Omega |\nabla(u-v)|^2 dx \le C(\alpha, v_i)\int_\Omega |u-v|^2$$

- Estimation of $h(u|v)$: $h(u|v) \ge c(M)|u-v|^2$ only if $u_i \le M$
- If u bounded then Gronwall implies that $\int_\Omega |(u-v)(t)|^2 dx = 0$
- Yields uniqueness of solutions u (bounded weak) and v (strong in the sense $\nabla \log v_i$ bounded)
- Question: Can we avoid boundedness of u? Yes, use Fischer 2017

$$h_L(u|v) = \sum_{i=1}^n \int_\Omega \big(u_i \log u_i - \phi_L(u) u_i \log v_i\big) dx$$

- Cut-off: $\phi_L(u) = 1$ if $\sum_{i=1}^n u_i \le L$, $\phi_L(u) = 0$ if $\sum_{i=1}^n u_i \ge L^K$
- Prove that

$$\frac{d}{dt}\int_\Omega h_L(u|v)dx \le \int_{\{\sum_{i=1}^n u_i \le L\}} |u-v|^2 dx \le C(L^K)\int_\Omega h_L(u|v)dx$$

- Implies that $(u-v)(t) = 0$ in $\{\sum_{i=1}^n u_i \le L\}$, $L \to \infty$: $u = v$ in Ω

Weak–strong uniqueness

$$\partial_t u_i = \mathrm{div}(u_i \nabla p_i(u)), \quad p_i(u) = \sum_{j=1}^n a_{ij} u_j$$

Theorem (Vetter 2024, PhD thesis)

Let u be nonnegative weak solution and v be weak solution such that $v_i, \log v_i \in L^\infty(0,T;W^{1,\infty})$. Then $u = v$ in Ω, $t > 0$.

- Fischer's method originally used for reaction–diffusion systems
- Laurençot–Matioc 2022 need u bounded weak solution
- Weak–strong uniqueness holds true for SKT model under detailed balance (X. Chen–AJ 2019)
- Weak–strong uniqueness holds true for Maxwell–Stefan models (Huo–AJ–Tzavaras 2022)
- Weak–weak uniqueness mainly open for cross-diffusion systems (few simple exceptions)

Large-time asymptotics

$$\partial_t u_i = \mathrm{div}(u_i \nabla p_i(u)), \quad p_i(u) = \sum_{j=1}^n a_{ij} u_j$$

- No-flux boundary conditions: steady state u^∞ is constant
- Relative entropy:
$$h(u|u^\infty) = \sum_{i=1}^n u_i \log \frac{u_i}{u_i^\infty}$$
- Relative entropy inequality: Assume that (a_{ij}) is positive definite
$$\frac{d}{dt}\int_\Omega h(u|u^\infty)dx = -\sum_{i,j=1}^n \int_\Omega a_{ij}\nabla u_i \cdot \nabla u_j dx \le -\alpha \sum_{i=1}^n \int_\Omega |\nabla u_i|^2 dx$$
- Logarithmic Sobolev inequality (Desvillettes–Fellner 2014):
$$-\int_\Omega |\nabla u_i|^2 dx \le -C_L \int_\Omega u_i^2 \log \frac{u_i^2}{\|u_i\|_{L^2}^2} dx \quad \text{if } |\Omega| = 1$$
- However, we cannot relate this to $h(u|u^\infty)$!

Large-time asymptotics

$$\frac{d}{dt}\int_\Omega h(u|u^\infty)dx \le -\alpha\sum_{i=1}^n\int_\Omega|\nabla u_i|^2dx \le -4\alpha\sum_{i=1}^n\int_\Omega u_i|\nabla\sqrt{u_i}|^2dx$$

- Wayout: Assume that u_i is bounded
- Logarithmic Sobolev inequality (if $|\Omega|=1$)

$$-\int_\Omega|\nabla\sqrt{u_i}|^2dx \le -C_L\int_\Omega u_i\log\frac{u_i}{\|u_i\|_{L^1}}dx = -C_L h(u|u^\infty)$$

- Gronwall:

$$\int_\Omega h(u(t)|u^\infty)dx \le h(u(0)|u^\infty)e^{-Ct}, \quad C = C(\alpha, C_L, \|u\|_{L^\infty})$$

- Csiszár–Kullback inequality:

$$\|u(t)-u^\infty\|_{L^1} \le C\int_\Omega h(u(t)|u^\infty)dx \le h(u(0)|u^\infty)e^{-Ct}$$

- Yields exponential decay to steady state with explicit rate
- Open problem: How to remove boundedness assumption

Overview

- Qualitative behavior of solutions
- Nonlocal variants
- Incomplete diffusion

① Nonlocal Busenberg–Travis model

$$\partial_t u_i = \sigma \Delta u_i + \mathrm{div}(u_i \nabla p_i[u]), \quad p_i[u](x) = \sum_{j=1}^n \int_{\mathbb{T}^d} K_{ij}(x-y) u_j(y) dy$$

