# Entropy dissipation methods for diffusion equations

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# Contents

# Literature

## Main references


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- J.A. Carrillo, A. Jüngel, P. Markowich, G. Toscani, and A. Unterreiter. Entropy dissipation methods for degenerate parabolic problems and generalized Sobolev inequalities. *Monats. Math.* 133 (2001), 1-82.
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# What mathematics skills are needed?

Entropy methods are intradisciplinary!

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

# Entropy in physics

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

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

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

# Entropy in information theory

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|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |

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|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 1 | 0 | 0 | 1 | 1 | 1 | 0 | 1 |

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

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

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

# Entropy in mathematics

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

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

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

# Entropy in literature

# Entropy and partial differential equations

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

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

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

- Euler equations in thermodynamics:

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

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

- Energy balance: $$\frac{d}{dt} \int_{\mathbb{R}^d} \left( \frac{\rho}{2} |v|^2 + \rho e \right) dx = 0$$

- Monoatomic ideal gas: energy density $\rho e = \frac{3}{2} \rho \theta$,
  entropy density $\rho s = -\rho \log(\rho / \theta^{3/2}) \Rightarrow \frac{\partial(\rho s)}{\partial(\rho e)} = \frac{1}{\theta} > 0$

# Aims of lecture course

- To introduce into several entropy methods for partial differential equations (PDEs)
- To use entropy methods to prove the qualitative behavior of solutions to PDEs (large-time asymptotics, existence analysis, $L^\infty$ bounds)
- To prove functional inequalities (convex Sobolev inequalities)
- To relate entropy methods to physical principles and the theory of stochastic processes
- To introduce into the theory of cross-diffusion systems

# Overview

# Example: Heat equation

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

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

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

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

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

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

# Example: Heat equation

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

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

First answer: Different "distances" admissible

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

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

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

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

# Example: Heat equation

Second answer: Method applicable to nonlinear equations

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

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

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

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

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

# Strategy

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

Strategy:

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

Entropy methods can do much more:

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

# Definitions

Setting:

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

Definitions:

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

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

Examples: $F_1$: Fisher information

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

# Heat equation revisited

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

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

Proof:

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

**Lemma (Csiszár-Kullback-Pinsker)**

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

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

Proof: Taylor expansion of $\phi$ around 1

# Overview

# Linear Fokker-Planck equation

$$\partial_t u = \operatorname{div}(\nabla u + u\nabla V) \quad \text{in } \mathbb{R}^d,\ t > 0, \quad u(u) = u_0 \geq 0$$

- Assumptions: $\int_{\mathbb{R}^d} u_0 dx = 1$, $\lim_{|x|\to\infty} V(x) = \infty$ (confinement)
- Steady state: $0 = \nabla u_\infty + u_\infty \nabla V = u_\infty \nabla(\log u_\infty + V) \Rightarrow$ $u_\infty = ce^{-V}$, where $c$ is such that $\int_{\mathbb{R}^d} u_\infty dx = 1$
- Entropy: Let $\phi \in C^4$ be convex

$$H_\phi[u] = \int_{\mathbb{R}^d} \phi\left(\frac{u}{u_\infty}\right) u_\infty dx - \phi\Big(\int_{\mathbb{R}^d} udx\Big)$$

**Theorem (Bakry/Emery '85, Arnold/Markowich/Toscani/Unterreiter '01)**

*Let* $u_0 \log u_0 \in L^1(\mathbb{R}^d)$, $\nabla^2 V \geq \lambda > 0$, $1/\phi''$ *concave. Then*

$$\|u(t) - u_\infty\|_{L^1} \leq e^{-\lambda t} C_\phi^{1/2} H_\phi[u_0]^{1/2}, \quad t > 0$$

Example ❶: $\phi(s) = s(\log s - 1) + 1$, $\phi(s) = s^\alpha - 1 - \alpha(s-1)$ $(1 < \alpha \leq 2)$

Example ❷: $\phi(s) = s\log s$, $V(x) = \frac{1}{2}|x|^2$ then $\lambda = 1$ (optimal!)

# Proof: First time derivative

$$\partial_t u = \operatorname{div}(\nabla u + u\nabla V) = \operatorname{div}\left(u_\infty \nabla \frac{u}{u_\infty}\right), \quad u_\infty = ce^{-V}$$

First time derivative: $H_\phi[u] = \int_{\mathbb{R}^d} \phi(u/u_\infty)u_\infty dx - \phi(1)$, set $\rho := \frac{u}{u_\infty}$

$$\frac{dH_\phi}{dt} = \int_{\mathbb{R}^d} \phi'(\rho)\partial_t u dx = -\int_{\mathbb{R}^d} \phi''(\rho)|\nabla\rho|^2 u_\infty dx \le 0$$

Second time derivative: (key idea!)

$$\frac{d^2 H_\phi}{dt^2}[u] = -\int_{\mathbb{R}^d} \left(\phi'''(\rho)\partial_t u|\nabla\rho|^2 + 2\phi''(\rho)\nabla\rho\cdot\nabla\partial_t\rho u_\infty\right)dx = -I_1 - I_2$$

First integral:

$$\begin{aligned} I_1 &= -\int_{\mathbb{R}^d} \nabla\left(\phi'''(\rho)|\nabla\rho|^2\right)\cdot(u_\infty\nabla\rho)dx \\ &= -\int_{\mathbb{R}^d} \left(\phi''''(\rho)|\nabla\rho|^4 + 2\phi'''(\rho)\nabla\rho\nabla^2\rho\nabla\rho\right)u_\infty dx \end{aligned}$$

# Proof: Second time derivative

$$\frac{d^2 H_\phi}{dt^2}[u] = -I_1 - I_2,\ \ I_1 = -\int_{\mathbb{R}^d} \big(\phi''''(\rho)|\nabla\rho|^4 + 2\phi'''(\rho)\nabla\rho\nabla^2\rho\nabla\rho\big)u_\infty dx$$

Second integral: compute $\nabla\partial_t\rho = \nabla\Delta\rho - \nabla^2\rho\cdot\nabla V - \nabla^2 V\nabla\rho$, $\rho = \frac{u}{u_\infty}$

$$\begin{aligned}
I_2 &= 2\int_{\mathbb{R}^d} \phi''(\rho)\nabla\rho\cdot\nabla\partial_t\rho u_\infty dx \\
&= 2\int_{\mathbb{R}^d} \phi''(\rho)\big(\nabla\rho\cdot\nabla\Delta\rho - \nabla\rho\nabla^2\rho\nabla V - \overbrace{\nabla\rho\nabla^2 V\nabla\rho}^{\geq\lambda|\nabla\rho|^2}\big)dx \\
&\leq 2\int_{\mathbb{R}^d} \phi''(\rho)\big(\mathrm{div}(\nabla^2\rho\nabla\rho) - |\nabla^2\rho|^2 - \nabla\rho\nabla^2\rho\nabla V - \lambda|\nabla\rho|^2\big)u_\infty dx \\
&= 2\int_{\mathbb{R}^d}\big(-\phi'''\nabla\rho\nabla^2\rho\nabla\rho u_\infty - \phi''\nabla\rho\nabla^2\rho\overbrace{(\nabla u_\infty + u_\infty\nabla V)}^{=0} - \phi''|\nabla^2\rho|^2 u_\infty\big)dx \\
&\quad - 2\lambda\int_{\mathbb{R}^d}\phi''(\rho)|\nabla\rho|^2 u_\infty dx, \quad \text{note: } \int_{\mathbb{R}^d}\phi''(\rho)|\nabla\rho|^2 u_\infty dx = \frac{dH_\phi}{dt}
\end{aligned}$$

# Proof: Second time derivative

Add both integrals $I_1$ and $I_2$ and use $\phi$ convex, $1/\phi''$ concave:

$$\frac{d^2H_\phi}{dt^2}[u] = \int_{\mathbb{R}^d} \left(\phi''''|\nabla\rho|^4 + 4\phi'''\nabla\rho\nabla^2\rho\nabla\rho + 2\phi''|\nabla^2\rho|^2\right)u_\infty dx - 2\lambda\frac{dH_\phi}{dt}$$

$$= \int_{\mathbb{R}^d}\Bigg(\underbrace{2\,\phi''\left|\nabla^2\rho + \frac{\phi'''}{\phi''}\nabla\rho\otimes\nabla\rho\right|^2}_{\geq 0} + \underbrace{\left(\phi'''' - 2\frac{(\phi''')^2}{\phi''}\right)}_{=-(\phi'')^2(1/\phi'')''\geq 0}|\nabla\rho|^4\Bigg)u_\infty dx$$

$$-2\lambda\frac{dH_\phi}{dt} \quad\Rightarrow\quad \frac{d^2H_\phi}{dt^2}[u] \geq -2\lambda\frac{dH_\phi}{dt}$$

Integrate over $(t,\infty)$:

$$\underbrace{\lim_{s\to\infty}\frac{dH_\phi}{dt}[u(s)]}_{=0} - \frac{dH_\phi}{dt}[u(t)] \geq -2\lambda\underbrace{\lim_{s\to\infty}H_\phi[u(s)]}_{=0} + 2\lambda H_\phi[u(t)]$$

