Dynamical cross-diffusion systems: modeling, analysis, numerics

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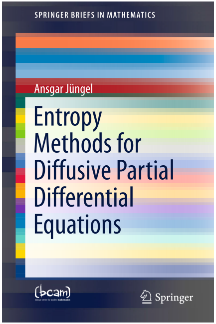
Literature

Main reference

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



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- A. Jüngel. Mathematische Modellierung mit Differentialgleichungen. Lecture Notes, 2003. https://www.asc.tuwien.ac.at/∼juengel
- E. Hairer, G. Wanner. Solving Ordinary Differential Equations I & II. Springer, 1993 & 1996.
- A. Jüngel. Cross-diffusion systems with entropy structure. *Proceedings of Equadiff 2017*, Bratislava, pp. 181-190.

What do I need to know?

Required:

- Linear algebra: matrices, eigenvalues
- Ordinary differential equations
- Analysis in $\mathbb{R}^d$: gradient, divergence theorem, Fourier analysis

Optional:

- Functional analysis: Hilbert spaces
- Partial differential equations: heat equation, Sobolev spaces
- Numerical analysis: differential equations, finite differences

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Most of these tools will be introduced during the lecture

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!

Mathematics: modeling → analysis → numerics → simulations

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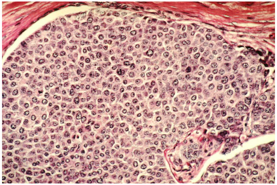
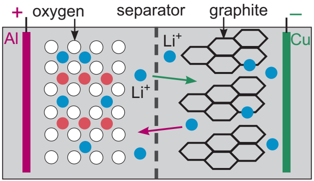


Image: Dr. Cecil Fox



How to model multi-species systems?

Microscopic models:

- Discrete-time Markov chains: $u_i(t_k)$ probability distribution at cell i

$$u_i(t_{k+1}) = \sum_{j=1}^N u_j(t_k)P_{ji}, \quad P_{ji} = \text{probability } j \to i, \quad \sum_{j=1}^N P_{ij} = 1$$

$$\Leftrightarrow \quad u_i(t_{k+1}) - u_i(t_k) = \sum_{j=1}^N \big(u_j(t_k)P_{ji} - u_i(t_k)P_{ij}\big)$$

$\to$ matrix-vector multiplication

- Time-continuous Markov chains: divide by $\triangle t$, replace $P_{ij} \to \triangle t P_{ij}$, and perform limit $\triangle t \to 0$:

$$\frac{du_i}{dt}(t) = \sum_{j=1}^N \big(u_j(t)P_{ji} - u_i(t)P_{ij}\big), \quad t > 0, \; i = 1, \ldots, N$$

$\to$ system of N differential equations

- Particle models: Newton's law for position of ith particle with mass

How to model multi-species systems?

Macroscopic models:

- Stochastic differential equations: $W_i(t)$ Brownian motion

$$u_i(t) - u_i(0) = \int_0^t \underbrace{F_i(u(s), s)ds}_{\text{Lebesgue integral}} + \int_0^t \underbrace{\sigma(u(s))dW_i(s)}_{\text{Itô integral}}, \quad i = 1, \dots, N$$

- Kinetic equations: distribution function $f(x, p, t)$ depends on (x, t) and trait parameter p (like age, size, maturity)

$$\frac{\partial f_i}{\partial t} + \underbrace{p \cdot \nabla_x f_i}_{\text{transport}} = \underbrace{Q(f)}_{\text{collisions}}, \quad i = 1, \dots, N$$

- Diffusive equations: deterministic dynamics for particle densities

$$\frac{\partial u_i}{\partial t} - \underbrace{\Delta u_i}_{\text{diffusion}} = \underbrace{f_i(u, t)}_{\text{reactions}}, \quad i = 1, \dots, N$$

$\rightarrow$ partial differential equations

History of population dynamics

Exponential growth: Malthus 1798

- Discrete: $u(t_{k+1}) = u(t_k) + \lambda \triangle t u(t_k)$, growth rate λ

$$\frac{1}{\triangle t}(u(t_{k+1}) - u(t_k)) = \lambda u(t_k), \quad \triangle t \to 0 : \quad u'(t) = \lambda u(t)$$

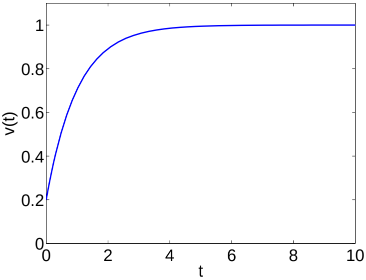
- Solution: $u(t) = u(0)e^{\lambda t}$, unrealistic for large times

Logistic growth: Verhulst 1838

- Carrying capacity $\kappa > 0$:

$$u' = \lambda u\left(1 - \frac{u}{\kappa}\right), \quad u(0) = u_0$$

- Solution: $u(t) = \frac{u_0 \kappa}{u_0 + (\kappa - u_0)e^{-\lambda t}}$, $t > 0$
- Large times $t \to \infty$: $u(t) \to \kappa$



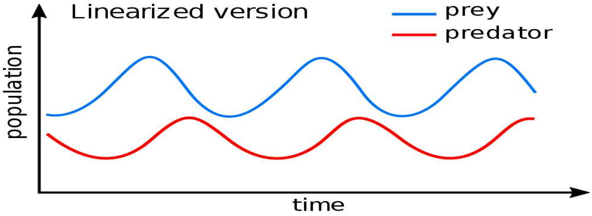
History of population dynamics

Predator-prey model: Lotka-Volterra 1925/26

- Number of preys: u_1 (e.g. rabbits), predators: u_2 (e.g. foxes)
- Equations:

$$u_1' = u_1(b_{10} - b_{12}u_2) = \text{exponential growth} - \text{predation}$$
$$u_2' = u_2(b_{21}u_1 - b_{20}) = \text{growth depending on preys} - \text{death rate}$$

- Solutions are periodic in time



Goal:
Include spatial effects (diffusion)

© AspidistraK, Lotka Volterra dynamics.svg

History of population dynamics

Fisher-Kolmorov model: (1937)

- Assume: temporal change = spatial diffusion + logistic growth
- Diffusion: net movement of particles from higher to lower concentration region (derivation below)
- Equation: population density $u(x,t)$, $\Delta u = \sum_{i=1}^{d} \frac{\partial^2 u}{\partial x_i^2}$

$$\partial_t u = \Delta u + u(1-u), \quad t > 0$$

- Large times: competition between diffusion $u(t) \to 0$ and reaction $u(x,t) \to 1$ (carrying capacity)
- Traveling-wave solutions: insert ansatz $u(x,t) = v(x-ct)$

$$v'(z) - v''(z) = v(z)(1-v(z)), \quad z = x - ct$$

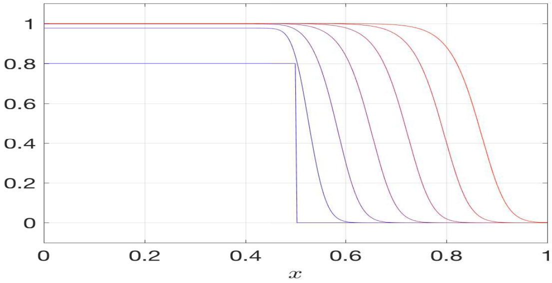
gives second-order differential equation
- There exist solutions $v(z)$ with $\lim_{z\to-\infty} v(z) = 0$, $\lim_{z\to\infty} v(z) = 1$ if $c \geq 2$

History of population dynamics

Fisher-Kolmorov model:

$$\partial_t u = \Delta u + u(1-u), \quad t > 0$$

- There exist solutions $v(z)$ with $\lim_{z\to-\infty} v(z) = 0$, $\lim_{z\to\infty} v(z) = 1$ if $c \geq 2$
- Interpretation: solution $u(x,t) = v(x-ct)$ switches from equilibrium state $u = 0$ to equilibrium state $u = 1$

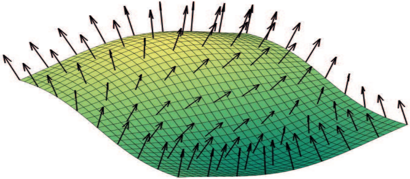


Bonizzoni-Braukhoff-A.J.-Perugia 2019

Elements of analysis

- Let $\Omega \subset \mathbb{R}^d$ be a bounded domain with smooth boundary, let $u : \Omega \to \mathbb{R}$ be "smooth"
- Gradient: $\nabla u = (\frac{\partial u}{\partial x_1}, \ldots, \frac{\partial u}{\partial x_d})^\top$
- Divergence: $\operatorname{div} v = \sum_{i=1}^n \frac{\partial v_i}{\partial x_i}$ for $v = (v_1, \ldots, v_n) : \Omega \to \mathbb{R}^n$
- Laplace-Operator: $\Delta u = \operatorname{div} \nabla u = \sum_{i=1}^n \frac{\partial^2 u}{\partial x_i^2}$
- Divergence theorem: let u, $v \in C^2(\Omega) \cap C^0(\overline{\Omega})$, ν: exterior unit normal vector to $\partial\Omega$

$$\int_\Omega \Delta u v dx = -\int_\Omega \nabla u \cdot \nabla v dx + \int_{\partial\Omega} (\nabla u \cdot \nu) v ds$$



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Partial differential equations:

- The equation

$$f\big(\partial_t u, \partial_x u, \partial_y u, \partial_{xx} u, \partial_{yy} u, \partial_{xxy} u, \ldots\big) = 0$$

  is called a partial differential equation
- Initial condition needed to determine constant from integrating $\partial_t u$
- Boundary conditions needed to determine constants from $\partial_x u$, etc.