- Initial conditions, solve in torus $\mathbb{T}^d$, $i = 1, \ldots, n$
- Kernel functions K_{ij}: applications in biology & neuroscience
  - $K_{ij} = a_{ij} K$ with $a_{ij} \in \mathbb{R}$: populations with nonlocal sensing
  - $M_{ij}(x,y) = \nabla K_{ij}(x-y)$: describes weight of neural connection between node x of species i and node y of species j
- Localization limit $K_{ij} \to a_{ij}\delta_0$ yields Busenberg–Travis model
- Assumptions: $K_{ij}(x-y) = K_{ji}(y-x)$ (symmetry) and

$$\sum_{i,j=1}^n \int_{\mathbb{T}^d} \int_{\mathbb{T}^d} K_{ij}(x-y) v_i(x) v_j(y) dx dy \geq 0 \quad \text{(positive definite)}$$

  $\to$ positive definiteness essential in reproducing kernel Hilbert theory
- Example that satisfies assumptions:

$$K_{ij}(x-y) = \frac{a_{ij}}{(2\pi\varepsilon)^{d/2}} \exp\left(-\frac{|x-y|^2}{2\varepsilon^2} \right), \quad (a_{ij}) \text{ positive definite}$$

Entropy structure

$$\partial_t u_i = \sigma\Delta u_i + \operatorname{div}(u_i\nabla p_i[u]), \quad p_i[u](x) = \sum_{j=1}^n \int_{\mathbb{T}^d} K_{ij}(x-y)u_j(y)dy$$

- Entropy densities:

$$h_1(u) = \sum_{i=1}^n u_i(\log u_i - 1)dx$$

$$h_2(u) = \frac{1}{2}\sum_{i,j=1}^n K_{ij}(x-y)u_i(x)u_j(y)dxdy$$

- Entropy inequalities:

$$\frac{d}{dt}\int_\Omega h_1(u)dx + 4\sigma\sum_{i=1}^n\int_{\mathbb{T}^d}|\nabla\sqrt{u_i}|^2dx = -\sum_{i,j=1}^n\int_{\mathbb{T}^d}\int_{\mathbb{T}^d}K_{ij}(x-y)\nabla u_i(x)\cdot\nabla u_j(y)dxdy$$

$$\frac{d}{dt}\int_\Omega h_2(u)dx + \sigma\sum_{i=1}^n\int_{\mathbb{T}^d}u_i|\nabla p_i[u]|^2dx = -\sigma\sum_{i,j=1}^n\int_{\mathbb{T}^d}\int_{\mathbb{T}^d}K_{ij}(x-y)\nabla u_i(x)\cdot\nabla u_j(y)dxdy$$

- $\sigma > 0$ needed to obtain estimate for $\nabla\sqrt{u_i}$
- Yields estimates for $\sqrt{u_i}$ in $L^2(0,T;H^1)$ and $L^\infty(0,T;L^4)$

Existence of global solutions

$$\partial_t u_i = \sigma \Delta u_i + \operatorname{div}(u_i \nabla p_i[u]), \quad p_i[u](x) = \sum_{j=1}^n \int_{\mathbb{T}^d} K_{ij}(x-y) u_j(y) dy$$

- $\sqrt{u_i^\varepsilon}$ bounded in $L^2(0,T;H^1) \cap L^\infty(0,T;L^4) \hookrightarrow L^{2+8/d}$
- $\sqrt{u_i^\varepsilon} \nabla p_i[u^\varepsilon]$ bounded in L^2

Theorem (AJ–Portisch-Zurek 2022)

Let $K_{ij} \in L^{d/2}(\mathbb{T}^d)$ $(d > 2)$ be symmetric and positive definite. Then $\exists$ global nonnegative weak solution.

Proof:

- Compactness: $\sqrt{u_i^\varepsilon} \nabla p_i[u^\varepsilon] \rightharpoonup z_i$ in L^2
- Nonlinear discrete Aubin–Lions: $u_i^\varepsilon \to u_i$ strongly in L^q, $q > 1$
- Implies that $p_i[u^\varepsilon] \to p_i[u]$ a.e.
- Young convolution inequality: $\nabla p_i[u^\varepsilon] \rightharpoonup \nabla p_i[u]$ weakly in L^q, $q > 1$
- Question: How to identify z_i with $\sqrt{u_i} \nabla p_i[u]$?

Identification of weak limit

$$\partial_t u_i = \sigma\Delta u_i + \operatorname{div}(u_i\nabla p_i[u]), \quad p_i[u](x) = \sum_{j=1}^n \int_{\mathbb{T}^d} K_{ij}(x-y)u_j(y)dy$$

Lemma

Let $1 \le q < 2$, $f^\varepsilon \ge 0$, $f^\varepsilon \to f$ strongly in L^q, $g^\varepsilon \rightharpoonup g$ weakly in L^q, $f^\varepsilon g^\varepsilon \rightharpoonup h$ weakly in L^q. Then $h = fg$.

Proof: Truncation for f^ε such that $T_k(f^\varepsilon)g^\varepsilon \rightharpoonup T_k(f)g$ weakly in L^1. Prove that $T_k(f)g = fg$ in $\{|f| \le k\}$. Now $k \to \infty$.