Gronwall lemma and Csiszár-Kullback inequality:

$$\|u(t)-u_\infty\|_{L^1}^2 \leq C_\phi H_\phi[u(t)] \leq C_\phi e^{-2\lambda t}H[u_0]$$

# Bakry-Emery: Remarks

**Theorem (Bakry/Emery '85, Arnold/Markowich/Toscani/Unterreiter '01)**

*Let* $u_0 \log u_0 \in L^1(\mathbb{R}^d)$, $\nabla^2 V \geq \lambda > 0$, $\phi$ *convex,* $1/\phi''$ *concave. Then*

$$\|u(t) - u_\infty\|_{L^1} \leq e^{-\lambda t} C_\phi^{1/2} H_\phi[u_0]^{1/2}$$

- Exponential $L^1$ decay with (optimal) rate $\lambda$
- Difficult part of proof: justify computations for weak solutions
- Proof yields convex Sobolev inequality for all (smooth) $u$ ($\rho = \frac{u}{u_\infty}$):

$$H_\phi[u] = \int_{\mathbb{R}^d} \phi(\rho) u_\infty dx - \phi(1) \leq -\frac{1}{2\lambda} \frac{dH_\phi}{dt}[u] = \frac{1}{2\lambda} \int_{\mathbb{R}^d} \phi''(\rho) |\nabla \rho|^2 u_\infty dx$$

- Example: $V(x) = \frac{1}{2}|x|^2$, $\phi(s) = s(\log s - 1) + 1$, then $\lambda = 1$

$$\int_{\mathbb{R}^d} u \log u dx + \frac{d}{2} \log(2\pi) + d \leq \frac{1}{2} \int_{\mathbb{R}^d} \frac{|\nabla u|^2}{u} dx, \quad \int_{\mathbb{R}^d} u dx = 1$$

- Benefit: Simultaneous proof of deacy rate and convex Sobolev ineq.

# Bakry-Emery for Markov processes

- Given Markov process $(X_t)_{t>0}$, semigroup $S_t f(x) = E[f(X_t)|X_0 = x]$, infinitesimal generator $Lf = \lim_{t\to 0}(S_t f - f)/t$
  Example: $Lf = \Delta f - x \cdot \nabla f$ on $\mathbb{R}^d$ (Fokker-Planck-type), $S_t f_0$ is solution to $\partial_t f = Lf$, $f(0) = f_0$
- Assume: $\exists$ invariant measure $\pi$: $\int f d\pi = \int S_t f d\pi$

Carré-du-champ operator: $\Gamma(f,g) = \frac{1}{2}(L(fg) - fLg - gLf)$
Example: $\Gamma(f,g) = \nabla f \cdot \nabla g$
Gamma-deux operator: $\Gamma_2(f,g) = \frac{1}{2}(L\Gamma(f,g) - \Gamma(Lf,g) - \Gamma(f,Lg))$
Example: $\Gamma_2(f,f) = |\nabla^2 f|^2 + |\nabla f|^2 \Rightarrow \Gamma_2(f,f) \geq \Gamma(f,f)$

**Theorem (Bakry/Emery 1985)**

*Let $\phi \in C^2$ be convex, $1/\phi''$ concave, and $\exists \lambda > 0$: $\Gamma_2(f,f) \geq \lambda \Gamma(f,f)$ for all $f \geq 0$. Then for probability density functions $\rho$,*

$$\int_{\mathbb{R}^d} \phi(\rho) d\pi - \phi\left( \int_{\mathbb{R}^d} \rho d\pi \right) \leq \frac{1}{2\lambda} \int_{\mathbb{R}^d} \phi''(\rho) \Gamma(\rho,\rho) d\pi$$

# Bakry-Emery for Markov processes

Example: Fokker-Planck-type equation

- We have $\Gamma(\rho,\rho) = |\nabla\rho|^2$ and $d\pi = u_\infty dx$ with $u_\infty = ce^{-V}$
- Choose $\rho = u/u_\infty$: $\int_{\mathbb{R}^d} \rho d\pi = \int_{\mathbb{R}^d} udx$
- Relation to previous convex Sobolev inequality:

$$\int_{\mathbb{R}^d} \phi(\rho) \underbrace{d\pi}_{=u_\infty dx} - \phi\left( \int_{\mathbb{R}^d} \underbrace{\rho d\pi}_{=udx} \right) \leq \frac{1}{\lambda} \int_{\mathbb{R}^d} \phi''(\rho) \underbrace{\Gamma(\rho,\rho)}_{=|\nabla\rho|^2} \underbrace{d\pi}_{=u_\infty dx}$$

Example ❶: $\phi(s) = s(\log s - 1)$ gives logarithmic Sobolev inequality

$$\int_{\mathbb{R}^d} \rho \log \rho d\pi - \int_{\mathbb{R}^d} \rho d\pi \log \int_{\mathbb{R}^d} \rho d\pi \leq \frac{1}{2\lambda} \int_{\mathbb{R}^d} \frac{\Gamma(\rho,\rho)}{\rho} d\pi$$

Example ❷: $\phi(s) = s^2$ gives Poincaré inequality

$$\int_{\mathbb{R}^d} \left( \rho - \int_{\mathbb{R}^d} udx \right)^2 d\pi \leq \frac{1}{\lambda} \int_{\mathbb{R}^d} \Gamma(\rho,\rho) d\pi$$

Benefit: Abstract framework for convex Sobolev inequalities

# Extensions of the Bakry-Emery method

1. More on convex Sobolev inequalities: Compare Poincaré, logarithmic Sobolev, and Beckner inequalities
2. Isoperimetric inequality for entropy: Relation to information theoretical approach (entropy power)
3. Relaxation to self-similarity: Analyze intermediate asymptotics of solution of heat equation
4. Linear Fokker-Planck equations with variable diffusion matrix
5. Nonlinear Fokker-Planck equations

# ❶ More on convex Sobolev inequalities

$$\int_{\mathbb{R}^d} \phi(\rho) u_\infty dx - \phi\left( \int_{\mathbb{R}^d} \rho u_\infty dx \right) \leq \frac{1}{2\lambda} \int_{\mathbb{R}^d} \phi''(\rho) |\nabla \rho|^2 u_\infty dx$$

- Logarithmic Sobolev inequality: $\phi(s) = s \log s$ (for $\int_{\mathbb{R}^d} \rho u_\infty dx = 1$)

$$\int_{\mathbb{R}^d} \rho \log \rho u_\infty dx \leq \frac{2}{\lambda} \int_{\mathbb{R}^d} |\nabla \rho^{1/2}|^2 u_\infty dx$$

- Poincaré inequality: $\phi(s) = s^2$

$$\int_{\mathbb{R}^d} \rho^2 u_\infty dx - \left( \int_{\mathbb{R}^d} \rho u_\infty dx \right)^2 \leq \frac{1}{\lambda} \int_{\mathbb{R}^d} |\nabla \rho|^2 u_\infty dx$$

- Beckner inequality: $\phi(s) = s^\alpha$, $1 < \alpha < 2$

$$\frac{1}{\alpha - 1} \left( \int_{\mathbb{R}^d} \rho^\alpha u_\infty dx - \left( \int_{\mathbb{R}^d} \rho u_\infty dx \right)^\alpha \right) \leq \frac{2}{\alpha\lambda} \int_{\mathbb{R}^d} |\nabla \rho^{\alpha/2}|^2 u_\infty dx$$

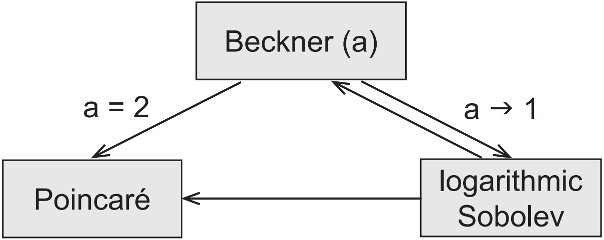
# Relations between functional inequalities

$$\frac{1}{\alpha-1}\left(\int_{\mathbb{R}^d}\rho^\alpha u_\infty dx - \left(\int_{\mathbb{R}^d}\rho u_\infty dx\right)^\alpha\right) \le \frac{2}{\alpha\lambda}\int_{\mathbb{R}^d}|\nabla\rho^{\alpha/2}|^2 u_\infty dx$$

- $\alpha \to 1$ in Beckner gives logarithmic Sobolev inequality since

$$\frac{1}{\alpha-1}\int_{\mathbb{R}^d}(\rho^{\alpha-1}-1)\rho u_\infty dx \to \int_{\mathbb{R}^d}\rho\log\rho u_\infty dx$$

- $\alpha \to 2$ in Beckner gives Poincaré inequality
- Logarithmic Sobolev implies Poincaré (use $\rho = 1+\varepsilon g$ with $\int_{\mathbb{R}^d} g u_\infty dx$ and $\varepsilon \to 0$) and Beckner (Latala/Oleszkiewicz 2000)



# ❷ Isoperimetric inequality for entropy

Aim: Relation between logarithmic Sobolev ineq. and isoperimetric ineq.