Parabolic equations:

- The equation

$$\partial_t u - \sum_{i,j=1}^{d} a_{ij}(x,t,u,\nabla u)\frac{\partial^2 u}{\partial x_i \partial x_j} = f(x,t,u,\nabla u)$$

  is parabolic if $A = (a_{ij})$ is symmetric & has only positive eigenvalues, i.e. if A is symmetric and positive definite
- Special case:

$$\partial_t u = \Delta u \quad \Rightarrow \quad A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ has one eigenvalue } \lambda = 1 > 0$$

Diffusion equation

$$\partial_t u = \Delta u \quad \text{in } \Omega,\ t > 0, \quad u(0) = u_0, \quad u = 0 \quad \text{on } \partial\Omega$$

How to solve this equation?

- Orthonormal basis (v_i) of eigenvectors of $-\Delta v_i = \lambda_i v_i$ in Ω, $v_i = 0$ on $\partial\Omega$ (existence guaranteed by spectral theorem)
- Fourier analysis: $u = \sum_{i=1}^\infty (u, v_i)v_i$, $(u, v_i) = \int_\Omega u v_i dx$
- Multiply equation by v_i, integrate over Ω, and integrate by parts

$$\partial_t(u, v_i) = (\Delta u, v_i) = (u, \Delta v_i) = -\lambda_i(u, v_i)$$

- Fourier coefficient $a_i(t) = (u(t), v_i)$ solves differential equation

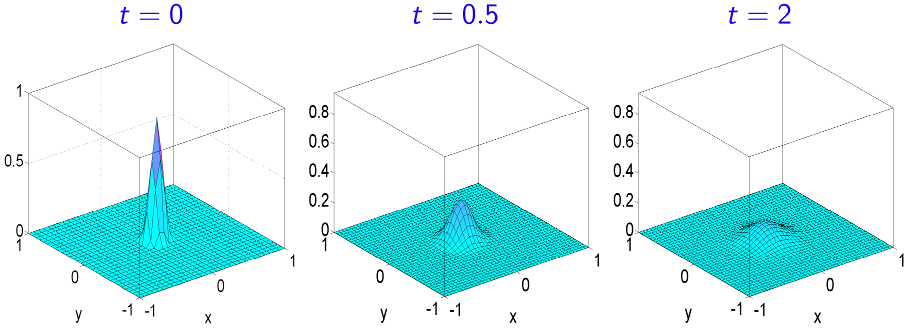
$$\partial_t a_i = -\lambda_i a_i \quad \Rightarrow \quad a_i(t) = e^{-\lambda_i t} a_i(0)$$

- Solution:

$$u(x, t) = \sum_{i=1}^\infty a_i(t) v_i(x) = \sum_{i=1}^\infty e^{-\lambda_i t}(u_0, v_i) v_i(x)$$

Diffusion equation

$$\partial_t u = \Delta u \quad \text{in } \Omega, \qquad u(0) = u_0, \qquad u = 0 \quad \text{on } \partial\Omega$$



Boundary conditions:

- Dirichlet condition: $u = 0$ on $\partial\Omega$, fixes values on boundary
- Neumann (no-flux) condition: $\nabla u \cdot \nu = 0$ on $\partial\Omega$, no outflow (ν: exterior unit vector on $\partial\Omega$)
- Robin condition: $\nabla u \cdot \nu + \alpha u = \beta$ on $\partial\Omega$

Overview

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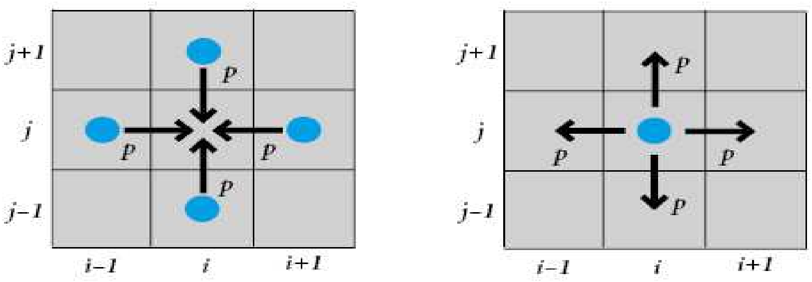
Derivation from lattice model: single species

- 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: $\partial_x u_{ij} = \frac{\partial u}{\partial x}(x_i, y_j)$, $\partial_{xx} u_{ij} = \frac{\partial^2 u}{\partial x^2}(x_i, x_j)$ etc.
- Taylor approximation of $u_{i\pm 1,j} = u(x_i \pm \eta, y_j)$, y_j fixed

$$
\begin{aligned}
u_{i+1,j} &= u_{ij} + \eta\partial_x u_{ij} + \tfrac{\eta^2}{2}\partial_{xx} u_{ij} + R_3(\eta) \\
u_{i-1,j} &= u_{ij} - \eta\partial_x u_{ij} + \tfrac{\eta^2}{2}\partial_{xx} u_{ij} + R_3(\eta) \\
\hline
\text{sum:}\quad u_{i+1,j} - 2u_{ij} + u_{i-1,j} &= \eta^2\partial_{xx} u_{ij} + R_3(\eta)
\end{aligned}
$$

- Taylor approximation of $u_{i,j\pm 1} = u(x_i, y_j \pm \eta)$, x_i fixed

$$u_{i,j+1} - 2u_{ij} + u_{i,j-1} = \eta^2\partial_{yy} u_{ij} + R_3(\eta)$$

- Master equation:

$$
\begin{aligned}
\frac{d}{dt} u_{ij} &= p(u_{i+1,j} - 2u_{ij} + u_{i-1,j}) + p(u_{i,j+1} - 2u_{ij} + u_{i,j-1}) \\
&= \eta^2 p\partial_{xx} u_{ij} + \eta^2 p\partial_{yy} u_{ij} + 2R_3(\eta) = \eta^2 p\Delta u_{ij} + 2R_3(\eta)
\end{aligned}
$$

Diffusion limit

$$\frac{d}{dt}u_{ij} = \eta^2 p\Delta u_{ij} + 2R_3(\eta), \quad \lim_{\eta\to 0} R_3(\eta)/\eta^2 = 0$$

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

$$\frac{d}{dt}u_{ij} = p\Delta u_{ij} + 2R_3(v)/\eta^2, \quad \lim_{h\to 0} R_3(\eta)/\eta^2 = 0$$

- Diffusion limit $\eta \to 0$:

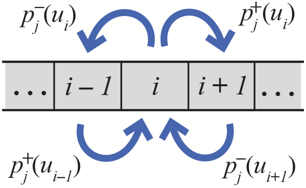
$$\partial_t u(x,y,t) = \Delta u(x,y,t) := \partial_{xx}u(x,y,t) + \partial_{yy}u(x,y,t)$$

- To be solved in bounded domain $\Omega \subset \mathbb{R}^2$
- Initial conditions: $u(x,y,0) = u_0(x,y)$ in Ω
- Boundary conditions: for instance $u(x,y,t) = 0$ on $\partial\Omega$

Derivation from lattice model: 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-A.J., *Ann. IHP* 2017)

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

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

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

- Multi-dimensional case analogous: $\partial_t u_i = \Delta(u_i p_i(u))$

Cross-diffusion systems

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

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

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

$\rightarrow$ not symmetric, not positive definite

General cross-diffusion systems: $\partial_t u - \mathrm{div}(A(u)\nabla u) = f$, i.e.

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

$\rightarrow$ nonlinear diffusion matrix $A(u)$, thus Fourier method does not apply!

Parabolicity: We call cross-diffusion system parabolic in the sense of Petrovskii if the real parts of all eigenvalues of $A(u)$ are positive.

Example: eigenvalues of $A(u)$ are $\lambda_{1/2} \geq (a_{10} + a_{20})/2 > 0$

Cross-diffusion systems

$$\partial_t u - \operatorname{div}(A(u)\nabla u) = f, \quad u = (u_1, \ldots, u_n)$$

Special cases:

- $A(u) =$ unit matrix: $\partial_t u_i - \Delta u_i = 0 \to$ (decoupled) diffusion eqs.
- $A(u) = \operatorname{diag}(a_1, \ldots, a_n)$:

$$\partial_t u_i - \operatorname{div}(a_i \nabla u_i) = f_i \quad \to \quad \text{reaction-diffusion equations}$$

- $A(u) =$ upper triangular matrix:

$$\begin{aligned} \partial_t u_n - \operatorname{div}(a_n \nabla u_n) &= f_n \quad \to \quad \text{gives solution } u_n \\ \partial_t u_{n-1} - \operatorname{div}(a_{n-1}\nabla u_{n-1} + a_n \nabla u_n) &= f_{n-1} \quad \to \quad \text{gives solution } u_{n-1} \\ &\vdots \\ \partial_t u_1 - \operatorname{div}(a_1 \nabla u_1 + \cdots + a_n \nabla u_n) &= f_1 \quad \to \quad \text{gives solution } u_1 \end{aligned}$$