Continuation of proof of existence result:

- $f^\varepsilon = \sqrt{u_i^\varepsilon} \rightharpoonup \sqrt{u_i}$ weakly in L^4, $g^\varepsilon = \nabla p_i[u^\varepsilon] \to \nabla p_i[u]$ weakly in L^q, $f^\varepsilon g^\varepsilon \rightharpoonup z_i$ weakly in L^2
- Apply lemma to conclude that $z_i = \sqrt{u_i}\nabla p_i[u]$
- Perform limit $\varepsilon \to 0$ in approximate problem

Weak–strong uniqueness

$$\partial_t u_i = \sigma \Delta u_i + \operatorname{div}(u_i \nabla p_i[u]), \quad p_i[u](x) = \sum_{j=1}^{n} \int_{\mathbb{T}^d} K_{ij}(x-y)u_j(y)dy$$

Theorem (AJ–Portisch–Zurek 2022)

Let $K_{ij} \in L^\infty(\mathbb{T}^d)$, u weak solution, v "strong" solution with $\log v_i \in L^\infty(0,T;W^{1,\infty}(\mathbb{T}^d))$. Then $u = v$.

Proof: Relative entropy density $h(u|v) = \sum_{i=1}^n u_i \log(u_i/v_i)dx$

- Exploit symmetry and positive definiteness of K_{ij}:

$$\frac{d}{dt}\int_{\mathbb{T}^d} h(u|v)dx \le C(v)\|u-v\|_{L^1}^2$$

- Apply Csiszár–Kullback inequality:

$$\|u-v\|_{L^1}^2 \le C(u(0))\int_{\mathbb{T}^d} h(u|v)dx$$

- Gronwall: $h(u|v)=0$ since $u(0)=v(0) \Rightarrow u(t)=v(t)$ for $t>0$

② Nonlocal Busenberg–Travis model

$$\partial_t u_i - \sigma\Delta u_i + \operatorname{div}(u_i v_i) = u_i f_i(u), \quad -\varepsilon\Delta v_i + v_i = -\nabla p_i(u) \quad \text{in } \Omega$$

- Pressure $p_i(u) = \sum_{j=1}^n a_{ij}u_j$, (a_{ij}) positive definite
- Lotka–Volterra: $f_i(u) = b_{i0} - \sum_{j=1}^n b_{ij}u_j$
- Initial and no-flux boundary conditions for u_i, Dirichlet cond. for v_i
- Brinkman law: regularization of Darcy law $v_i = -\nabla p_i(u)$
- Solution operator $L_\varepsilon(\nabla p_i(u)) = v_i$, square root K_ε $(K_\varepsilon \circ K_\varepsilon = L_\varepsilon)$
- Boltzmann–Shannon entropy density:

$$h_1(u) = \sum_{i=1}^n u_i(\log u_i - 1)$$

- Entropy inequality:

$$\frac{d}{dt}\int_\Omega h_1(u)dx + \int_\Omega 4\sigma\sum_{i=1}^n|\nabla\sqrt{u_i}|^2dx + \sum_{i,j=1}^n\int_\Omega a_{ij}K_\varepsilon(\nabla u_i)\cdot K_\varepsilon(\nabla u_j)dx$$
$$+\sum_{i=1}^n\int_\Omega b_{ii}u_i^2\log u_i dx \le C$$

- Yields L^2 bounds for $\nabla\sqrt{u_i}$ and u_i (if $b_{ii} > 0$)

Entropy structure

$$\partial_t u_i - \sigma\Delta u_i + \operatorname{div}(u_i v_i) = u_i f_i(u), \quad -\varepsilon\Delta v_i + v_i = -\nabla p_i(u) \quad \text{in } \Omega$$

- Nonlocal Rao entropy density:

$$h_2(u) = \sum_{i,j=1}^n \int_\Omega a_{ij} K_\varepsilon(u_i) K_\varepsilon(u_j)dx$$

- Rao entropy inequality not useful for existence analysis:

$$\frac{d}{dt}\int_\Omega h_2(u) + \sigma \sum_{i,j=1}^n a_{ij} K_\varepsilon(\nabla u_i)\cdot K_\varepsilon(\nabla u_j)dx + \sum_{i=1}^n \int_\Omega u_i |\nabla L_\varepsilon(u_i)|^2 dx = (\cdots)$$

Theorem (AJ–Vetter–Portisch 2024)

Let $b_{ii} > 0$, (a_{ij}) pos. def. $\exists$ weak solution u with $v_i \in L^2(0,T; H^1(\Omega))$.

Proof: Regularize $L_\varepsilon^\eta : H^1(\Omega)' \to H^m(\Omega) \hookrightarrow L^\infty(\Omega)$

- Difficulty: $\partial_t u_i^\eta \in L^1(0,T; W^{1,\infty}(\Omega)')$ (not reflexive)
- Helly's selection theorem: $\partial_t u_i^\eta \rightharpoonup \partial_t u_i$ weakly in $\mathcal{M}([0,T]; H^m(\Omega)')$

Boundedness & uniqueness

$$\partial_t u_i - \sigma\Delta u_i + \operatorname{div}(u_i v_i) = u_i f_i(u), \quad -\varepsilon\Delta v_i + v_i = -\nabla p_i(u) \quad \text{in } \Omega$$

Recall $L_\varepsilon(g) = v$ with $-\varepsilon\Delta v + v = g$ in Ω, $v = 0$ on $\partial\Omega$

Theorem (AJ–Vetter–Zurek 2024)

Let $d = 1$. Then $\exists$ bounded weak solution u.