- Entropy: $H[u] = \int_{\mathbb{R}^d} u \log u dx$
- Fisher information: $I[u] = 4 \int_{\mathbb{R}^d} |\nabla u^{1/2}|^2 dx$
- Entropy power: $N[u] = \exp(-\frac{2}{d} H[u])$

**Theorem (Isoperimetric inequality for entropy)**

*For all probability density functions $u$, $N[u]I[u] \geq 2\pi e d$.*

- Equivalent formulation: $4\pi \exp(\frac{2}{d} H[u]) \leq \frac{8}{ed} \int_{\mathbb{R}^d} |\nabla u^{1/2}|^2 dx$
- Compare with isoperimetric inequality on $\mathbb{R}^2$: $4\pi A \leq L^2$ for closed curve with length $L$ and enclosed area $A$
- Approximating $e^z \geq z$ gives logarithmic Sobolev inequality:

$$\frac{2}{d} \int_{\mathbb{R}^d} u \log u dx = \frac{2}{d} H[u] \leq \frac{2}{\pi e d} \int_{\mathbb{R}^d} |\nabla u^{1/2}|^2 dx$$

# Isoperimetric inequality for entropy

**Theorem (Isoperimetric inequality for entropy)**

*For all probability density functions $u$, $N[u]I[u] \geq 2\pi e d$.*

Proof:

- $N[u]$ is concave (Costa 1985, Villani 2000) since
$$\frac{d^2N}{dt^2} = \left(\frac{2}{d}\right)^2 N\left(\left(\frac{dH}{dt}\right)^2 - \frac{d}{2}\frac{d^2H}{dt^2}\right) \leq 0$$
- Let $v$ solve $\partial_t v = \Delta v$, $v(0) = u$:
$$\frac{d}{dt}(N[v]I[v]) = \frac{2}{d}N\left(I^2 + \frac{d}{2}\frac{dI}{dt}\right) = \frac{2}{d}N\left(\left(\frac{dH}{dt}\right)^2 - \frac{d}{2}\frac{d^2H}{dt^2}\right) \leq 0$$
- $N[v(t)]I[v(t)]$ reaches minimum as $t \to \infty \Rightarrow N[v(t)]I[v(t)] \geq m$
- Scaling argument: $m = N[M]I[M]$, where $M(x) = \frac{1}{(2\pi t)^{d/2}}\exp(-\frac{|x|^2}{2t})$
- Conclusion: $N[u]I[u] = N[v(0)]I[v(0)] \geq N[M]I[M] = 2\pi e d$

# ❸ Relaxation to self-similarity

Consider heat equation in whole space:

$$\partial_t u = \Delta u \quad \text{in } \mathbb{R}^d,\ t>0, \quad u(0)=u_0, \quad \int_{\mathbb{R}^d} u_0 dx = 1$$

- Explicit solution:
  $u(x,t) = (4\pi t)^{-d/2}\int_{\mathbb{R}^d}\exp(-|x-y|^2/(4t))u_0(y)dy$, thus
  $u(t)\to 0$ in $L^\infty$ as $t\to\infty$
- Entropy is decreasing but

$$H_1[u(t)] = \int_{\mathbb{R}^d} u\log u dx \le \int_{\mathbb{R}^d} u(t)dx \log\|u(t)\|_{L^\infty} \to -\infty \quad (t\to\infty)$$

- Entropy method fails! Problem: $u_\infty = 0$ has not unit mass
- Solution: Analyze $u(t) - U(t)\to 0$, where self-similar solution

$$U(x,t) = \frac{1}{(2\pi(2t+1))^{d/2}}\exp\left(-\frac{|x|^2}{2(2t+1)}\right)$$

- Idea: Transform variables to make $U$ stationary: $y = x/\sqrt{2t+1}$,
  $s = \log\sqrt{2t+1}$, and $v(y,s) = e^{ds}u(e^s y, \frac{1}{2}(e^{2s}-1))$

# Relaxation to self-similarity

$$\partial_t u = \Delta u \quad \text{in } \mathbb{R}^d, \quad v(y,s) = e^{ds} u(e^s y, \tfrac{1}{2}(e^{2s}-1))$$

- Function $v$ solves $\partial_s v = \mathrm{div}_y(\nabla_y v + yv)$ in $\mathbb{R}^d$
- Self-similar solution becomes $M(y) = (2t+1)^{d/2} U(x,t) = (2\pi)^{-d/2}\exp(-|y|^2/2)$
- Bakry-Emery shows:

$$\|v(s) - M\|_{L^1}^2 \le 2e^{-2s} H_1[u_0], \quad s > 0$$

- Back-transformation:

$$\|v(s) - M\|_{L^1}^2 = \|u(t) - U(t)\|_{L^1}^2, \quad 2e^{-2s} = 2(2t+1)^{-1}$$

**Theorem**

*Let $\int_{\mathbb{R}^d} u_0 dx = 1$, $u$ solves $\partial_t u = \Delta u$ in $\mathbb{R}^d$, $u(0) = u_0$, and $U(x,t) = (2\pi(2t+1))^{-d/2}\exp(-|x|^2/(2(2t+1)))$. Then*

$$\|u(t) - U(t)\|_{L^1} \le (2t+1)^{-1/2}(2H_1[u(0)])^{1/2} \sim t^{-1/2} \ (t \to \infty)$$

# ❹ Variable diffusion matrix

$$\partial_t u = \operatorname{div}(D(x)(\nabla u + u\nabla V)) = \operatorname{div}(D(x)u_\infty\nabla\rho) \quad \text{in } \mathbb{R}^d, \qquad D(x)\in\mathbb{R}^{d\times d}$$

- Steady state: $u_\infty = ce^{-V}$, $\rho = \frac{u}{u_\infty}$
- Assumptions: $D(x)$ pos. definite, $\lim_{|x|\to\infty} V(x) = \infty$, $\int_{\mathbb{R}^d} u_\infty dx = 1$
- Entropy: $H[u] = \int_{\mathbb{R}^d}\phi(\rho)u_\infty dx$, $\phi$ convex, $\phi(1)=0$, $1/\phi''$ concave
- Entropy production:

$$\frac{dH}{dt}[u] = -\int_{\mathbb{R}^d}\phi''(\rho)\nabla\rho^\top D\nabla\rho u_\infty dx \le 0$$

**Theorem (Arnold/Markowich/Toscani/Unterreiter 2001)**

*Assume $H[u(0)]<\infty$ and*

$$\begin{aligned} &D(x) = const., && \nabla^2 V \ge \lambda D^{-1} \quad \text{or} \\ &D(x) = a(x)I, && \left(\tfrac12 - \tfrac d4\right)\tfrac1a\nabla a\otimes\nabla a + \tfrac12(\Delta a - \nabla a\cdot\nabla V)I \\ & && + a\nabla^2 V + \tfrac12(\nabla V\otimes\nabla a + \nabla a\otimes\nabla D) \ge \lambda I \end{aligned}$$

*Then*

$$H[u(t)] \le e^{-2\lambda t}H[u(0)], \quad t\ge 0$$

# Nonsymmetric Fokker-Planck equations

$$\partial_t u = \mathrm{div}[D(x)(\nabla u + u(\nabla V + F(x)))] \quad \text{in } \mathbb{R}^d,$$

- Assume: $\mathrm{div}(DFu_\infty) = 0$ in $\mathbb{R}^d \Rightarrow u_\infty = ce^{-V}$ is still steady state
- Operator $\mathrm{div}(D(\nabla u + u\nabla V)) = \mathrm{div}(Du_\infty \nabla(u/u_\infty))$ symm. in $L^2(u_\infty^{-1})$
- Operator $\mathrm{div}(DuF)$ is skew-symmetric in $L^2(u_\infty^{-1})$
  $\Rightarrow$ evolution $=$ symmetric $+$ skew-symmetric
- Entropy production: (some computations needed)

$$\frac{dH}{dt}[u] = -\int_{\mathbb{R}^d} \phi(\rho)\nabla\rho^\top D\nabla\rho u_\infty dx - \int_{\mathbb{R}^d} \phi(\rho) \underbrace{\mathrm{div}(DFu_\infty)}_{=0} dx$$

- Entropy and entropy production are independent of $F$
- Prove as before that $\frac{d^2H}{dt^2} + 2\lambda\frac{dH}{dt} \geq 0$
- Implies exponential decay for non-symmetric equation
- Bolley/Gentil 2010: Assumption $\mathrm{div}(DFu_\infty) = 0$ not necessary

# Degenerate Fokker-Planck equations

$$\partial_t u = \mathrm{div}(D\nabla u + Cxu) \quad \text{in } \mathbb{R}^d, \qquad u(0) = u_0$$

- Matrix $D \in \mathbb{R}^{d\times d}$ constant and degenerate, $C \in \mathbb{R}^{d\times d}$
- Assumption ❶: $\forall v$: $C^\top v = \lambda_C v \Rightarrow v \notin \ker(D)$
  Consequence: $u_0 \in L^1 \Rightarrow u \in C^\infty(\mathbb{R}_+ \times \mathbb{R}^d)$ (hypoellipticity)
- Assumption ❷: $\forall \lambda_C$ eigenvalues of $C^\top$: $\mathrm{Re}(\lambda_C) > 0$
  Consequence: Drift towards $x = 0$ due to confinement potential