- $A(u) =$ full matrix: full cross-diffusion system

Derivation from fluid 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
- Force term: $f_i = \sum_{j=1}^n k_{ij} u_i u_j (v_j - v_i)$
- Mass balance: by divergence theorem $\partial_t \int_{\mathbb{R}^d} u_i dx = 0$
  $\Rightarrow$ mass $\int_\Omega u_i(t) dx$ conserved for all time
- Momentum balance: $\varepsilon \ll 1$ means small inertia effects

Example 1: $\varepsilon = 0$ and $S_i = u_i p_i(u)$, nonlinear pressure p_i
Simplification: $k_{ij} = 1$ gives $\sum_{j=1}^n k_{ij} u_i u_j (v_j - v_i) = -u_i v_i$

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

Derivation from fluid 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: $\varepsilon = 0$ and $S_i = u_i$, $\sum_{i=1}^n u_i = 1$, $\sum_{j=1}^n u_i v_i = 0$

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

$\to$ Maxwell-Stefan diffusion system

- Problem: $\sum_{i=1}^n \nabla u_i = 0$, 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

❶ Population model of Shigesada-Kawasaki-Teramoto

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

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

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

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

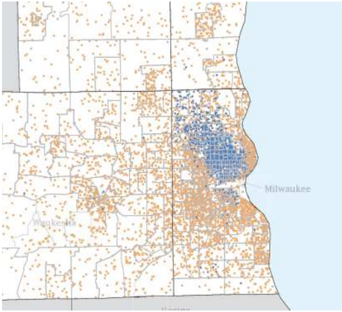


Figure: Black residential segregation in Milwaukee (blue dots) US Census Bureau 2002

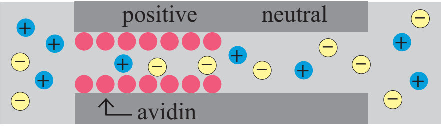
❷ Ion transport through membranes

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

- 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 $n=4$:

$$A(u) = \begin{pmatrix} D_1(1-u_2-u_3) & D_1u_1 & D_1u_1 \\ D_2u_2 & D_2(1-u_1-u_3) & D_2u_2 \\ D_3u_3 & D_3u_3 & D_3(1-u_2-u_3) \end{pmatrix}$$

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



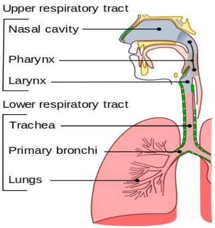
❸ Multicomponent gas mixtures

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

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

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

- Application: Patients with airway obstruction inhale Heliox to speed up diffusion
- Proposed by Maxwell 1866/Stefan 1871
- Duncan-Toor 1962: Fick's law ($J_i \sim \nabla u_i$) not sufficient, include cross-diffusion terms
- Boudin-Grec-Salvarani 2015: Derivation from Boltzmann equation for simple mixtures



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Overview

1. Introduction
   - Multi-species systems
   - Short primer on diffusion equations
2. Modeling
   - Derivation from lattice model
   - Derivation from fluid model
   - Examples
3. Analysis
   - Entropy structure
   - Weak formulation – weak solutions
   - Large-time asymptotics
   - How to find entropies?
4. Numerics
   - Methods and aims
   - Time discretizations
   - Space discretizations

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

What makes cross-diffusion systems special?

Diffusion-induced instability:

- ODE system $u_i' = f_i(u)$ has linearly stable constant equilibrium
- Adding (cross-) diffusion, constant equilibrium may become unstable
- May lead to physically desired pattern formation (Turing 1952)

Uphill diffusion:

- Fick's law: $J_i \sim \nabla u_i$, i.e., flux proportional to density gradient
- Cross-diffusion: $J_i \sim \nabla u_j$ $(i \neq j)$, i.e., density gradient of a species causes change of flux of different species

Segregation:

- Solutions may be segregated, i.e. if $u_1^0 u_2^0 = 0$ then $u_1(t)u_2(t) = 0$ for all $t > 0$ (Bertsch et al. 1985)

Blow-up in finite time:

- Solutions may lose Hölder continuity in finite time, i.e., $u^0 \in C^{0,\alpha} \Rightarrow \exists T^* > 0$: $u(T^*) \notin C^{0,\alpha}$ (Stará-John 1995)

Getting ideas from thermodynamics

$$\partial_t u_i + \mathrm{div}(u_i v_i) = 0, \quad i = 1, \ldots, n$$

Assumption: dynamics driven by Helmholtz free energy $\mathcal{E} = \mathcal{E}(u)$

- Chemical potentials: $\mu_i := \partial\mathcal{E}/\partial u_i$
- Pressure: $p := -\mathcal{E} + \sum_{i=1}^n u_i \mu_i$
- Entropy density: $s := -\mathcal{E}$ (constant temperature)
- Darcy law: $v_i = -\nabla p$, pressure $p = p(u)$

$$\nabla p = -\sum_{i=1}^n \frac{\partial \mathcal{E}}{\partial u_i} \nabla u_i + \sum_{i=1}^n \nabla u_i \mu_i + \sum_{i=1}^n u_i \nabla \mu_i = \sum_{i=1}^n u_i \nabla \mu_i$$

- Cross-diffusion equations:

$$\partial_i u_i = \mathrm{div}(u_i \nabla p) = \mathrm{div} \sum_{j=1}^n u_i u_j \nabla \mu_i = \mathrm{div} \sum_{j=1}^n u_i u_j \nabla \frac{\partial \mathcal{E}}{\partial u_i}$$

- Formal gradient flow with diffusion matrix $B_{ij} = u_i u_j$ which is symmetric and positive semidefinite (Onsager principle)

Gradient flows

- Definition: $\partial_t u = -\operatorname{grad}\mathcal{E}(u)$ on differential manifold
- Example: $\mathbb{R}^d$ with Euclidean structure $\Rightarrow \partial_t u = -\mathcal{E}'(u)$

$$\partial_t \mathcal{E}(u) = \mathcal{E}'(u)\partial_t u = -|\mathcal{E}(u)|^2 \le 0 \ \Rightarrow\ \mathcal{E}(u) \text{ is Lyapunov functional}$$

Generalized gradient flow: (Otto 2001)

$$\partial_t u = -\mathcal{A}(\operatorname{grad}\mathcal{E}(u)) \quad \text{with} \quad \mathcal{A}(w) = -\operatorname{div}(u\nabla w)$$

- Entropy $\mathcal{E}(u) = \int_{\mathbb{R}^d} u \log u dx \Rightarrow \operatorname{grad}\mathcal{E}(u) = \frac{\partial \mathcal{E}}{\partial u} = \log u$

$$\partial_t u = \operatorname{div}\left(u\nabla\frac{\partial\mathcal{E}}{\partial u}\right) = \operatorname{div}(u\nabla\log u) = \Delta u$$

- Cross-diffusion system with gradient-flow structure:

$$\partial_t u_i = \operatorname{div}\sum_{j=1}^n B_{ij}(u)\nabla\frac{\partial\mathcal{E}}{\partial u_j}$$

- Onsager principle: (B_{ij}) is positive (semi-) definite

Entropy structure

Main assumption

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

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

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

- Derivative of entropy:
$$\frac{\partial H}{\partial u}(u)\xi = \int_\Omega h'(u)\xi dx, \quad \frac{\partial H}{\partial u}(u) \simeq h'(u) =: w = (w_1, \ldots, w_n)$$
- Formulation with entropy variables or chemical potentials w:
$$\partial_t u - \mathrm{div}(B\nabla w) = f(u), \quad B = A(u)h''(u)^{-1}$$

Lyapunov functional: let $f = 0$ to simplify

$$\frac{dH}{dt} = \int_\Omega \partial_t u \cdot \underbrace{h'(u)}_{=w} dx = -\int_\Omega \underbrace{\nabla w : B\nabla w dx}_{\text{sum over both indices}} \leq 0$$

❶ Population model

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

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

- Entropy: $H(u) = \int_\Omega h(u)dx = \int_\Omega \sum_{i=1}^2 u_i(\log u_i - 1)dx,\ u \in (0,\infty)^2$
- Entropy production: if $f = 0$

$$\frac{dH}{dt} + C\sum_{i=1}^2 \int_\Omega \big(a_{i0}|\nabla\sqrt{u_i}|^2 + a_{ii}|\nabla u_i|^2\big)dx \leq 0$$

- Entropy variables: $w_i = \partial h/\partial u_i = \log u_i \Rightarrow u_i = \exp(w_i) > 0$
  $\rightarrow$ solve system in w-variables, conclude positivity for density u_i

❷ Ion transport through membranes

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

$A_{ij}(u) = D_i \delta_{ij} u_n + D_i u_i, \quad i, j = 1, \ldots, n$

- Solvent concentration: $u_n = 1 - \sum_{i=1}^{n-1} u_i$
- Entropy: $H(u) = \int_\Omega h(u)dx = \int_\Omega \sum_{i=1}^{n} u_i(\log u_i - 1)$ but replace $u_n = 1 - \sum_{i=1}^{n-1} u_i \Rightarrow u = (u_1, \ldots, u_{n-1})$
- Entropy production: if $f = 0$

$$\frac{dH}{dt} + C \int_\Omega \left(u_n^2 \sum_{i=1}^{n-1} |\nabla \sqrt{u_i}|^2 + |\nabla \sqrt{u_n}|^2 \right) dx \le 0$$

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

$$u_i = \frac{e^{w_i}}{1 + \sum_{j=1}^{n-1} e^{w_j}} \in (0, 1)$$

- We obtain lower and upper bounds although generally no maximum principle applies!