Proof:

- General result for $d = 1$: $g \in L^1(\Omega) \Rightarrow \exists\ v \in W_0^{1,1}(\Omega)$: $-\varepsilon v'' + v = g'$ in Ω, $v = 0$ on $\partial\Omega$
- Apply result for $g = \nabla p_i(u) \in L^1(\Omega) \Rightarrow v_i \in W_0^{1,1}(\Omega) \hookrightarrow L^\infty(\Omega)$
- Alikakos estimate yields $u_i \in L^q(\Omega)$ uniformly in q

Theorem (AJ–Vetter–Zurek 2024)

Let $d = 1$. Then $\exists$ unique bounded weak solution.

Proof: Relative entropy method with nonlocal Rao entropy

Overview

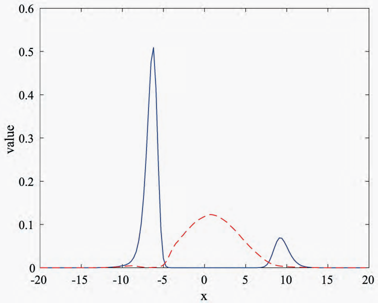
- Qualitative behavior of solutions
- Nonlocal variants
- Incomplete diffusion

Incomplete diffusion

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

- Assume: rank of $(a_{ij}) < n$
- Why bother? Complete segregation possible $(u_1(t)u_2(t) = 0)$

Full rank case



Chen–Daus–Holzinger–AJ 2021

Non full rank case

Bertsch–Dal Passo–Mimura 2010

Finite-volume scheme: Carrillo–Filbet–Schmidtchen 2020

Special rank-one case

$$\partial_t u_1 = \operatorname{div}(u_1 \nabla(u_1+u_2)), \quad \partial_t u_2 = \operatorname{div}(u_2 \nabla(u_1+u_2)) \quad \text{in } \Omega$$

- Key idea: separate hyperbolic & parabolic parts (Bertsch et al. 1985)
- Transform $v_1 = u_1 + u_2$, $v_2 = u_1/(u_1+u_2)$ $\to$ yields porous-medium equation & transport equation with velocity ∇v_1

$$\partial_t v_1 = \tfrac{1}{2}\Delta(v_1^2), \quad \partial_t v_2 - \nabla v_1 \cdot \nabla v_2 = 0$$

- Generalization to $n \geq 2$:

$$\partial_t u_i = \operatorname{div}(u_i \nabla p), \quad p = G(\textstyle\sum_{j=1}^n u_j), \quad G \text{ increasing}$$

- Transform $v_1 = \sum_{j=1}^n u_j$, $v_i = u_i/v_1$, $i = 2, \ldots, n$

$$\partial_t v_1 = \operatorname{div}(v_1 G'(v_1)\nabla v_1), \quad \partial_t v_i - \nabla p \cdot \nabla v_i = 0, \quad i = 2, \ldots, n$$

Theorem (Druet–AJ 2020)

$\sum_{j=1}^n u_j(0) \geq c > 0$, $u_i(0)$ *smooth* $\Rightarrow$ *global classical nonneg. solutions*

Variational splitting & reactions in 1D: Carrillo et al. 2018

General rank-one case (Druet–Hopf–AJ 2023)

$$\partial_t u_i = \operatorname{div}(u_i \nabla p_i(u)), \quad p(u) = \sum_{j=1}^n a_{ij} u_j$$

Rank-one case: (a_{ij}) has rank one

- $a_{ij} = 1$: Carrillo et al. 2018 (BV solutions), Druet–AJ 2020
- $a_{ij} = a_i$: change $v = \Phi(u)$ more involved; set $v' = (v_2, \ldots, v_n)$

$$\partial_t v_1 = \operatorname{div}(A(v)\nabla v_1), \quad \partial_t v' = \nabla v_1 Y(v) \nabla v' + Y_1(v)|\nabla v_1|^2$$

- Explicitly: $v_i = \log(u_i^{1/a_i}/u_1^{1/a_1})$, $i = 2, \ldots, n$
- Symmetrizable hyperbolic part since $\exists A_0(v)$: $A_0(v)Y(v)$ symmetric
- Local existence & uniqueness of strong solutions

General rank-r case: (a_{ij}) has rank $r < n$

- Parabolic in r variables & symmetric hyperbolic in $n - r$ variables
- Local existence of classical solutions

→ Busenberg–Travis system can be written as symmetric hyperbolic–parabolic system if (a_{ij}) has not full rank

Global solutions: motivation

$$\partial_t u_i = \operatorname{div}(u_i \nabla p_i(u)), \quad p_i(u) = \textstyle\sum_{j=1}^n a_{ij} u_j, \quad A = (a_{ij})$$