**Theorem (Erb/Arnold 2014)**

*Let assumptions hold, $\mu = \min\{Re(\lambda_C)\}$. Then $\exists\ c_0 > 0$:*

$$H[u(t)] \le c_0 e^{-2\mu t} H[u_0], \quad t > 0$$

*if all $\lambda \in \sigma(C)$ with $Re(\lambda) = \mu$ are non-defective (i.e. geometric = algebraic multiplicity), otherwise reduced rate $2(\mu - \varepsilon)$, $\varepsilon > 0$.*

Idea of proof: $\frac{dH}{dt}[u] = 0$ for $u \neq u_\infty$ possible, thus use modified functional

$$I[u] = \int_{\mathbb{R}^d} \phi''(\rho)\nabla\rho^\top P \nabla\rho u_\infty dx, \qquad P \text{ positive definite}$$

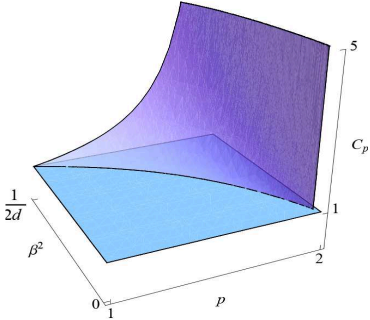
# Generalized Beckner inequalities

$$\frac{1}{\alpha-1}\left(\int_{\mathbb{R}^d} u^\alpha \mu dx - \left(\int_{\mathbb{R}^d} u\mu dx\right)^\alpha\right) \le \frac{2}{\alpha\lambda}\int_{\mathbb{R}^d} D(x)|\nabla u^{\alpha/2}|^2 \mu dx$$

- Valid for $u^{\alpha/2} \in H^1(\mathbb{R}^d;\mu)\cap L^{2/\alpha}(\mathbb{R}^d;\mu)$, $1<\alpha\le 2$
- If $\mu(x) = e^{-|x|^2/2}$, $D(x)=1$ then $\lambda = 1$ for all $1<\alpha\le 2$
- Question: Determine $\lambda$ for $D(x)\neq$ const.? (Matthes/A.J./Toscani '11)

Example: Linearized fast-diffusion eq. $\partial_t u = D(x)\Delta u - x\cdot\nabla u$

- $D(x) = \alpha^2 + \beta^2|x|^2$
- $\mu(x) = C(\alpha^2+\beta^2|x|^2)^{-1-1/(2\beta^2)}$
- $\beta > 0$: no Sobolev inequality and $\lambda \to 0$ as $\alpha \to 1$
- Pointwise Bakry-Emery approach ($\Gamma_2 \ge \lambda\Gamma$) does not work
- Idea: Use integral expressions
- Figure: $p = 2/\alpha$, $C_p = 2/(\alpha\lambda)$



# ❺ Nonlinear Fokker-Planck equations

Aim: Extend Bakry-Emery method to

$$\partial_t u = \operatorname{div}(\nabla f(u) + u\nabla V) \quad \text{in } \Omega,\ t > 0, \quad u(0) = u_0 \geq 0$$

where $\Omega = \mathbb{R}^d$ or $\Omega$ bounded (with no-flux boundary cond.). Assume

- $f \in C^3$ strictly increasing, $f(0) = 0$, $f(s) \leq \frac{d}{d-1} s f'(s)$, $f''(0) > 0$
- $\Omega$ convex, $\nabla^2 V \geq \lambda > 0$, $\inf_\Omega V = 0$

Example: $f(s) = s^m$ $(m \geq \frac{d}{d-1})$, $V(x) = \frac{\lambda}{2}|x|^2$ for $x \in \mathbb{R}^d$

- Steady state: $u_\infty(x) = (N - \frac{m-1}{2m}|x|^2)_+^{1/(m-1)}$, $N > 0$
- Relative entropy: $H^*[u] = H[u] - H[u_\infty]$, where

$$H[u] = \int_{\mathbb{R}^d} (\Phi(u) + uV(x))dx, \quad \Phi''(u) = \frac{f'(u)}{u}$$

**Theorem (Carrillo/A.J./Markowich/Toscani/Unterreiter 2001)**

*Let $H[u_0] < \infty$. Then, for $t > 0$, $\|u(t) - u_\infty\|_{L^1} \leq e^{-\lambda t} C(H^*[u_0])$.*

# Proof $(f(u) = u^m,\ V(x) = \frac{\lambda}{2}|x|^2)$

**Theorem (Carrillo/A.J./Markowich/Toscani/Unterreiter 2001)**

*Let $H[u_0] < \infty$. Then, for $t > 0$, $\|u(t) - u_\infty\|_{L^1} \le e^{-\lambda t} C(H^*[u_0])$.*

- Step 1. First time derivative (entropy production)

$$\frac{dH^*}{dt}[u] = -\int_{\mathbb{R}^d} u|\nabla(h(u) + V)|^2 dx \le 0, \quad h(u) = \frac{m}{m-1}u^{m-1}$$

- Step 2. Second time derivative

$$\frac{d^2H^*}{dt^2}[u] = -2\lambda\frac{dH^*}{dt}[u] - 2R(t)$$

$$R(t) = \int_{\mathbb{R}^d} u^m\big((m-1)(\Delta(h(u) + V))^2 + |\nabla^2(h(u) + V)|^2\big)dx \ge 0$$

$$\Rightarrow \quad \frac{d^2H^*}{dt^2}[u] \ge -2\lambda\frac{dH^*}{dt}[u]$$

# Proof $(f(u) = u^m,\ V(x) = \frac{\lambda}{2}|x|^2)$

$$\frac{d^2 H^*}{dt^2}[u] \geq -2\lambda \frac{dH^*}{dt}[u]$$

- Step 3. Functional inequality: integrate, use $\lim_{t\to\infty} \frac{dH^*}{dt}[u(t)] = 0$

$$\frac{dH^*}{dt}[u(t)] \leq -2\lambda H^*[u_0] \ \Rightarrow H^*[u(t)] \leq e^{-2\lambda t} H^*[u_0]$$

- Step 4. Csiszár-Kullback inequality: introduce $\widehat{u} = \alpha u 1_{\{|x|\leq R\}}$

$$\|u - u_\infty\|_{L^1} \leq \underbrace{\|u - \widehat{u}\|_{L^1}}_{\leq H^*[u]^{1/2}} + \underbrace{\|\widehat{u} - u_\infty\|_{L^1}}_{Ce^{-\lambda t}} \leq Ce^{-\lambda t}$$

Question: Does entropy production ineq. relate to functional ineq.? Yes:

Gagliardo-Nirenberg inequality: Let $1 < p < 2$, $u \in H^1(\mathbb{R}^d) \cap L^p(\mathbb{R}^d)$:

$$\|u\|_{L^{p/2+1}} \leq C\|\nabla u\|_{L^1}^{\theta} \|u\|_{L^p}^{1-\theta}, \quad \theta = \frac{d(2-p)}{(2+p)(d(2-p)+2p)}$$

Proof: Show $\int_{\mathbb{R}^d} v^m dx \leq A \int_{\mathbb{R}^d} |\nabla v^{m-1/2}|^2 dx + B(\int_{\mathbb{R}^d} v dx)^\gamma$, $m = \frac{p+2}{2p}$

# Summary

Let $u(t)$ solve $\partial_t u + A(u) = 0$, let $u_\infty$ solve $A(u_\infty) = 0$.
Define entropy $H[u]$. Entropy method:

- Compute $dH/dt$ and $d^2H/dt^2$
- Show that $d^2H/dt^2 + \kappa dH/dt \geq 0 \Rightarrow H[u(t)] \leq e^{-\kappa t} H[u(0)]$

- Csiszár-Kullback inequality gives exponential $L^1$ decay rate:

$$\|u(t) - u_\infty\|_{L^1} \leq e^{-(\kappa/2)t} C(H[u(0)]), \quad t > 0$$

- Also yields convex Sobolev inequality with explicit constant:

$$\text{entropy} = H[u] \leq \kappa^{-1}\Big(-\frac{dH}{dt}[u]\Big) = \kappa^{-1} \times \text{entropy production}$$

- Applies to Markov processes (see book of Bakry/Gentil/Ledoux '14)
- Also yields intermediate asymptotics of type $\|u(t) - U(t)\|_{L^1} \leq Ct^{-\gamma}$
- Very robust for nonsymm./degenerate/nonlinear diffusion equations

Problem: Many integration by parts are needed – make them systematic!

# Overview

1. Introduction
2. Entropies
3. Fokker-Planck equations
   - Bakry-Emery approach
   - Extensions
4. Systematic integration by parts
5. Cross-diffusion systems
   - Examples from physics and biology
   - Derivation, gradient flows
   - Boundedness-by-entropy method
   - Extensions
6. Uniqueness of weak solutions
7. Towards discrete entropy methods
   - Time-continuous Markov chains
   - Time-discrete entropy methods

# Systematic integration by parts: Motivation

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

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

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

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

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

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

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

# Idea of method

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

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

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

- Standard integration by parts:

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

- Formalization of integration by parts:

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

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

# Integration-by-parts rules

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

Question: How many independent rules of integration by parts?