❸ Multicomponent gas mixtures

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

$$\nabla u_i = -\sum_{j=1}^{n} k_{ij}(u_i J_j - u_j J_i), \quad i, j = 1, \ldots, n$$

- Invert using Perron-Frobenius: $J^* = A(u)\nabla u^*$, where $u^* = (u_1, \ldots, u_{n-1})$, $J^* = (J_1, \ldots, J_{n-1})$
- Entropy: $H(u) = \int_\Omega h(u)dx = \int_\Omega \sum_{i=1}^n u_i(\log u_i - 1)$ with $u_n = 1 - \sum_{i=1}^{n-1} u_i$
- Entropy production: if $f = 0$

$$\frac{dH}{dt} + C \int_\Omega \sum_{i=1}^{n-1} |\nabla \sqrt{u_i}|^2 dx \le 0$$

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

$$u_i = \frac{e^{w_i}}{1 + \sum_{j=1}^{n-1} e^{w_j}} \in (0, 1)$$

Intermediate summary

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

- Assume that there exists entropy density $h(u)$ such that

$$\partial_t u(w) - \mathrm{div}(B(w)\nabla w) = f(u(w)), \quad t > 0$$

- Entropy variables: $w = h'(u)$, inverse: $u(w) = (h')^{-1}(w)$
- Entropy production:

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

  $t \mapsto H(u(t))$ Lyapunov fct. if B pos. semidef. & $f(u) \cdot h'(u) \le 0$
- Lower/upper bounds: if $h' : D \to \mathbb{R}^n$ and D bounded then $u(x,t) = (h')^{-1}(w(x,t)) \in D$, gives L^∞ bounds

Weak solutions

$$-\Delta u + u = f \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega \tag{1}$$

- Let $f \in L^2(\Omega) = \{f : \Omega \to \mathbb{R} : f^2 \text{ integrable}\}$
- Solution u cannot be C^2! Generally, weaker solution concept needed
- Let $u \in C^2(\Omega) \cap C^0(\overline{\Omega})$ be a classical solution
- Multiply equation by $v \in H := \{v \in C^1(\overline{\Omega}) : v = 0 \text{ on } \partial\Omega\}$ and integrate by parts:

$$\int_\Omega f v dx = \int_\Omega (-\Delta u + u) v dx = \int_\Omega (\nabla u \cdot \nabla v + uv) dx \tag{2}$$

- Advantage: only one derivative needed

Definition

A function $u \in u \in C^2(\Omega) \cap C^0(\overline{\Omega})$ to (1) is called a classical solution.
A function $u \in H$ to (2) is called a weak solution.

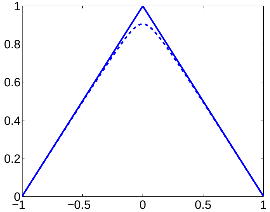
Weak solutions

$$(u, v) := \int_\Omega (\nabla u \cdot \nabla v + uv)dx = \int_\Omega fv =: F(v)$$

Theorem (Riesz)

Let H be a Hilbert space with inner product $(\cdot,\cdot)$, $F : H \to \mathbb{R}$ linear bounded. Then $\exists! u \in H : \forall v \in H : (u, v) = F(v)$.

- Hilbert space = every Cauchy sequence is convergent in H
- Norm of $H = \{v \in C^1(\overline{\Omega}) : v = 0 \text{ on } \partial\Omega\}$: $\|u\|_H^2 := \|u\|_{L^2}^2 + \|\nabla u\|_{L^2}^2$
- Problem: H is not a Hilbert space
- Counterexample: $u_n(x) = \sqrt{1 + \frac{1}{n}} - \sqrt{x^2 + \frac{1}{n}}$, $x \in \Omega = (-1, 1)$ converges in C^1 norm to $u(x) = 1 - |x| \notin H$
- Solution: complete space $\overline{H}$ with respect to norm of H



Sobolev space

Definitions:

- Inner product: $(u,v)_{H_0^1} := \int_\Omega (\nabla u \cdot \nabla v + uv)dx$, $u,\ v \in C^\infty(\Omega)$
- Norm: $\|u\|_{H^1} := (u,u)_{H_0^1}^{1/2}$, $u \in C^\infty(\Omega)$
- Sobolev space: $H_0^1(\Omega)$ equals completion of $\{u \in C_0^\infty(\Omega) : \|u\|_{H^1} < \infty\}$ with respect to norm $\|\cdot\|_{H_0^1}$

Properties:

- $H_0^1(\Omega)$ is a Hilbert space (every Cauchy sequence converges)
- Characterization: $H_0^1(\Omega) = \{u \in L^2(\Omega) : \nabla u \in L^2(\Omega),\ u = 0 \text{ on } \partial\Omega\}$ (∇u is defined in the sense of distributions, $u = 0$ in a weak sense)
- Every function in $H_0^1(\Omega)$ can be approximated by C_0^∞ functions

Examples:

- $u(x) = 1 - |x|$ is an element of $H_0^1(-1,1)$ with $u'(x) = 1$ for $x < 0$ and $u'(x) = -1$ for $x > 0$ ($u'(0)$ is not defined)
- $u(x) = 0$ for $x \in (-1, -\frac{1}{2}) \cup (\frac{1}{2}, 1)$, $u(x) = 1$ for $x \in (-\frac{1}{2}, \frac{1}{2})$ is not an element of $H_0^1(-1,1)$ (because of the jumps at $x = \pm\frac{1}{2}$)

Weak solutions

$$(u,v) := \int_\Omega (\nabla u \cdot \nabla v + uv)dx = \int_\Omega fv =: F(v)$$

Theorem (Riesz)

Let H be a Hilbert space with inner product $(\cdot,\cdot)$, $F: H \to \mathbb{R}$ linear bounded. Then $\exists! u \in H : \forall v \in H : (u,v) = F(v)$.

$\to \exists!\ u \in H_0^1(\Omega)$ such that $(u,v) = F(v)$ for $v \in H_0^1(\Omega)$

Parabolic equations:

$$\int_\Omega \partial_t uvdx + \int_\Omega (\nabla u \cdot \nabla v + uv)dx = \int_\Omega fvdx$$

- We need Bochner-Sobolev spaces

$$L^2(0,T;H^1(\Omega)) = \left\{u : (0,T) \to \mathbb{R} : t \mapsto \|u(t)\|_{H_0^1} \text{ integrable}\right\}$$

- Difficulty: $\partial_t u$ is generally not a function (but $\in H_0^1(\Omega)'$)
- Details: Evans, Partial Differential Equations, 2010

Weak formulation of cross-diffusion systems

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

- Weak formulation in density variables u:

$$(\partial_t u, v) + \int_\Omega \nabla v : A(u)\nabla u dx = \int_\Omega f(u)\cdot v dx$$

with smooth test function $v = (v_1, \ldots, v_n)$. More precisely:

$$\sum_{i=1}^n (\partial_t u_i, v_i) + \int_\Omega \sum_{i,j=1}^n A_{ij}(u)\nabla u_i \cdot \nabla v_j dx = \int_\Omega \sum_{i=1}^n f_i(u) v_i dx$$

- Weak formulation in entropy variables $w = h'(u)$:

$$(\partial_t u(w), v) + \int_\Omega \nabla v : B(w)\nabla w dx = \int_\Omega f(u(w))\cdot v dx$$

- Initial condition: $u(x,0) = u^0(x)$ for $x \in \Omega$
- Boundary condition: hidden in functional space $L^2(0,T;H_0^1(\Omega))$ (Dirichlet) or $L^2(0,T;H^1(\Omega))$ (no-flux)

For experts only: global existence of solutions

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

Assumptions:

- $\exists\ h \in C^2(D;[0,\infty)^n)$ convex, h' invertible on $D \subset \mathbb{R}^n$
- $\forall u \in D$: $z^\top h''(u)A(u)z \geq C\sum_{i=1}^n u_i^{2(m-1)} z_i^2$, $m \geq 1/2$
- A continuous, $f(u)\cdot h'(u) \leq C(1+h(u))$ for all $u \in D$

Theorem (Boundedness-by-entropy method, A.J. 2015)

Let the above assumptions hold, $D \subset \mathbb{R}^n$ be bounded, $u^0 \in L^1(\Omega)\cap \overline{D}$. Then $\exists$ global bounded weak solution such that $u(x,t)\in\overline{D}$ and

$$u \in L^2(0,T;H^1(\Omega)), \quad \partial_t u \in L^2(0,T;H^1(\Omega)')$$

Tools for proof: Lax-Milgram lemma, Leray-Schauder fixed-point theorem, entropy production inequality, Aubin-Lions compactness

Population model for $n > 2$ species

$$\partial_t u - \operatorname{div}(A(u)\nabla u) = 0 \text{ in } \Omega,\ t > 0, \quad u(0) = u_0, \quad \text{no-flux b.c.}$$
$$A_{ij}(u) = (a_{i0} + a_{i1}u_1 + \cdots a_{in}u_n)\delta_{ij} + a_{ij}u_i$$

- Problem: entropy density $h(u) = \sum_{i=1}^n u_i(\log u_i - 1)$ does not work
- Idea: try $h(u) = \sum_{i=1}^n \pi_i u_i(\log u_i - 1)$ for some $\pi_i > 0$
- Entropy production: only works if $\pi_i a_{ij} = \pi_j a_{ji}$ $\forall i, j$

$$\frac{dH}{dt} + \int_\Omega \sum_{i=1}^n \pi_i a_{i0} |\nabla \sqrt{u_i}|^2 dx \le 0$$

Why the condition $\pi_i a_{ij} = \pi_j a_{ji}$?