- Entropy inequality: (P_L : projection onto $L = \operatorname{ran} A$, h_1: Boltzmann entropy)
$$\frac{d}{dt}\int_\Omega h_1(u)dx + \int_\Omega |\nabla(A^{1/2}u)|^2 dx = 0$$
$$\Rightarrow \quad \text{gives } L^2 \text{ bound for } \nabla(P_L u)$$
- Let (u_m) be approximate solutions, $y_m := \nabla(P_L u_m)$
- Weak compactness: $u_m \rightharpoonup u$, $y_m \rightharpoonup y = \nabla(P_L u)$ weakly in L^2
- Aubin–Lions compactness: $P_L u_m \to P_L u$ strongly in L^2
- Problem: limit in $u_m \nabla(A u_m)$
- Key idea: Solve problem in larger space of Young measures
  $(u_m, \nabla u_m)$ generates Young measure $(\mu_{x,t}) \in L^\infty(\Omega \times (0,T); \mathcal{P}(W))$
  $\mathcal{P}(W)$ = probability measures on $W := [0,\infty)^n \times L^d$

Global solutions: existence (Hopf–AJ 2023)

$$\partial_t u_i = \operatorname{div}(u_i \nabla p_i(u)), \quad p_i(u) = \textstyle\sum_{j=1}^n a_{ij} u_j, \quad A = (a_{ij})$$

- Recall $L = \operatorname{ran} A \in \{1, \ldots, n-1\}$, $\mathcal{P}(W)$ probability measures
- Define $\langle \nu, f(s,p) \rangle = \int_W f(s,p) d\nu(s,p)$, $\nu \in \mathcal{P}(W)$, $f \in C_0(W)$

Dissipative measure-valued solution: $\mu \in L^\infty_w(\Omega \times [0,\infty); \mathcal{P}(W))$ with

- $u_i := \langle \mu, s_i \rangle \in L^\infty(0,T; L^2(\Omega))$, $y := \nabla(P_L u) \in L^2(\Omega \times (0,T); L^d)$
- Weak formulation: for $\phi \in C_0^1(\overline{\Omega} \times [0,T))$

$$\int_0^T \int_\Omega u_i \partial_t \phi dx dt + \int_\Omega u_i(0)\phi(0) dx = \int_0^T \int_\Omega \langle \mu_{x,t}, s_i (Ap)_i \rangle \cdot \nabla \phi dx dt$$

entropy ineq. $$\frac{d}{dt}\int_\Omega \langle \mu_{x,t}, \underbrace{h_1(s)}_{\text{Boltzmann}} \rangle dx + \int_\Omega \langle \mu_{x,t}, |A^{1/2}p|^2 \rangle dx \le 0$$

$$\frac{d}{dt}\int_\Omega \underbrace{h_2(u)}_{\text{Rao}} dx + \int_\Omega \sum_{i=1}^n \langle \mu_{x,t}, s_i |(Ap)_i|^2 \rangle dx \le 0$$

Global solutions: proof & further results

$$\partial_t u_i = \operatorname{div}(u_i \nabla p_i(u)), \quad p_i(u) = \textstyle\sum_{j=1}^n a_{ij} u_j, \quad 1 \le \operatorname{ran} A < n$$

- Implicit Euler finite-volume scheme: flux discretized by upwind scheme & artificial diff. $\eta^\alpha \nabla^\eta u_i$, where $\eta = \max\{\Delta x, \Delta t\}$, $0 < \alpha < 2$
- Artificial diffusion needed for η-dependent bound for gradient
- Existence of finite-volume solutions u_m: fixed-point theorem
- Convergence: $(u_m, \nabla^\eta(P_L u_m))$ generates Young measure μ

Theorem (Weak–strong uniqueness)

Let μ be dissipative measure-valued solution & v be positive weak solution. Then $\mu_{x,t} = \delta_{v(x,t)} \otimes \delta_{\nabla P_L v(x,t)}$ a.e.

Theorem (Long-time behavior)

$\exists\ u^* \in L^2$, $\int_\Omega u^* dx = m$, $\nabla(Au^*) = 0$ *such that*

$$P_L u(t) \to P_L u^* \quad \text{strongly in } L^2(\Omega) \text{ as } t \to \infty$$

Overview

1. Introduction
2. Derivation of population models
3. Analysis of cross-diffusion systems
4. More about the Busenberg–Travis model
5. Numerical approximation
    - Time discretization: implicit Euler and BFD2
    - Space discretization: finite-volume method

Motivation

Aim: Derive structure-preserving numerical schemes

Entropy inequality: Use test function $h'(u)$ in weak formulation of $\partial_t u = \mathrm{div}(A(u)\nabla u)$:

$$\int_\Omega \underbrace{\partial_t u \cdot h'(u)}_{=\partial_t h(u)} dx + \int_\Omega \underbrace{\nabla h'(u)^T}_{=\nabla u^T h''(u)} A(u)\nabla u dx = 0$$

Aim: Translate the chain rules $\partial_t h(u) = \partial_t u \cdot h'(u)$ and $\nabla h(u) = h''(u)\nabla u$ to the discrete level

Implicit Euler & BDF2 methods

$$\partial_t u - \mathrm{div}(A(u)\nabla u) = 0 \quad \text{in } \Omega, \quad \text{no-flux boundary conditions}$$

Implicit Euler method: (also used in existence analysis)

$$\frac{1}{\Delta t}(u^k - u^{k-1}) = \mathrm{div}(A(u^k)\nabla u^k), \quad u^k \approx u(k\Delta t)$$