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

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

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

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

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

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

# Integration-by-parts rules

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

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

Nonnegativity of entropy production follows ...

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

... from solution of decision problem:

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

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

# Solution of decision problem

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

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

Reductions:

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

# Entropies for thin-film equation

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

- Shift polynomials:

$$T_1(\xi) = (\alpha+\beta-3)\xi_1^4 + 3\xi_1^2\xi_2,$$
$$T_2(\xi) = (\alpha+\beta-2)\xi_1^2\xi_2 + \xi_2^2 + \xi_1\xi_3$$
$$T_3(\xi) = (\alpha+\beta-1)\xi_1\xi_3 + \xi_4$$

- Decision problem:

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

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

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

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

# Bakry-Emery revisited

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

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

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

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

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

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

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

# Shift polynomials

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

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

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

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

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

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

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

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

# Solution of decision problem

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

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

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

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

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

**Theorem**

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

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

# Summary

## Systematic integration by parts

- Formulate $\int_\Omega(\cdots)dx \geq 0$ as polynomial $S(\xi)$
- Determine shift polynomials $T_1(\xi), \ldots, T_n(\xi)$
- Solve decision problem $\exists c_1, \ldots, c_n \in \mathbb{R} : \forall \xi \in \mathbb{R}^m$:

$$(S + c_1 T_1 + \cdots + c_n T_n)(\xi) \geq 0$$

- Can be solved by quantifier elimination in an algorithmic way

**What comes next?** Entropy methods are also useful for ...

- Structural information for diffusion systems (gradient flows)
- Gradient estimates and existence analysis for cross-diffusion systems
- Positivity, $L^\infty$ bounds, uniqueness of weak solutions, structure-preserving numerical discretizations

# Overview

# Cross-diffusion systems

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

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

Why study cross-diffusion systems?

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

# Example ❶: Cross-diffusion population dynamics

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

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

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

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

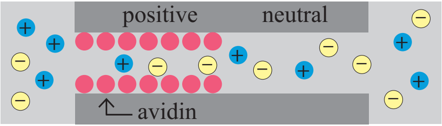
# Example ❷: Ion transport through nano-pores

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

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

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

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



# Example ❸: Tumor-growth modeling

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

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

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

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

# Example ❹: Multicomponent gas mixtures

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

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

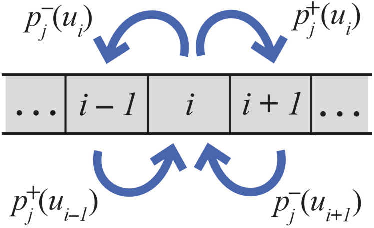
$$A(u) = \frac{1}{\delta(u)} \begin{pmatrix} d_2 + (d_0 - d_2)u_1 & (d_0 - d_1)u_1 \\ (d_0 - d_2)u_2 & d_1 + (d_0 - d_1)u_2 \end{pmatrix}$$

- Application: Patients with airway obstruction inhale Heliox (helium-oxygen mixture) 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
- Uphill diffusion possible
- Boudin/Grec/Salvarani 2013: Derivation from Boltzmann equation for simple mixtures

# Derivation of cross-diffusion models

Starting models:

1. Random-walk lattice model
2. Continuum fluid model
3. System of Boltzmann equations
4. Stochastic differential equations describing many-particle system




## ❶ Random-walk lattice model:

Single species: one space dimension to simplify

- Master equation: time variation = incoming − outgoing

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

- Taylor expansion: ($h$ = grid size)

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

# Derivation from on-lattice model

- Taylor expansion: $u(x_{i\pm 1}) - u(x_i) = \pm h\partial_x u(x_i) + \frac{1}{2}h^2\partial_x^2 u(x_i) + O(h^3)$
- Diffusion scaling: $t \mapsto t/h^2 \Rightarrow \partial_t \rightsquigarrow h^2\partial_t$

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

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

Multiple species:

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

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

- Taylor expansion, diffusion scaling and limit $h \to 0$ leads to system of diffusion equations $\partial_t u_j = \partial_x(\sum_k A_{jk}(u)\partial_x u_k)$
- Multi-dimensional case analogous

# Derivation from continuum fluid model

Example: two-species system

- Transition rates $p_j(u) = a_{j0} + a_{j1}u_1 + a_{j2}u_2$, $j = 1, 2$
- Diffusion matrix $A = (A_{jk}(u)) \rightsquigarrow$ population model

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

❷ Continuum fluid model:

- Mass and force balance equations:

$$\partial_t\rho_i + \operatorname{div}(\rho_i v_i) = 0, \ \varepsilon(\partial_t(\rho_i v_i) + \operatorname{div}(\rho_i v_i \otimes v_i)) - \operatorname{div} T_i - p\nabla\rho_i = f_i$$
$$f_i = \sum_{j=1}^N k_{ij}(v_j - v_i)\rho_i\rho_j, \quad i = 1, \ldots, N$$

- Properties: $\sum_{i=1}^N \rho_i = 1$, $\sum_{i=1}^N \rho_i v_i = 0$, $\sum_{i=1}^N f_i = 0$
- Interphase pressure: $p\nabla\rho_i$, $p$: phase pressure (Drew/Segel 1971)
- Assumptions: inertia approximation ($\varepsilon = 0$), $k := k_{ij}$, stress tensor: $T_i = -\rho_i(p\mathrm{Id} + P_i)$, $P_i$: isotropic pressures, $P_N = 0$

# Derivation from continuum fluid model

$$\partial_t \rho_i + \operatorname{div}(\rho_i v_i) = 0, \quad -\operatorname{div} T_i - p\nabla\rho_i = f_i = \sum_{j=1}^N k_{ij}(v_j - v_i)\rho_i\rho_j$$

- Consequence of $k := k_{ij}$: $f_i = -k\rho_i v_i$
- Consequence of pressure: $-\operatorname{div} T_i - p\nabla\rho_i = \rho_i\nabla p + \operatorname{div}(\rho_i P_i)$
- Add all force balance equations:

$$0 = \sum_{i=1}^N f_i = \sum_{i=1}^N \big(\rho_i\nabla p + \operatorname{div}(\rho_i P_i)\big) = \nabla p + \sum_{i=1}^{N-1} \operatorname{div}(\rho_i P_i)$$

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

$$\partial_t \rho_i + \sum_{j=1}^{N-1} \operatorname{div}(A_{ij}(\rho)\nabla\rho_j) = 0, \quad i = 1, \ldots, N-1$$

Example: $N = 3$, $P_1 = \rho_1$, $P_2 = \beta\rho_2(1+\theta\rho_1)$ $\rightsquigarrow$ tumor-growth model

$$A(\rho) = \begin{pmatrix} 2\rho_1(1-\rho_1) - \beta\theta\rho_1\rho_2^2 & -2\beta\rho_1\rho_2(1+\theta\rho_1) \\ -2\rho_1\rho_2 + \beta\theta\rho_2^2(1-\rho_2) & 2\beta\rho_2(1-\rho_2)(1+\theta\rho_1) \end{pmatrix}$$

# Cross-diffusion systems

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

Main features:

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

Objectives:

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

Mathematical difficulties:

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

# Previous results

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

Global existence if . . .

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

Unexpected behavior:

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

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

# Abstract gradient flows

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

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

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

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

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

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

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

# Gradient flows: Cross-diffusion systems

## Main assumption

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

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

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

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

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

Consequences:

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

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

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

# Example ❶: Population-dynamics model

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

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

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

- Entropy:

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

- Entropy production:

$$\begin{aligned}\frac{dH}{dt}[u] &= \int_\Omega \left(\frac{\log u_1}{a_{12}}\partial_t u_1 + \frac{\log u_2}{a_{21}}\partial_t u_2\right)dx \\ &= -2\int_\Omega \bigg(\frac{2}{a_{12}}(a_{10}+a_{11}u_1)|\nabla\sqrt{u_1}|^2 + \frac{2}{a_{21}}(a_{20}+a_{22}u_2)|\nabla\sqrt{u_2}|^2 \\ &\qquad + |\nabla\sqrt{u_1u_2}|^2\bigg)dx \le 0\end{aligned}$$

# Example ❶: Population-dynamics model

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

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

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

Answer: Yes!