- Detailed-balance condition for Markov chain associated to (a_{ij})
- (π_i) is reversible measure, i.e. (π_i) does not change the dynamics
- Detailed balance $\Leftrightarrow$ Onsager matrix $A(u)h''(u)^{-1}$ symmetric
- Detailed balance $\Rightarrow$ $t \mapsto H(u(t))$ is Lyapunov functional

Large-time asymptotics

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

General strategy:

- Entropy production:

$$\frac{dH}{dt} + (\mathcal{A}(u), h'(u)) = (f(u), h'(u))$$

- Assume: $(f(u), h'(u)) \le 0$ and $(\mathcal{A}(u), h'(u)) \ge \lambda H$ with $\lambda > 0$. Then

$$\frac{dH}{dt} + \lambda H \le 0, \quad t > 0$$

- Integrate inequality over $(0, t)$ (Gronwall lemma):

$$H(u(t)) \le H(u^0)e^{-\lambda t}, \quad t > 0$$

- Consequence: entropy converges exponentially fast to zero
- Question: Does $(\mathcal{A}(u), h'(u)) \ge \lambda H$ hold?

Large-time asymptotics: examples

Diffusion equation: $\partial_t u = \Delta u$ with no-flux b.c., $u(0) = u^0$

- Equilibrium state: $u_\infty = \text{const.} = |\Omega|^{-1}\int_\Omega u^0 dx$
- Entropy production from entropy $H(u) = \int_\Omega (u-u_\infty)^2 dx$:

$$\frac{dH}{dt} = 2\int_\Omega (u-u_\infty)\Delta u dx = -2\int_\Omega |\nabla u|^2 dx$$

- Poincaré-Wirtinger inequality: for all $v \in H^1(\Omega)$,

$$\left\| v - \frac{1}{|\Omega|}\int_\Omega v dx \right\|_{L^2} \le C_P \|\nabla u\|_{L^2}$$

- Conclusion:

$$\frac{dH}{dt} \le -2C_P^{-2}\left\| u - \frac{1}{|\Omega|}\int_\Omega u dx \right\|_{L^2}^2 = -2C_P^{-2}\|u-u_\infty\|_{L^2}^2 = -2C_P^2 H$$

- Integration over $(0,t)$:

$$\|u(t)-u_\infty\|_{L^2} = H(u(t))^{1/2} \le H(u^0)^{1/2} e^{-t/C_P^2}, \quad t > 0$$

- Same result from $u(t) = \sum_{i=1}^\infty e^{-\lambda_i t}(u^0, v_i)v_i$ since $\lambda_1 = 1/C_P^2$

Large-time asymptotics: examples

Population model: $\partial_t - \operatorname{div}(A(u)\nabla u) = 0$ with no-flux b.c., $u(0) = u^0$

- Equilibrium state: $u_{\infty,i} = \text{const.} = |\Omega|^{-1} \int_\Omega u_i^0 dx$
- Entropy production from entropy $H(u) = \int_\Omega \sum_{i=1}^2 u_i \log(u_i/u_{\infty,i}) dx$:

$$\frac{dH}{dt} \leq -\alpha \int_\Omega \sum_{i=1}^2 |\nabla \sqrt{u_i}|^2 dx \leq 0, \quad \alpha := \min\{a_{10}, a_{20}\}$$

- Logarithmic Sobolev inequality: for all $\sqrt{v} \in H^1(\Omega)$

$$\int_\Omega v \log v d\mu \leq C_L \int_\Omega |\nabla \sqrt{v}|^2 d\mu, \quad \mu : \text{probability measure}$$

- With $v = u_i/u_{\infty,i}$ and $d\mu = u_{\infty,i} dx$:

$$\frac{dH}{dt} \leq -\alpha C_L^{-1} \int_\Omega \sum_{i=1}^2 u_i \log \frac{u_i}{u_{\infty,i}} dx = -\alpha C_L^{-1} H$$

- Integration over $(0,t)$: $H(u(t)) \leq H(u^0) e^{-\alpha t/C_L}$, $t > 0$
- Result cannot be (easily) obtained from spectral theory

How to find entropies?

$$\frac{dH}{dt} + \int_\Omega \nabla u : h''(u)A(u)\nabla u dx \le 0$$

Goal: find $h(u)$ such that $h''(u)A(u) \ge 0$ (positive semidefinite)

- $h''(u)A(u) \ge 0$: algebraic condition, in contrast to existence analysis
- Thermodynamics: often $h(u) = \sum_{i=1}^n u_i(\log u_i - 1)$ is entropy density
- There is no general strategy to find entropy density in given system
- One option: set up thermodynamics which gives free energy $\mathcal{E} \Rightarrow$ entropy density $h(u) = -\mathcal{E}(u)$

Example: population model with nonlinear transition rates ($s > 0$)

$$A(u) = \begin{pmatrix} a_{10} + (s+1)a_{11}u_1^s + a_{12}u_2^s & sa_{12}u_1u_2^{s-1} \\ sa_{21}u_1^{s-1}u_2 & a_{20} + a_{21}u_1^s + (s+1)a_{22}u_2^s \end{pmatrix}$$

Entropy: $H(u) = \int_\Omega (a_{21}u_1^s + a_{12}u_2^s)dx$ if $(1 - \frac{1}{s})a_{12}a_{21} \le a_{11}a_{22}$ then

$$\nabla u : h''(u)A(u)\nabla u \ge a_{21}a_{10}u_1^{s-1}|\nabla u_1|^2 + a_{12}a_{20}u_2^{s-1}|\nabla u_2|^2$$

How to find entropies?

$$(\star) \quad \partial_t u = \operatorname{div}(A(u)\nabla u), \qquad \frac{dH}{dt} + \int_\Omega \nabla u : h''(u)A(u)\nabla u dx = 0$$

Definition:

- $(\star)$ has entropy structure $\Leftrightarrow \exists$ convex h: $(h''A + A^\top h'')(u)$ pos. def.
- $A(u)$ normally elliptic $\Leftrightarrow$ eigenvalues of $A(u)$ have positive real part

Benefit:

- Normal ellipticity gives local classical solutions (Amann 1990)
- Entropy structure helps to obtain global weak solutions (A.J. 2015)

Theorem (X. Chen-A.J. 2019)

- *$(\star)$ has entropy structure $\Rightarrow$ $A(u)$ is normally elliptic*
- *$A(u)$ normally elliptic & $h''(u)A(u)$ symm. $\Rightarrow$ $(\star)$ has entropy structure*

If A is constant: A normally elliptic $\Leftrightarrow$ $(\star)$ has entropy structure

Thermodynamics: symmetry of $h''(u)A(u)$ expresses Onsager's principle

Intermediate summary

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

- Classical solutions cannot be expected: weak formulation

$$(\partial_t u, v) + \int_\Omega \nabla v : A(u)\nabla u dx = \int_\Omega f(u) \cdot v dx, \ v \text{ smooth}$$

$$(\partial_t u(w), v) + \int_\Omega \nabla v : B(w)\nabla w dx = \int_\Omega f(u(w)) \cdot v dx$$

- Global-in-time existence of bounded weak solutions possible
- Difficulty: to find entropy such that $h''(u)A(u) \geq 0$
- Exponential decay to equilibrium if entropy production $\geq$ entropy $\Leftrightarrow$ functional inequality
- Weak formulation needed for numerical approximation

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Time discretization

$$\partial_t u = \mathcal{A}(u), \quad t > 0, \quad u(0) = u^0$$

Implicit Euler method: $t_k = k\tau$, $k \in \mathbb{N}$, $\tau > 0$ (time step size)

- Replace $\partial_t u(t_k)$ by $\tau^{-1}(u(t_k) - u(t_{k-1}))$:
$$u^k - u^{k-1} = \tau \mathcal{A}(u^k), \quad k \in \mathbb{N}$$
- Solve nonlinear system for $u_k \approx u(t_k)$
- Error estimate: $\|u(t_k) - u_k\| \le C\|\partial_{tt} u\|\tau$, but first order only

Backward Differentiation Formula BDF-2:

- Replace $\partial_t u(t_k)$ by $\tau^{-1}(\frac{3}{2}u(t_k) - 2u(t_{k-1}) + \frac{1}{2}u(t_{k-2}))$:
$$\tfrac{3}{2}u^k - 2u^{k-1} + \tfrac{1}{2}u^{k-2} = \tau \mathcal{A}(u^k), \quad k \in \mathbb{N}$$
- Error estimate: $\|u(t_k) - u_k\| \le C\tau^2$

Explicit Runge-Kutta approximation: error order four

- Idea: $u^k - u^{k-1} = \tau \sum_{i=1}^4 b_i K_i$, $(b_1, b_2, b_3) = (\frac{1}{6}, \frac{1}{3}, \frac{1}{3}, \frac{1}{6})$
$K_1 = \mathcal{A}(u^{k-1})$, $K_2 = \mathcal{A}(u^{k-1} + \frac{\tau}{2}k_1)$, $K_3 = \mathcal{A}(u^{k-1} + \frac{\tau}{2}k_2)$, $K_4 = \mathcal{A}(u^{k-1} + \tau k_3)$

Space discretization

$$-\Delta u = f \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \partial\Omega$$