- Test function $h'(u^k)$:
$$(u^k - u^{k-1}) \cdot h'(u^k) \geq h(u^k) - h(u^{k-1}) \quad \text{if } h \text{ convex}$$
- Discrete entropy inequality:
$$\frac{1}{\Delta t}\int_\Omega (h(u^k) - h(u^{k-1}))dx + \int_\Omega \nabla u^T h''(u)A(u)\nabla u dx \leq 0$$

Higher-order discretization: BDF2 = Backward Differential Formula

$$\frac{1}{\Delta t}\left(\frac{3}{2}u^k - 2u^{k-1} + \frac{1}{2}u^{k-1}\right) = \mathrm{div}(A(u^k)\nabla u^k)$$

Problem: $h(u^k) - h(u^{k-1}) \not\leq (\frac{2}{3}u^k - 2u^{k-1} + \frac{1}{2}u^{k-1}) \cdot h'(u^k)$

BDF2 method: single-species case

$$\frac{1}{\Delta t}\left(\frac{3}{2}u^k - 2u^{k-1} + \frac{1}{2}u^{k-1}\right) = \operatorname{div}(A(u^k)\nabla u^k)$$

- Assume: entropy density $h(u) = \sum_{i=1}^n u_i^\alpha$, $\alpha > 1$
- Use "magic" inequality:

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

- Modify entropy density: $h(u^k, u^{k-1}) = \frac{1}{2}((u^k)^\alpha + (2u^k - u^{k-1})^\alpha)$

$$\frac{1}{\Delta t}\int_\Omega \left(h(u^k, u^{k-1}) - h(u^{k-1}, u^{k-2})\right)dx + \int_\Omega h''(u)A(u)|\nabla u|^2 dx = 0$$

- Logic behind "magic" inequality: scheme is G-stable if $\exists$ positive definite matrix G (Dahlquist 1978)

$$a^2 + (2a-b)^2 = \begin{pmatrix} a \\ b \end{pmatrix}^T \begin{pmatrix} 5 & -2 \\ -2 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} =: \begin{pmatrix} a \\ b \end{pmatrix}^T G \begin{pmatrix} a \\ b \end{pmatrix}$$

- References: Hill 1987, Bukal–Emmrich–AJ 2014, AJ–Milišić 2015

BDF2 method: multi-species case

$$\frac{1}{\Delta t}\left(\frac{3}{2}u_i^k - 2u_i^{k-1} + \frac{1}{2}u_i^{k-1}\right) = \operatorname{div}(u_i^k \nabla p_i(u^k)), \quad p_i(u^k) = \sum_{j=1}^n a_{ij}u_j$$

- Assume $A := (a_{ij})$ positive definite
- Discrete Rao entropy density: $h(u,v) = \frac{1}{4}(5u^TAu - 4u^TAv + v^TAv)$
- "Magic" inequality:

$$\sum_{i=1}^n \left(\frac{3}{2}u_i^k - 2u_i^{k-1} + \frac{1}{2}u_i^{k-1}\right)p_i(u^k) \geq h(u^k, u^{k-1}) - h(u^{k-1}, u^{k-2})$$

- Discrete Rao entropy inequality:

$$\int_\Omega h(u^k, u^{k-1})dx + c\int_\Omega |\nabla u^k|^2 dx \leq \int_\Omega h(u^{k-1}, u^{k-2})dx$$

- Existence of semidiscrete solutions & convergence
- Generalization to BDF2 finite-volume scheme: AJ–Vetter 2024
- Open problems: BFD2 scheme preserving Boltzmann entropy structure, Runge–Kutta methods, ...

Overview

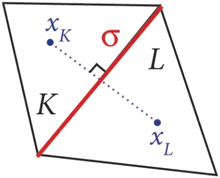
- Time discretization
- Space discretization

Finite-volume method: scalar equation

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

Admissible mesh:

- $\Omega = \cup_{K\in\mathcal{T}} K$, K: polygonal control volume
- $\mathcal{E}$ = family of edges σ, $\mathcal{E}_K$ = edges of K
- Family of points $(x_K)_{K\in\mathcal{T}}$ such that $\overline{x_K x_L}$ orthogonal to $\sigma = K|L$ (e.g. Voronoï mesh)



Idea of method: integrate over K and integrate by parts

$$\partial_t \int_K u dx - \int_\sigma \underbrace{A(u)\nabla u}_{=-F} \cdot \nu ds = \int_K f(u) dx$$

- Def. $u_K^k \approx \mathrm{m}(K)^{-1} \int_K u(x, k\Delta t) dx$, $F_{K,\sigma}^k \approx -\mathrm{m}(\sigma)^{-1} \int_\sigma F \cdot \nu ds$
- Numerical scheme: implicit Euler in time & finite-volume in space

$$\mathrm{m}(K)\frac{u_K^k - u_K^{k-1}}{\Delta t} + \sum_{\sigma\in\mathcal{E}_K} F_{K,\sigma}^k = \mathrm{m}(K) f(u_K^k)$$

Numerical flux: scalar equation

$$\mathrm{m}(K)\frac{u_K^k - u_K^{k-1}}{\Delta t} + \sum_{\sigma\in\mathcal{E}_K} F_{K,\sigma}^k = \mathrm{m}(K) f(u_K^k)$$