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

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

- New diffusion matrix:

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

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

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

# Example ❷: Ion-transport model

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

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

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

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

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

- Entropy production:

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

# Example ❷: Ion-transport model

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

- Entropy production:

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

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

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

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

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

# Relation to nonequilibrium thermodynamics

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

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

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

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

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

- Open problem: Include nonconstant temperature

# Boundedness-by-entropy method

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

Assumptions:

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

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

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

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

# Boundedness-by-entropy method

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

Assumptions:

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

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

**Theorem (A.J. 2014)**

*Let the above assumptions hold, let $D \subset \mathbb{R}^n$ be bounded, $u_0 \in L^1(\Omega) \cap \overline{D}$. Then $\exists$ global weak solution such that $u(x, t) \in \overline{D}$ and*
$$u \in L^2_{\mathrm{loc}}(0, \infty; H^1(\Omega)), \quad \partial_t u \in L^2_{\mathrm{loc}}(0, \infty; H^1(\Omega)')$$

# Boundedness-by-entropy method

**Theorem (A.J. 2014)**

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

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

Remarks:

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

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

# Proof of existence theorem

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

Key ideas:

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

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

# Proof of existence theorem

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

More details:

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

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

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

# Step ❶: Lax-Milgram argument

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

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

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

**Theorem (Leray-Schauder)**

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

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

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

# Step ❷: Leray-Schauder argument

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

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

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

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

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

# Step ❸: Uniform estimates

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

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

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

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

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

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

Remarks:

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

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

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

- Nonlinear Aubin-Lions lemma:

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

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

# Summary

**Theorem (A.J. 2014)**

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

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

Strategy of the proof:

- Implicit Euler discretization and $\Delta^m$ regularization
- Entropy formulation gives a priori estimates and $L^\infty$ bounds
- Compactness from nonlinear Aubin-Lions lemma

Benefits:

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

Limitations:

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

# ❶ Population model of Shigesada-Kawasaki-Teramoto

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

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

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

- Yields estimate for $(\sqrt{u_i})$ in $H^1(\Omega)$: Previous proof applies
- Main difference: We do not have $(u_i)$ bounded in $L^\infty(\Omega)$ but only $(u_i)$ bounded in $L^6(\Omega)$ (if space dimension $\leq 3$)
- Assumption: Transition rates $p_i(u) = a_{i0} + a_{i1}u_1 + a_{i2}u_2$
- What about more general transition rates?

# General population models

- General systems derived from on-lattice model can be written as

$$\partial_t u_i = \mathrm{div}(A(u)\nabla u)_i = \Delta(u_i p_i(u)), \quad p_i: \text{ transition rates}$$

- Population model of Shigesada-Kawasaki-Teramoto: $p_i(u) = a_{i0} + a_{i1}u_1 + a_{i2}u_2$, $i = 1, 2$
- Nonlinear transition rates: $p_i(u) = a_{i0} + a_{i1}u_1^s + a_{i2}u_2^s$, $s > 0$
- Desvillettes/Lepoutre/Moussa 2014: $0 < s < 1$
- A.J. 2014: $0 < s < 4$, $(1 - \frac{1}{s})a_{12}a_{21} \le a_{11}a_{22}$ (weak cross-diffusion)
- Desvillettes/Lepoutre/Moussa/Trescases 2015: $s > 1$ and $(\frac{s-1}{s+1})^2 a_{12}a_{21} \le a_{11}a_{22}$ (less restrictive than above)
- Key idea: Exploit extra regularity using duality method for $\Delta(u_i p_i(u))$

Further generalization: $n \ge 3$ equations

Existence result only under conditions on $a_{ij}$, related to detailed balance principle (Daus/A.J., in progress)

# ❷ Ion-transport model

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

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

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

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

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

- Consequence ❷: By nonlinear Aubin-Lions lemma,

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

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

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

# ❷ Ion-transport model

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

- Aim: Perform limit in

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

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

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

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

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

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

# General ion-transport model

- Existence result valid for $n = 4$ species and transition rate $q_i(u_4) = u_4$
- Generalizes result by Burger/DiFrancesco/Pietschmann/Schlake 2010
- Extension: Let $q_i(u_n) = \beta_i q(u_n)$, $\beta_i > 0$ (Zamponi/A.J. 2015)

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

- Entropy density:

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

- Extension: Transition rates $T_i = p_i(u_i)q(u_n)$ (Zamponi/A.J. 2015)
- Also other choices possible, e.g. $T_i = p_i(u_i) + q_i(u_n)$ (Painter 2009)

Open problems:

- General functions $q_i(u_4)$ or general transition rates $T_i$
- How to determine entropy for general $T_i$? $\forall T_i : \exists$ entropy?

# ❸ Tumor-growth model

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

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

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

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

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

- Entropy production inequality:

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

and $C_\theta > 0$ if and only if $\theta < \theta^* := 4/\sqrt{\beta}$

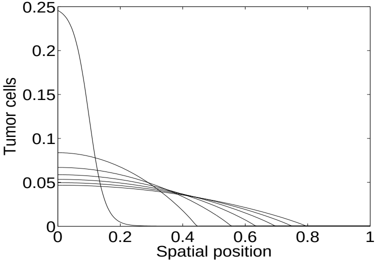
# ❸ Tumor-growth model

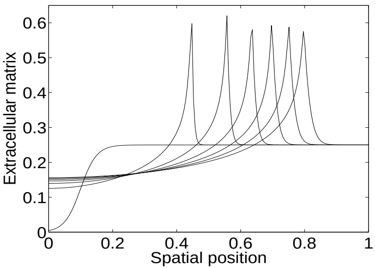
**Theorem (A.J./Stelzer 2012)**

*Let $\theta < 4/\sqrt{\beta}$, $H[u_0] < \infty \Rightarrow \exists$ bounded weak solution with $0 \le u_1, u_2 \le 1$*

Question: What happens for $\theta > \theta^*$?

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




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

# ❹ Multicomponent gas mixtures

$$\partial_t u_i - \operatorname{div} J_i = f_i(u), \quad \nabla u_i = \sum_{j\neq i} c_{ij}(u_j J_i - u_i J_j), \quad i = 1, \ldots, n$$

- No-flux boundary conditions, $u(0) = u_0$ in $\Omega$
- Assume: Isothermal ideal gas mixture, equal molar masses
- Volume fractions $u_i$, fluxes $J_i$
- Problem: $\nabla u_i$ depends on $J_j$ not vice versa, need to invert relation
- Solution: Use linear algebra (Perron-Frobenius theorem)

**Theorem (Perron-Frobenius, special case)**

*Let $C = (C_{ij})$ be quasi-positive ($C_{ij} > 0$ for $i \neq j$), irreducible, $\sum_j C_{ij} = 0$. Then spectrum $\sigma(C) \subset \{0\} \cap \{z \in \mathbb{C} : \mathrm{Re}(\lambda) < 0\}$*

# Matrix analysis

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

- Formulate: $\nabla u = -C(u)J$, $u = (u_1, \ldots, u_n)$, $J = (J_1, \ldots, J_n)$

$$C_{ij} = c_{ij} u_i \text{ for } i \neq j, \quad C_{ii} = -\sum_{j\neq i} c_{ij} u_j, \quad \sum_{i=1}^n J_i = 0$$

- $\sum_j C_{ij} = 0 \Rightarrow C$ has eigenvalue zero $\Rightarrow C$ not invertible
- Perron-Frobenius: Matrix is quasi-positive, irreducible $\Rightarrow$ spectrum $\sigma(-C) \subset \{0\} \cup [\delta, \infty)$ with $\delta = \min_{i,j} c_{ij} > 0$, eigenvalue 0 simple
- Reduction to $n-1$ eqs.: Because of zero eigenvalue, $\exists X \in \mathbb{R}^{n\times n}$:

$$-X^{-1}CX = \begin{pmatrix} C_0 & b \\ 0 & 0 \end{pmatrix}, \quad C_0 \in \mathbb{R}^{(n-1)\times(n-1)}$$

- Matrices $-X^{-1}CX$ and $-C$ are similar:

$$\sigma(C_0) \cup \{0\} = \sigma(-X^{-1}CX) = \sigma(-C) \subset \{0\} \cup [\delta, \infty)$$

- Consequence: $\sigma(C_0) \subset [\delta, \infty)$ and $C_0$ is invertible

# Entropy structure

$$\partial_t u - \operatorname{div} J = f(u), \quad \nabla u = -C(u)J$$

- Let $u' = (u_1, \ldots, u_{n-1})$: $\nabla u' = C_0 J' \Rightarrow J' = C_0^{-1}\nabla u'$
- Solve $\partial_t u' - \operatorname{div}(C_0^{-1}\nabla u') = f'(u)$

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

- Entropy variables: $w_i = \partial h/\partial u_i$ $(i = 1, \ldots, n-1)$
- New diffusion matrix: $B(w) = C_0^{-1}(\nabla^2 h)^{-1}$ symm., positive definite

$$\partial_t u'(w) - \operatorname{div}(B(w)\nabla w) = f'(u'(w)), \ u(w(0)) = u_0, \text{ no-flux b.c.}$$

- Boundedness-by-entropy method applies with $D = (0,1)^n$

**Theorem (A.J./Stelzer 2014)**

*Let $(c_{ij})$ symmetric, $\sum_{i=1}^n f_i(u)\log u_i \le 0$. Then $\exists$ global weak solution $u_i^{1/2} \in L^2_{\mathrm{loc}}(0,\infty; H^1)$, $0 \le u_i \le 1$, $\sum_{i=1}^{n-1} u_i \le 1$*

# Extensions of Maxwell-Stefan models

Limitations: zero barycentric velocity, equal molar masses, isothermal

More realistic models: (see Bothe/Dreyer 2015)