Finite differences: one-dimensional, $x_i = i\eta$, $i \in I$, $\eta > 0$

- Replace $\Delta u(x_i)$ by $\eta^{-2}(u(x_{i+1}) - 2u(x_i) + u(x_{i-1}))$:

$$-u_{i+1} + 2u_i - u_{i-1} = \eta^2 f(x_i), \quad i \in I$$

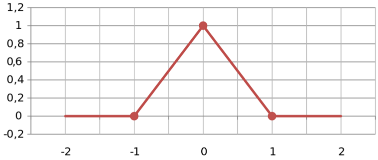
- Solve linear system in (u_i), convergence order η^2
- Sparse matrix, but unflexible in several dimensions

Finite elements:

- Idea: solve weak formulation in finite-dimensional space H_m (Galerkin)

$$\int_\Omega \nabla u \cdot \nabla v dx = \int_\Omega f v dx, \ v \in H_m$$

- Example: $H_m = \text{span}\{\text{hat fct.}\}$
- Advantage: leads to sparse matrices



Schwammerl-Bob, Hat function.svg

Space discretization

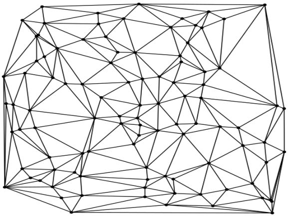
$$\int_\Omega \nabla u \cdot \nabla v dx = \int_\Omega f v dx, \quad v \in H_m$$

Finite elements:

- Let $H_m = \mathrm{span}(v_1, \ldots, v_m)$, $u = \sum_{i=1}^m u_i v_i$

$$\sum_{i=1}^m u_i \underbrace{\int_\Omega \nabla v_i \cdot \nabla v_j dx}_{=a_{ij}} = \underbrace{\int_\Omega f v_j dx}_{=b_j}$$

- Linear system $AU = b$, where $A = (a_{ij})$, $U = (u_i)$, and $b = (b_i)$
- Triangulation: Ω = set of triangles
- Ansatz functions = hat functions
- Small support $\to$ A is sparse matrix
- Efficient solution, triangulation flexible



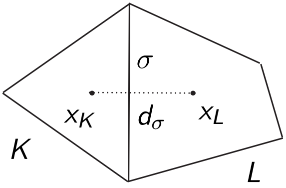
Inductiveload @Wikipedia

Space discretization

$$\operatorname{div} J = f, \quad J = -\nabla u \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \partial\Omega$$

Finite volumes:

- Triangulation $\mathcal{T}$: $\Omega = \cup_{K\in\mathcal{T}} K$, $\mathcal{E}_K$ = set of edges of K
- $u|_K$ approximated by $u_K \approx |K|^{-1}\int_K u dx$
- Idea: integrate over K_i and apply divergence theorem
$$\int_{\partial K} J\cdot\nu ds = \int_K f dx, \quad K \in \mathcal{T}$$
- Approximation:
$$\sum_{\sigma\in\mathcal{E}_K} J_\sigma = \int_K f dx, \quad J_\sigma = -\tau_\sigma(u_L - u_K) \text{ for } \sigma = K|L$$
- Transmissibility coeff.: $\tau_\sigma = \text{meas}(\sigma)/d_\sigma$
- Flux J conserved through ∂K
- Reduces in 1D to finite-difference method
- Very flexible, efficient implementation



Aims of numerical discretization

Consider time-space discretization of $\partial_t u + \mathcal{A}(u) = f$:

$$\partial_t^\tau u_K^k + \mathcal{A}_K(u_K^k) = f_K^k, \quad u_K^k \approx u(x_K, t_k)$$

Aim: Reproduce numerically as many features of the PDE as possible:

- mass conservation or mass control:

$$\sum_{K\in\mathcal{T}} u_K^k dx = \sum_{K\in\mathcal{T}} u_K^0 dx \quad \text{or} \quad \sum_{K\in\mathcal{T}} u_K^k dx \le C$$

- nonnegativity and/or upper bounds:

$$0 \le u_K^k \le C \quad \text{for all } K \in \mathcal{T},\ k \in \mathbb{N}$$

- discrete energy dissipation or entropy production:

$$H(u^k) + P(u^k) \le H(u^{k-1}), \quad k \in \mathbb{N}, \quad P(u^k) \ge 0$$

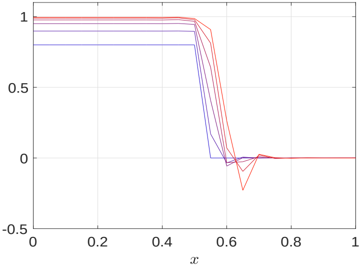
- discrete large-time asymptotics:

$$H(u^k) \le H(u^0)e^{-\kappa t_k}, \quad k \in \mathbb{N}$$

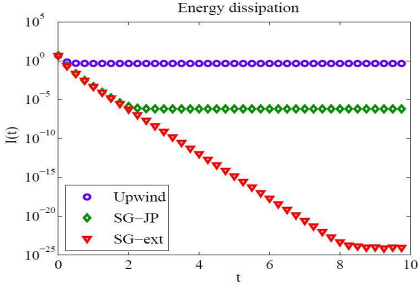
What can go wrong?

- Fisher-KPP equation:
  $\partial_t u - \Delta u = u(1-u)$
- Implicit Euler $P1$ finite elements
- Nonnegativity not preserved!

- Drift-diffusion equation:
  $\partial_t u = \mathrm{div}(\nabla u^{5/3} - u\nabla\Phi)$
  $\Delta\Phi = u - f(x)$
- Implicit Euler finite volumes
- Large-time asymptotics may be poor!



Bonizzoni-Braukhoff-A.J.-Perugia 2019



Bessemoulin 2012

Mathematical difficulties: time discretization

Assume that $H(u)$ is entropy for $\partial_t u + \mathcal{A}(u) = 0$ (multiply by $H'(u)$):

$$\frac{dH}{dt} = (\partial_t u, H'(u)) = -(\mathcal{A}, H'(u)) \leq 0$$

- Implicit Euler scheme: $u^k - u^{k-1} = \tau \mathcal{A}(u^k)$
- Multiply by $H'(u^k)$ for convex H:

$$H(u^k) - H(u^{k-1}) \leq (u^k - u^{k-1}, H'(u^k)) = -\tau(\mathcal{A}(u^k), H'(u^k)) \leq 0$$

  $\rightarrow$ entropy is nonincreasing if it is convex
- Problem: higher-order time discretizations like BDF-2

$$\begin{aligned} H(u^k) - H(u^{k-1}) &\not\leq \left(\tfrac{3}{2}u^k - 2u^{k-1} + \tfrac{1}{2}u^{k-2}, H'(u^k)\right) \\ &= -\tau(\mathcal{A}(u^k), H'(u^k)) \leq 0 \end{aligned}$$

- Ideas: modify $H(u^k) \rightarrow H(u^k, u^{k-1})$ or Taylor expansion for $\tau \mapsto H(u(t)) - H(u(t-\tau))$

Mathematical difficulties: space discretization

Entropy $H(u) = \int_\Omega h(u)$ for $\partial_t u = \Delta u$ in Ω, $u = 0$ on $\partial\Omega$:

$$\frac{dH}{dt} = \int_\Omega h'(u)\Delta u dx = -\int_\Omega \nabla h'(u) \cdot \nabla u dx = -\int_\Omega h''(u)\nabla u \cdot \nabla u dx$$

- Finite-difference discretization in one space dimension:

$$\partial_t u_i + \eta^{-2}\big(- u_{i+1} + 2u_i - u_{i-1}\big) = 0, \quad i \in I$$

- Multiply by $h'(u_i)$:

$$\begin{aligned}\frac{d}{dt}\sum_{i\in I} h(u_i) &= \sum_{i\in I} \partial_t u_i h'(u_i) = -\eta^{-2}\sum_{i\in I}(-u_{i+1} + 2u_i - u_{i-1})h'(u_i) \\ &\overset{?}{\leq} -\eta^{-2}\sum_{i\in I} h''(u_i)(u_i - u_{i-1})^2\end{aligned}$$

- Problem: discrete chain rule for $\nabla h'(u) = h''(u)\nabla u$ unclear
- Idea: redefine $h''(u)$ to enforce discrete version of $\nabla h'(u) = h''(u)\nabla u$

Time discretizations: implicit Euler, BDF-2

Implicit Euler scheme:

$$\tau^{-1}(u^k - u^{k-1}) + \mathcal{A}(u^k) = f(u^k), \quad \mathcal{A}(u) = -\operatorname{div}(A(u)\nabla u)$$

Let $H = \frac{1}{2}\int_\Omega \sum_{i=1}^n (u_i^k)^2 \ f(u)\cdot u \le 0$. Then

$$\underbrace{(u^k - u^{k-1})\cdot u^k}_{\ge H(u^k)-H(u^{k-1})} + \underbrace{(\mathcal{A}(u^k), u^k)}_{\ge 0} \le 0, \quad k \in \mathbb{N}$$

BDF-2 scheme: $\tau^{-1}\big(\frac{3}{2}u^k - 2u^{k-1} + \frac{1}{2}u^{k-2}\big) + \mathcal{A}(u^k) = f(u^k) \mid \cdot u^k$

- "Magic" inequality: for all a, b, $c \ge 0$

$$\big(\tfrac{3}{2}a - 2b + \tfrac{1}{4}c\big)a \ge \tfrac{1}{4}\big(a^2 + (2a-b)^2\big) - \tfrac{1}{4}\big(b^2 + (2b-c)^2\big)$$