Definitions and assumption:

- Distance: $\mathrm{d}_\sigma = \mathrm{dist}(x_K, x_L)$ if $\sigma = K|L$, $\mathrm{d}_\sigma = \mathrm{dist}(x_K,\sigma)$ if $\sigma\subset\partial\Omega$
- Mesh regularity: $\exists\zeta>0$, $\forall K\in\mathcal{T}$, $\sigma\in\mathcal{E}_K$: $\mathrm{dist}(x_K,\sigma)\ge\zeta\mathrm{d}_\sigma$
- Difference: $\mathrm{D}_{K,\sigma}u := u_L - u_K$ if $\sigma = K|L$ and $\mathrm{D}_{K,\sigma}u := 0$ if $\sigma\subset\partial\Omega$

$$F_{K,\sigma}^k = -\tau_\sigma A(\widetilde{u}_\sigma^k)\mathrm{D}_{K,\sigma}u^k, \quad \tau_\sigma := \frac{\mathrm{m}(\sigma)}{\mathrm{d}_\sigma}$$

Entropy inequality: $h(u) = u(\log u - 1)$

- Test function $h'(u)$ translates to $\mathrm{D}_{\sigma,K}\log u^k = \log u_L^k - \log u_K^k$

$$\frac{\mathrm{m}(K)}{\Delta t}\underbrace{(u_K^k - u_K^{k-1})(\log u_L^k - \log u_K^k)}_{\ge h(u_K^k)-h(u_K^{k-1})} + \sum_{\sigma\in\mathcal{E}_K}\underbrace{F_{K,\sigma}^k\mathrm{D}_{\sigma,K}\log u^k}_{\ge ???}$$
$$= \mathrm{m}(K)f(u_K^k)\mathrm{D}_{\sigma,K}\log u^k \le C$$

Discrete chain rule: scalar equation

$$\frac{\mathrm{m}(K)}{\Delta t}\big(h(u_K^k) - h(u_K^{k-1})\big) + \sum_{\sigma\in\mathcal{E}_K} F_{K,\sigma}^k \mathrm{D}_{\sigma,K}\log u^k \le C$$
$$F_{K,\sigma}^k = -\tau_\sigma A(\widetilde{u}_\sigma^k)\mathrm{D}_{K,\sigma}u^k$$

Goal: Define $\widetilde{u}_\sigma^k$ such that discrete chain rule holds $(h''(u)\nabla u = \nabla h'(u))$

- Logarithmic mean $\widetilde{u}_\sigma^k = \frac{u_L^k - u_K^k}{\log u_L^k - \log u_K^k}$ $\Leftrightarrow$ $h''(\widetilde{u}_\sigma^k)\mathrm{D}_{K,\sigma}u^k = \mathrm{D}_{K,\sigma}h'(u^k)$
- Numerical flux:

$$\begin{aligned} F_{K,\sigma}\mathrm{D}_{\sigma,K}\log u^k &= -\tau_\sigma A(\widetilde{u}_\sigma^k)(u_L^k - u_K^k)(\log u_L^k - \log u_K^k) \\ &= -\tau_\sigma A(\widetilde{u}_\sigma^k)(u_L^k - u_K^k)^2\frac{1}{\widetilde{u}_\sigma^k} \\ &= -\tau_\sigma A(\widetilde{u}_\sigma^k)h''(\widetilde{u}_\sigma^k)(u_L^k - u_K^k)^2 \le 0 \end{aligned}$$

- If $f(u) = 0$: $h(u_K^k) \le h(u_K^{k-1}) \to$ discrete entropy structure
- Aim: discrete chain rule for cross-diffusion systems

Finite-volume scheme for systems

$$\mathrm{m}(K)\frac{u_{i,K}^k - u_{i,K}^{k-1}}{\Delta t} + \sum_{\sigma\in\mathcal{E}_K} F_{i,K,\sigma}^k = \mathrm{m}(K) f_i(u_K^k)$$

$$F_{i,K,\sigma}^k = -\sum_{j=1}^n \tau_\sigma A_{ij}(\widetilde{u}_\sigma^k)\mathrm{D}_{K,\sigma} u_j^k, \quad i = 1,\ldots,n$$

Assumption: h'' invertible, $h(u) = \sum_{i=1}^n h_i(u_i)$

- Implies that $h'' = \mathrm{diag}(h_1''(u_1),\ldots,h_n''(u_n))$ is diagonal matrix
- Define $\widetilde{u}_{i,K}^\sigma$ by $h_i''(\widetilde{u}_{i,\sigma}^k)\mathrm{D}_{K,\sigma} u_i^k = \mathrm{D}_{K,\sigma} h_i'(u_i^k)$
- Entropy production:

$$\sum_{i=1}^n F_{i,K,\sigma}^k \mathrm{D}_{K,\sigma} h_i'(u_i^k) = -\sum_{i,j=1}^n \tau_\sigma \underbrace{\mathrm{D}_{K,\sigma} h_i'(u_i^k)}_{=h_i''(\widetilde{u}_{i,\sigma}^k)\mathrm{D}_{K,\sigma} u_i^k} A_{ij}(\widetilde{u}_\sigma^k)\mathrm{D}_{K,\sigma} u_j^k$$

$$= -\sum_{i,j=1}^n \tau_\sigma \underbrace{h_i''(\widetilde{u}_{i,\sigma}^k) A_{ij}(\widetilde{u}_\sigma^k)}_{\text{positive semidefinite}} \mathrm{D}_{K,\sigma} u_i^k \mathrm{D}_{K,\sigma} u_j^k \le 0$$