- Include barycentric velocity $v$:

$$\partial_t \rho_i + \operatorname{div}(\rho_i v - J_i) = 0, \quad i = 1, \ldots, n$$
$$\partial_t \rho + \operatorname{div}(\rho v) = 0, \quad \partial_t(\rho v) + \operatorname{div}(\rho v \otimes v) + \nabla p = \rho f + \nu \Delta v$$

  where $\rho$: total mass density, $p$: pressure
- Include molar masses $m_i$: $\rho_i = m_i c_i$ with number densities $c_i$
- Include pressure in driving forces:

$$-\rho_i \nabla \log \frac{c_i}{c} + \nabla p = \sum_{j=1}^{n} c_{ij}(\rho_j J_i - \rho_i J_j), \quad i = 1, \ldots, n$$

  where $c = \sum_{i=1}^{n} c_i$: total number density

Mathematical difficulties and open problems:

- Pressure in compressible Navier-Stokes eqs. not a function of $\rho$
- Maxwell-Stefan relations include $\nabla p$ (regularity issues)

# Summary

Extensions of boundedness-by-entropy method:

1. Population model: Transition rates $p_i(u) = a_{i0} + a_{i1}u_1^s + a_{i2}u_2^s$ with $s < 1$ or $s > 1$, the case $n \geq 3$ being work in progress
2. Ion-transport model: Transition rates $q_i(u_n) = \beta_i u_n$ or nonlinear, valid for all $n \in \mathbb{N}$, yields bounded weak solutions
3. Tumor-growth model: Entropy structure only for pressure coefficients $\theta < \theta^*$, the case $\theta > \theta^*$ being not well understood
4. Maxwell-Stefan model: Needs matrix inversion, extension to more general cases (Navier-Stokes coupling) delicate

Further extensions/questions:

- Different boundary conditions: Dirichlet or Robin conditions
- Drift terms in cross-diffusion systems (e.g. due to electric forces)
- Include general reaction terms (Fischer 2015: renormalized solutions)
- Are weak solutions to population models bounded?

# Supplement: Energy-transport equations

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

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

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

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

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

# Entropy structure

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

Mathematical difficulties:

- Equations are not in divergence form (loss of regularity)
- Equations are strongly coupled and degenerate at $\theta = 0$

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

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

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

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

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

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

# Entropy structure

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

Key ideas:

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

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

- Nonlogarithmic entropies:

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

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

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

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

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

# Global existence

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

**Theorem (Zamponi/A.J. 2015)**

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

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

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

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

- Equilibration to constant steady state $(\rho_D, \theta_D)$:

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

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

# Overview

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3. Fokker-Planck equations
   - Bakry-Emery approach
   - Extensions
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   - Time-continuous Markov chains
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# Uniqueness of weak solutions

Entropy methods useful for ...

- Large.time asymptotics (Bakry-Emery method)
- Understanding the structure of diffusion systems (gradient flows)
- Existence analysis, $L^\infty$ bounds for the solutions

Surprisingly, entropy concept may help to prove uniqueness of solutions

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

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

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

# Example

First idea: Integration by parts

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

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

Second idea: Cauchy-Schwarz inequality

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

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

Third idea: Entropy method (Gajewski 1994)

# Example

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

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

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

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

- Integrate over $t$:

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

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

# A cross-diffusion example

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

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

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

Step ❶: Uniqueness for $u_n$

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

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

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

# $H^{-1}$ method for $u_n$

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

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

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

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

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

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

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

# Entropy method for $u_i$

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

- It holds $d(u,v)\ge\frac{1}{8}\|u-v\|_{L^2}^2$ and

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

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

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

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

**Theorem (Zamponi/A.J. 2015)**

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

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

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

# Overview

# Towards discrete entropy methods

Aims:

- Extend entropy methods to the discrete setting
- Goal: Develop structure-preserving numerical schemes (stable, highly efficient, higher-order accurate)

Main difficulties:

- Proofs need integration by parts and chain rules
- Integration by parts $\rightsquigarrow$ summation by parts
- Extension of chain rule to discrete case is challenging:

$$\nabla f(u) = f'(u)\nabla u \;\rightsquigarrow\; f(u_i) - f(u_{i-1}) = \frac{f(u_i) - f(u_{i-1})}{u_i - u_{i-1}}(u_i - u_{i-1})$$

Problem: many choices for approx. of $f'(u)$, multi-dimens. case?

Possible solutions:

- Design numerical discretizations satisfying particular chain rules
- Minimize use of integrations by parts and chain rules
- Exploit finite-state Markov chain theory

# Discrete-time Markov chains

Markov chain: Describes change of state from time $t$ to $t+1$ of stochastic process $X_t$, $t \in \Sigma$ (finite or countable state space)

- Markov property: transition probability depends on $t$ only
- Transition probability: $p_{ij} = P(X_{t+1} = s_j | X_t = s_i)$
- Transition matrix: $P = (p_{ij})$, $\sum_j p_{ij} = 1$
- Markov chain irreducible if any state reachable from any state
- Markov chain is positive recurrent if first return time is finite
- $\pi$ is stationary distribution (invariant measure) if $\pi P = \pi$ (row vector)

Theorem: If Markov chain is irreducible, positive recurrent, and aperiodic then $\lim_{n\to\infty} P^n = (\pi, \ldots, \pi)^\top$, $\pi$ stationary

# Time-continuous Markov chains

- Let $\Sigma$ be finite or countable state space, $X_t$ time-homogeneous Markov process (i.e. jump probabilities depend on elapsed time)
- Transition probability: $p_t(\xi,\eta) = \delta_\xi(\eta) + tQ(\xi,\eta) + o(t)$ $(t \to 0)$
- Semigroup $S_t$: $(S_t f)(x) = E[f(X_t)|X_0 = x]$ for $f \in L^2(\Sigma)$
- Generator $L$: operator on $L^2(\Sigma)$ such that $S_t = e^{tL}$

Example ❶: Let $Q$ be a (finite or infinite) matrix, $\sum_\eta Q(\xi,\eta) = 0$

- Generator: $(Lf)(\xi) = \sum_\eta Q(\xi,\eta)f(\eta)$ can be identified with $Q$
- Semigroup: $S_t f = e^{tQ} f$ solves ODE system $\partial_t u = Qu$, $u_0 = f$
- Relation to transition probabilities: $(S_t f)(\xi) = \sum_\eta p_t(\xi,\eta)f(\eta)$

Example ❷: Let $Lu = \operatorname{div}(\nabla u + xu)$ be Fokker-Planck operator in $\mathbb{R}^d$

- Semigroup: $S_t f = e^{tL} f$ solves PDE $\partial_t u = Lu$, $u_0 = f$
- Relation to Markov chain: discretize PDE, then $L \rightsquigarrow$ matrix

# Time-continuous Markov chains

- Dual semigroup $S_t^*$: defined by $\int S_t f d\mu = \int f d(S_t^* \mu)$ for measures $\mu$
- Given $\pi > 0$, $S_t^*$ can be identified with $\rho_t$ via $S_t^* \mu = \rho_t \pi$, where $\rho_t$ solves $\partial_t \rho = L^* \rho$ and $L^*$ is adjoint of $L$ in $L^2(\pi)$
- Invariant measure $\pi$: $S_t^* \pi = \pi$ or
$$\int_\Sigma L f d\pi = 0 \quad \text{or} \quad \int_\Sigma S_t f d\pi = \int_\Sigma f d\pi \quad \text{for all } f$$
- Detailed balance or reversible measure: $\exists$ measure $\pi$ such that $\pi(\xi)Q(\xi,\eta) = \pi(\eta)Q(\eta,\xi)$ for all $\xi, \eta \in \Sigma \Leftrightarrow L^* = L$ on $L^2(\pi)$

Example ❶: ODE system $\partial_t u = Qu$

- Dual semigroup: $S_t^* = e^{tL^*}$, where $L^*$ adjoint to $L = Q$ in $L^2(\pi)$
- Invariant measure:
$$0 = \sum_\xi (Lf)(\xi)\pi(\xi) = \sum_{\xi,\eta} Q(\xi,\eta) f(\eta)\pi(\xi) = \sum_\eta \Big( \sum_\xi \pi(\xi) Q(\xi,\eta) \Big) f(\eta)$$
$\Rightarrow \pi Q = 0$ or $\pi = P\pi$, where $P = (p(\xi,\eta))$
- $\pi$ reversible measure satisfies $\pi(\xi)Q(\xi,\eta) = \pi(\eta)Q(\eta,\xi)$

# Time-continuous Markov chains

- Dual semigroup $S_t^*$: defined by $\int S_t f d\mu = \int f d(S_t^*\mu)$ for measures $\mu$
- Given $\pi > 0$, $S_t^*$ can be identified with $\rho_t$ via $(S_t^*\mu) = \rho_t\pi$, where $\rho_t$ solves $\partial_t\rho = L^*\rho$ and $L^*$ is adjoint of $L$ in $L^2(\pi)$
- Invariant measure $\pi$: $S_t^*\pi = \pi$ or
$$\int_\Sigma Lfd\pi = 0 \quad \text{or} \quad \int_\Sigma S_t f d\pi = \int_\Sigma f d\pi \quad \text{for all } f$$
- Detailed balance or reversible measure: $\exists$ measure $\pi$ such that $\pi(\xi)Q(\xi,\eta) = \pi(\eta)Q(\eta,\xi)$ for all $\xi,\eta \in \Sigma \Leftrightarrow L^* = L$ on $L^2(\pi)$