- Modified entropy $H(u^k, u^{k-1}) = \frac{1}{2}\int_\Omega \sum_{i=1}^n ((u_i^k)^2 + (2u_i^k - u_i^{k-1})^2)dx$

$$H(u^k, u^{k-1}) - H(u^{k-1}, u^{k-2}) + \tau(\mathcal{A}(u^k), H'(u^k)) \le 0$$

- Can be generalized for $H(u) = \int_\Omega \sum_{i=1}^n u_i^\alpha dx$ and general multistep methods

Runge-Kutta scheme

Motivation: re-definition of entropy is unsatisfactory - can we do better?
Answer: Runge-Kutta methods for

$$\partial_t u + \mathcal{A}(u) = 0, \quad H(u) = \int_\Omega h(u)dx$$

- Runge-Kutta method with uniform time step $\tau > 0$ (to simplify):

$$u^k - u^{k-1} = \tau \sum_{i=1}^s b_i K_i, \quad K_i = \mathcal{A}\Big(u^k + \tau \sum_{j=1}^s a_{ij} K_k \Big)$$

- Implicit Euler: $s = 1$, $b_1 = a_{11} = 1$ gives $u^k - u^{k-1} = \tau\mathcal{A}(u^k)$
- Classical Runge-Kutta: $s = 4$, $b = (\frac{1}{6}, \frac{1}{3}, \frac{1}{3}, \frac{1}{6})$, $a_{21} = a_{32} = 1$, $a_{43} = 1$, and $a_{ij} = 0$ else
- Aim: $H(u^k) - H(u^{k-1}) \leq 0$
- Idea: fix $u := u^k$, interpret $v(\tau) := u^{k-1}$ as function of τ
- Define $G(\tau) = H(u) - H(v(\tau))$ and Taylor expansion

$$G(\tau) = \underbrace{G(0)}_{=0} + \tau \underbrace{G'(0)}_{\leq 0} + \tfrac{1}{2}\tau^2 \underbrace{G''(\xi)}_{\leq 0} \leq \tau G'(0), \quad 0 < \xi < \tau$$

Runge-Kutta scheme

$$H(u^k) - H(u^{k-1}) = \tau \underbrace{G'(0)}_{\le 0} + \tfrac{1}{2}\tau^2 \underbrace{G''(\xi)}_{\le 0}$$

- To show:

$$G'(0) = \int_\Omega \mathcal{A}(u)h'(u)dx, \quad C_{\mathrm{RK}} = 2\sum_{i=1}^{s} b_i\Big(1 - \sum_{j=1}^{s} a_{ij}\Big)$$

$$G''(0) = -\int_\Omega \big(C_{\mathrm{RK}} h'(u)D\mathcal{A}(u)(\mathcal{A}(u)) + h''(u)(\mathcal{A}(u))^2\big)dx < 0$$

  where $D\mathcal{A}(u) =$ Fréchet derivative of $\mathcal{A}$ at u

- Runge-Kutta constant C_{RK}:

$$C_{\mathrm{RK}} = 2 \text{ (explicit Euler)}, \ 1 \text{ (Runge-Kutta} \ge 2), \ 0 \text{ (implicit Euler)}$$

Theorem (A.J.-Schuchnigg 2017)

Let u^k be Runge-Kutta solution. If $G''(0) < 0$ then $\exists \tau^k > 0$: $\forall 0 < \tau \le \tau^k$:

$$H(u^k) + \tau\int_\Omega \mathcal{A}(u^k)h'(u^k)dx \le H(u^{k-1})$$

Runge-Kutta scheme: linear diffusion system

$$\partial_t u_1 - \Delta u_1 = u_2 - u_1, \quad \partial_t u_2 - \Delta u_2 = u_1 - u_2 \; + \; \text{no-flux b.c.}$$

Question: do we have $G''(0) < 0$?

$$G''(0) = -\int_\Omega \big(C_{\mathrm{RK}} h'(u) D\mathcal{A}(u)(\mathcal{A}(u)) + h''(u)(\mathcal{A}(u))^2 \big) dx$$

- Operator: $\mathcal{A}(u) = (\Delta u_1 + u_2 - u_1, \Delta u_2 + u_1 - u_2)$
- Since $D\mathcal{A}(u)(\mathcal{A}(u)) = \mathcal{A}(\mathcal{A}(u))$, deal with fourth-order derivatives
- Use systematic integration by parts & tedious computations

Theorem

Let u^k Runge-Kutta solution of order ≥ 2, $H(u) = \int_\Omega h(u)dx$. Then $\exists \tau^k > 0$: $\forall 0 < \tau \leq \tau^k$:

$$H(u^k) + \tau \int_\Omega \Big(\sum_{i=1}^{2} \frac{|\nabla u_i^k|^2}{u_i^k} + (\log u_1^k - \log u_2^k)(u_1^k - u_2^k) \Big) \leq H(u^{k-1})$$

Space discretizations: aims and difficulties

Finite-element method:

$$\partial_t u_\eta + \mathcal{A}_\eta(u_\eta) = 0 \quad \text{in } V_\eta,\ \dim V_\eta < \infty$$

- Aim: discrete entropy dissipation $\frac{dH}{dt} = -(\mathcal{A}_\eta(u_\eta), h'(u_\eta)) \leq 0$
- Problem: Generally, $h'(u_\eta) \notin V_\eta$ cannot be used as a test function
- Idea: Solve problem in entropy variable $w_\eta := h'(u_\eta) \in V_\eta$
- Discrete L^∞ bounds may be obtained without use of max. principle

Finite-volume method:

$$\partial_t u_K + \sum_\sigma J_{K,\sigma} = 0, \quad J_{K,\sigma} \text{ flux on edge } \sigma \in K$$

- Problem: entropy dissipation $\sum_K \sum_\sigma J_{K,\sigma} \cdot h'(u_K) \geq 0$ not clear
- Aim: obtain discrete analog of entropy dissipation
- Idea: adapt numerical scheme (e.g. upwinding)
- Discrete L^∞ bounds from discrete maximum principle

❷ Ion transport model

$$\partial_t u_i = \operatorname{div}\big(D_i(u_n\nabla u_i - u_i\nabla u_n + u_n u_i z_i \nabla\phi)\big) \quad \text{in } \Omega,\ t>0$$
$$-\Delta\phi = \textstyle\sum_{i=1}^n z_i u_i + f(x), \quad u_i(0) = u_i^0, \quad \text{no-flux b.c.}$$

- Can be written as $\partial_t u = \operatorname{div}(A(u)\nabla u + D(u)\nabla\phi)$
- Solvent density: $u_n = 1 - \sum_{i=1}^{n-1} u_i \Rightarrow$ consider $u = (u_1,\ldots,u_{n-1})$
- Entropy $H(u) = \int_\Omega h(u)dx$, $h(u) = \sum_{i=1}^n u_i(\log u_i - 1) + \frac{1}{2}|\nabla\phi|^2$
- Entropy variables: $w_i = \partial h/\partial u_i = \log(u_i/u_n) + z_i\phi$ gives

$$\partial_t u = \operatorname{div}(B\nabla w), \quad B = A(u)h''(u)^{-1} \in \mathbb{R}^{(n-1)\times(n-1)} \text{ pos. semidef.}$$

Consequences:

- H is Lyapunov functional: $dH/dt \le 0$
- L^∞ bounds for u:

$$w_i = \log\frac{u_i}{u_n} + z_i\phi \quad \Rightarrow \quad u_i = \frac{e^{w_i - z_i\phi}}{1 + \sum_{j=1}^{n-1} e^{w_i - z_i\phi}} \in (0,1)$$

Aim: derive discrete L^∞ bounds and discrete entropy dissipation

Ion transport model: finite-volume scheme

$$\partial_t u_i = \operatorname{div} J_i, \quad J_i = D_i(u_n \nabla u_i - u_i \nabla u_n + u_n u_i z_i \Phi)$$
$$-\Delta\Phi = \textstyle\sum_{i=1}^n z_i u_i + f(x) \quad \text{in } \Omega, \quad \text{no-flux b.c.}$$

- Implicit-Euler finite-volume scheme for $D_i = 1$, $\Phi = 0$: (K: cells, σ: edges)
$$(u_{i,K}^k - u_{i,K}^{k-1}) + \frac{\tau}{|K|}\sum_\sigma \big(u_{n,\sigma}^k(u_{i,L}^k - u_{i,K}^k) - u_{i,\sigma}^k(u_{n,L}^k - u_{n,K}^k)\big) = 0$$
upwind: $u_{i,\sigma}^k = u_{i,K}^k$ $(u_{i,L}^k)$ if $u_{n,K}^k - u_{n,L}^k \le 0$ (> 0)
- Discrete entropy: $H(u^k) = \sum_K |K| \sum_{i=1}^n u_{i,K}^k(\log u_{i,K}^k - 1)$

Theorem (Cancès-Chainais-Gerstenmayer-A.J. 2018)

- *There exists discrete solution* $u_{i,K}^k \ge 0$ *with* $\sum_{i=1}^{n-1} u_{i,K}^k \le 1$
- (u_K^k) *converges to continuous solution and*

$$H(u^k) + \tau\kappa \sum_\sigma \tau_\sigma \left(\sum_{i=1}^n u_{n,\sigma}^k \big((u_{i,K}^k)^{1/2} - (u_{i,L}^k)^{1/2}\big)^2 + (u_{n,K}^k - u_{n,L}^k)^2 \right) \le H(u^{k-1})$$

Ion transport model: finite-element scheme

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

- Time step size $\tau > 0$, Galerkin space V_η with dimension $< \infty$
- Given $w^{k-1} \in V_\eta$, solve for $w^k \in V_\eta$ and $u_i^k := u_i(w^k)$:

$$\frac{1}{\tau}(u(w^k) - u(w^{k-1})) - \mathrm{div}(B(w^k)\nabla w^k) + \varepsilon w^k = r(u(w^k)) \text{ in } V_\eta$$

- L^∞ bounds $0 < u_i^k < 1$ automatically fulfilled
- D_i may be different, ε-term needed for coercivity
- Iteration: full Newton needed

Theorem (A.J.-Gerstenmayer 2018)

Bounds $0 < u_i^k < 1$, *numerical convergence, discrete entropy production:*

$$H(u^k) + \kappa\tau \int_\Omega \sum_{i=1}^n u_n^k |\nabla (u_i^k)^{1/2}|^2 dx \le H(u^{k-1})$$

Comparison: finite volumes and finite elements

Question: solve system with concentrations u_i or entropy variables w_i?