SKT model: existence of discrete solutions

- Diffusion matrix and Hessian of Boltzmann entropy density:

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

$$\Rightarrow \quad \nabla u^T h''(u)A(u)\nabla u \geq a_{11}a_{21}|\nabla u_1|^2 + a_{22}a_{12}|\nabla u_2|^2$$

- Discrete gradient estimate: gives discrete $H^1(\Omega)$ estimate for u_i^k

Theorem (AJ–Zurek, SINUM 2021)

Let $a_{ii} > 0$ for $i = 1,2$, $f(u)\cdot h'(u) \leq C_f(1+h(u))$, and $\Delta t < 1/C_f$. Then $\exists\ u_{i,K}^k \geq 0$ satisfying discrete entropy inequality

$$(1 - C_f\Delta t)H(u^k) + C\Delta t \sum_{i=1}^n \sum_{\sigma\in\mathcal{E}} \tau_\sigma (\mathrm{D}_{K,\sigma}u_i^k)^2 \leq H(u^{k-1}) + C\Delta t$$

- Discrete entropy: $H(u^k) = \sum_{i=1}^2 \sum_{K\in\mathcal{T}} \mathrm{m}(K)u_{i,K}(\log u_{i,K}^k - 1)$
- Scheme preserves positivity, mass, and entropy structure

Population model: convergence of the scheme

Theorem (AJ–Zurek, SINUM 2021)

If (u_m) solves scheme with Δx_m, $\Delta t_m \to 0$ then, for a subsequence,

$$u_{i,m} \to u \quad \text{in } L^2, \quad \nabla^m u_{i,m} \rightharpoonup \nabla u \quad \text{in } L^2,$$

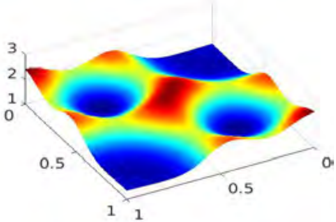
where u solves the population model and ∇^m is the approximate gradient (defined on dual mesh).

Ideas of proof:

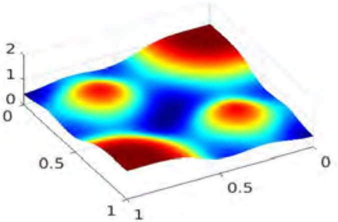
- Discrete entropy inequality gives uniform bounds in (discrete) $L^\infty(0,T;L^1(\Omega))$ and $L^2(0,T;H^1(\Omega))$
- Gagliardo–Nirenberg inequality gives uniform bound in $L^3(\Omega \times (0,T))$
- Discrete time derivative in (discrete) $L^1(0,T;W^{1,6}(\Omega)')$
- Apply discrete Aubin–Lions lemma by Gallouët & Latché 2012
- Limit $m \to \infty$: estimate for $(A_{ij}(\widetilde{u}_\sigma^k) - A_{ij}(u_K^k))\mathrm{D}_{K,\sigma} u_j^k$ delicate, exploit linearity of $A_{ij}(u)$

Numerical experiments

- 3584 triangles, Newton method, time-adaptive strategy
- Spatial pattern formation in two-species model (steady state)

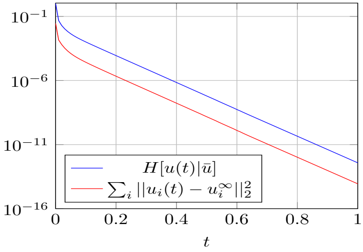


u_1



u_2

- Convergence to constant steady state for three-species model
- $H(u^k|\bar{u})$ = relative log. entropy, $\bar{u}$ = constant steady state
- Exponential decay of H and L^2-norm



Intermediate summary

Derivation of discrete entropy inequality possible if …

… implicit Euler scheme for convex entropies

… BDF2 method for Rao-type entropies

… finite-volume method for entropy densities $h(u) = \sum_{i=1}^n h_i(u_i)$

Generalization to size-exclusion models possible (AJ–Zurek 2023)

Generalization to general cross-diffusion systems open

Summary & open problems

Summary:

- Derivation of population systems from lattice models, fluid mixture models, and interacting particle systems
- Global existence analysis relies on entropy structure
- Boundedness-by-entropy method yields bounded weak solutions
- Analysis of (local and nonlocal) Busenberg–Travis systems
- Numerical analysis relies on discrete entropy inequality, which relies on discrete chain rule

Some open problems:

- Derivation of cross-diffusion systems from kinetic equations
- Classify matrix sets *positively stable*, *entropy structure*, *pos. def.*
- Stochastic cross-diffusion systems: derivation, space-time noise
- Higher-order time and space discretizations, general chain rule

Thank you!

Adobe Firefly: A mathematician's viewpoint at the Calanques