Solve system with concentrations u_i:

- Advantages: no inversion of $w \mapsto u$, drift-diffusion structure may be exploited (upwind meth.), bounds can be preserved, fast algorithm
- Drawbacks: simplifying assumptions needed for numerical analysis, discretization needs to be adapted to satisfy properties

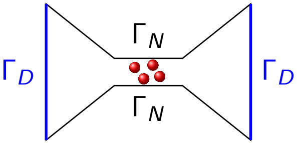
Solve system with entropy variables w_i:

- Advantages: thermodynamic interpretation (w_i = chemical potential), diffusion matrix positive (semi-) definite, straightforward discretization, numerical analysis possible under natural conditions
- Drawbacks: need to invert $w \mapsto u$, theory needs ε-regularization (only asymptotically mass-conserving), slow algorithm (highly nonlinear)

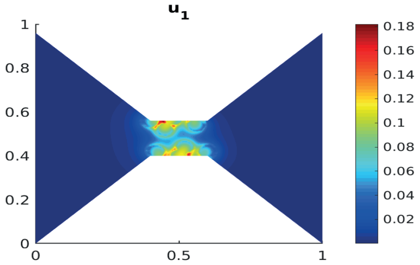
In both cases, discrete L^∞ bounds and discrete entropy dissipation

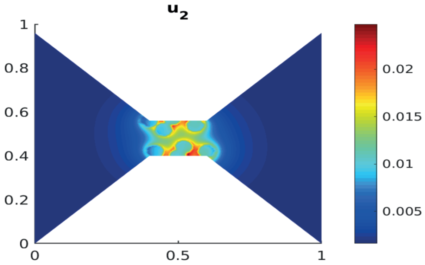
Application: calcium-selective ion channel

- Confined oxygen ions in channel
- Ions: calcium u_1, sodium u_2, chloride u_3
- Finite volumes, full Newton, Delauney mesh of 4736 elements



- Asymmetric charge distribution in ion channel
- Equilibrium: calcium ions (u_1) are selected over sodium ions (u_2)





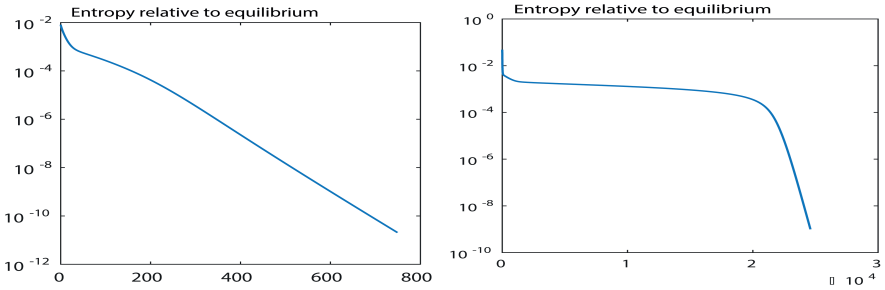
Gerstenmayer-A.J. 2019

Application: calcium-selective ion channel

- Recall flux: $J_i = D_i(u_4 \nabla u_i - u_i \nabla u_4 + u_4 u_i z_i \Phi)$
- Relative entropy:

$$H^k = \sum_K |K| \sum_{i=1}^4 u_{i,K}^k \log\left(\frac{u_{i,K}^k}{u_{i,K}^\infty}\right) + \frac{\lambda^2}{2} \sum_\sigma \tau_\sigma \mathrm{D}_{K,\sigma}(\Phi^k - \Phi^\infty)^2$$

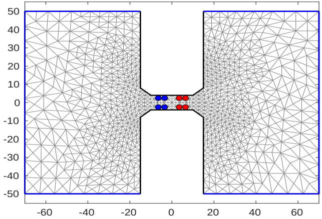
- Degeneracy $(u_4 \nabla u_i)$ may prevent exponential decay rate

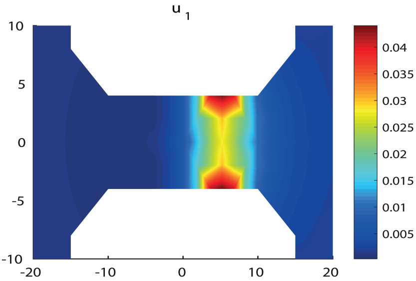


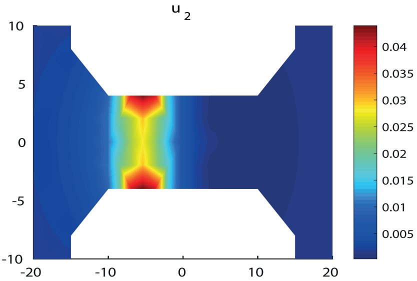
Cancès-Chainais-Gerstenmayer-A.J. 2019

Application: bipolar ion channel

- Nanochannel with 1 nm diameter
- Blue: positively charged ions,
  red: negatively charged ions
- Na^+: u_1, Cl^-: u_2
- Finite elements, mesh of 2080 triangles, full Newton







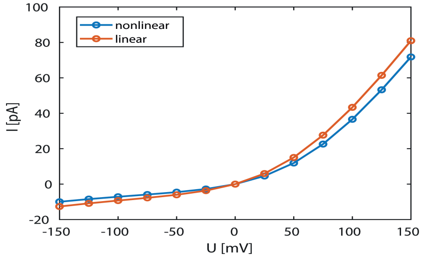
Application: bipolar ion channel

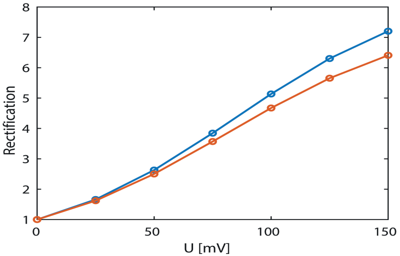
Question: What about the rectification behavior?

- Rectification = converting bidirectional current flow
- Current flow through pore with cross section A:

$$\text{apply voltage } U, \text{ obtain } I(U) = -\sum_{i=1}^{n} z_i \int_A J_i \cdot \nu ds$$

- Rectification: $r(U) := |I(U)/I(-U)|$
- Compare with standard Nernst-Planck model ($u_n = 1$)





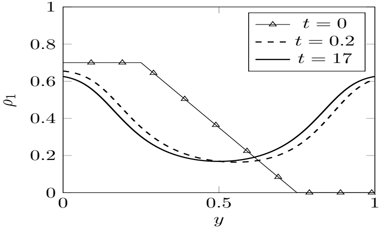
Gerstenmayer-A.J. 2019

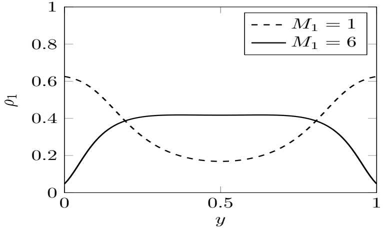
Multicomponent gas mixtures

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

$$\nabla u_i = -\sum_{j=1}^{n} k_{ij}(u_i J_j - u_j J_i), \quad i,j = 1,\ldots,n$$

- Implicit Euler & P1 finite elements, formulation in entropy variables
- Linearize $u(w^k, \Phi^k)$, use $B(w^{k-1})$ (semi-implicit)
- Different molar masses M_i





A.J.-Leingang 2018

Intermediate summary

We discussed…

- Time discretizations: implicit Euler, BDF-2, Runge-Kutta
  - Problem: there is no general discrete chain rule
  - Change definition of discrete entropy (BDF-2)
  - Show that $G''(0) < 0$ (Runge-Kutta)
- Space discretizations: finite volumes, finite element
  - Finite volumes: flux conservation through edges, fast algorithms
  - Finite elements: automatic lower/upper bounds for entropy variables, slow algorithm
- Structure-preservation: mass conservation, lower/upper bounds, discrete entropy production

Summary

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

Modeling:

- Many examples from physics and biology
- Derivation from lattice or fluid models
- Cross diffusion may show pattern formation, loss of regularity

Analysis:

- Entropy structure inspired by thermodynamics
- Missing regularity makes weak formulation necessary
- Mathematical formulation needs functional analysis

Numerics:

- Need for structure-preserving numerical schemes
- Higher-order time discretizations possible under conditions
- Space discretizations: obtain entropy-producing schemes
- Advantage: stable and efficient numerical algorithms compared to standard discretizations