Example ❷: Fokker-Planck operator $Lu = \operatorname{div}(\nabla u + xu)$ in $\mathbb{R}^d$

- $L$ symmetric with respect to $d\pi = e^{|x|^2/2}dx$:
$$\int_{\mathbb{R}^d} Luve^{|x|^2/2}dx = -\int_{\mathbb{R}^d}(\nabla u + xu)\cdot(\nabla v + xv)e^{|x|^2/2}dx = \int_{\mathbb{R}^d} uLve^{|x|^2/2}dx$$
$\Rightarrow \pi$ is reversible measure
- Invariant measure $d\pi = \rho dx$ solves $0 = \int_{\mathbb{R}^d} Lf\rho dx = \int_{\mathbb{R}^d} fL'\rho dx \Rightarrow$ $0 = L'\rho = \Delta\rho - x\cdot\nabla\rho \Rightarrow \rho = \text{const.}$

# Entropy and entropy production

- Relative entropy: $H[\mu|\pi] = \int_\Sigma \rho \log \rho d\pi$, where $\rho = \frac{d\mu}{d\pi}$
- Entropy for functions: For $f \log f \in L^1(\pi)$,

$$\mathrm{Ent}_\pi[f] = \int_\Sigma f \log f d\pi - \int_\Sigma f d\pi \log \int_\Sigma f d\pi$$

  If $f = \frac{d\mu}{d\pi}$ then $\mathrm{Ent}_\pi[f] = H[\mu|\pi]$ ($\pi$ is probability measure)
- $\rho_t = \frac{dS_t^*\mu}{d\pi}$ solves $\partial_t \rho = L^*\rho$, where $L^*$ is adjoint of $L$ in $L^2(\pi)$
- Entropy production:

$$\frac{dH}{dt}[S_t^*\mu|\pi] = \int_\Sigma \partial_t \rho_t \log \rho_t d\pi = \int_\Sigma L^*\rho_t \log \rho_t d\pi = \int_\Sigma \rho_t L \log \rho_t d\pi$$

- Under detailed balance (i.e. $L = L^*$), $\rho_t = \frac{dS_t^*\mu}{d\pi} = S_t \frac{d\mu}{d\pi} =: S_t f$:

$$\frac{dH}{dt}[S_t^*\mu|\pi] = \int_\Sigma S_t f \, L \log S_t f d\pi =: -\mathcal{E}(S_t f, \log S_t f)$$

# Exponential decay

$$\frac{dH}{dt}[S_t^*\mu|\pi] = -\mathcal{E}(S_t f, \log S_t f), \quad S_t f = \frac{dS_t^*\mu}{d\pi}$$

- Exponential decay: If $\mathrm{Ent}_\pi[f] \le \kappa^{-1}\mathcal{E}(f, \log f)$ then

$$\frac{dH}{dt}[S_t^*\mu|\pi] \le -\kappa\,\mathrm{Ent}_\pi[S_t f] = -\kappa H[S_t^*\mu|\pi] \;\Rightarrow\; H[S_t^*\mu|\pi] \le e^{-\kappa t} H[\mu|\pi]$$

- Question: How to prove $\mathrm{Ent}_\pi[f] \le \kappa^{-1}\mathcal{E}(f, \log f)$?
- Dai Pra/Posta 2014: Compute second time derivative

$$\frac{d^2}{dt^2}\mathrm{Ent}_\pi[S_t f] = \int_\Sigma \left( L^2 S_t f \log S_t f + \frac{(LS_t f)^2}{S_t f} \right) d\pi$$
$$\ge \kappa \mathcal{E}(S_t f, \log S_t f) = -\kappa \frac{d}{dt}\mathrm{Ent}_\pi[S_t f]$$

- Integration from 0 to $\infty$ yields

$$-\mathcal{E}(S_0 f, \log S_0 f) = \frac{d}{dt}\mathrm{Ent}_\pi[S_0 f] \le -\kappa\,\mathrm{Ent}_\pi[S_0 f]$$

$\Rightarrow$ Desired estimate $\mathrm{Ent}_\pi[S_0 f] = \mathrm{Ent}_\pi[f] \le \kappa^{-1}\mathcal{E}(f, \log f)$

# Verification of inequality

It remains to prove:

$$\kappa\mathcal{E}(f,\log f) \leq \int_\Sigma (L^2 f \log f + f^{-1}(Lf)^2)d\pi$$

- Generator: $Lf(\xi) = \sum_\eta Q(\xi,\eta)(f(\xi) - f(\eta))$, $Q$: jump rates
- Under detailed balance,

  $$\mathcal{E}(f,\log f) = -\frac{1}{2}\sum_{\xi,\eta} Q(\xi,\eta)(f(\xi) - f(\eta))(\log f(\xi) - \log f(\eta)) \geq 0$$

  and thus, $\frac{dH}{dt}[S_t^*\mu|\pi] = -\mathcal{E}(f,\log f) \leq 0$, $f = \frac{d\mu}{d\pi}$
- Computation of $L^2 f \log f + f^{-1}(Lf)^2$ much more involved!

Approach ❶: Caputo/Dai Pra/Posta 2009

- Employ certain (Bochner) identity and convexity of log terms
- Involves $R(\xi,\eta)$, can to be determined in special cases

Approach ❷: Mielke 2013

Write Markov chain as a gradient flow, apply gradient-flow techniques

# Discretized Fokker-Planck equation

One-dimensional Fokker-Planck equation: $u_\infty(x) = e^{-V(x)}$ (Mielke 2013)

$$\partial_t u = \partial_x(\partial_x u + u\partial_x V) = \partial_x\left(u_\infty \frac{u}{u_\infty}\partial_x\left(\log\frac{u}{u_\infty}\right)\right) \text{ in } \Omega, \text{ no-flux b.c.}$$

Finite-volume approx.: $u_i(t) = h^{-1}\int_{x_{i-1}}^{x_i} u(x,t)dx$, $x_i = hi$, $\rho_i = \frac{u_i}{u_{\infty,i}}$

$$\partial_t u = -D^\top L D \log\rho, \quad L = \operatorname{diag}(\kappa_i L_i), \quad L_i = \frac{\rho_{i+1}-\rho_i}{\log\rho_{i+1} - \log\rho_i}$$

$\rightarrow$ gives Markov chain model with $Q$: tridiagonal matrix

- Discrete gradient: $(Du)_i = -h^{-1}(u_{i+1} - u_i)$
- Approximations: $\kappa_i = u_{\infty,i+1}^{1/2} u_{\infty,i}^{1/2}$ approximates $u_{\infty,i}$, $L_i$ approx. $\rho_i$
- Choice of $L$ allows for nonlinear chain rule $\rho\nabla\log\rho = \nabla\rho$:

$$\begin{aligned}(LD\log\rho)_i &= \sum_j L_{ij}(D\log\rho)_j \\ &= -\kappa_i\frac{\rho_{i+1}-\rho_i}{\log\rho_{i+1}-\log\rho_i} h^{-1}(\log\rho_{i+1} - \log\rho_i) = \kappa_i(D\rho)_i\end{aligned}$$

# Discretized Fokker-Planck equation

$$\partial_t u = -D^\top L D \log \rho$$

- Discrete entropy: $H[u] = \sum_i u_i \log(u_i/u_{\infty,i}) =: \langle u, \log \rho\rangle$
- Discrete entropy production:

$$\frac{dH}{dt}[u] = \langle \partial_t u, \log\rho\rangle = -\langle D^\top L D \log\rho, \log\rho\rangle = -\langle D\log\rho, LD\log\rho\rangle$$

- Second time derivative: $\frac{d^2H}{dt^2}[u] = \langle D\log\rho, MD\log\rho\rangle$
- Show that $M \geq 2\mu L \Rightarrow \frac{d^2H}{dt^2} \geq -2\mu\frac{dH}{dt} \Rightarrow$ exponential decay

**Theorem (Mielke 2013)**

*Let $V_{i+1} - 2V_i + V_{i-1} \geq \lambda h^2$. Then $H[u(t)] \leq e^{-2\mu t}H[u(0)]$, where*

$$\mu = \frac{2}{h^2}\Phi\left(\frac{h^2}{8}\lambda\right) \to \lambda \quad \text{as } h\to 0, \qquad \Phi(s) = \frac{3\,\mathrm{Erf}(s^{1/2}) - \mathrm{Erf}(3s^{1/2})}{2\,\mathrm{Erf}(s^{1/2})}$$

Error function: $\mathrm{Erf}(s) = 2\pi^{-1/2}\int_0^s \exp(-t^2)dt$

# Time-discrete entropy methods

Open problems:

- Markov chain approach only possible for linear equations
- Mielke 2013: restricted to one-dimensional eq., quasi-uniform grids
- Erbar-Maas 2014: porous-medium equation, but no exponential decay

New idea: Time discretization instead of space discretization

Motivation: Implicit Euler scheme for $u_k = u(t_k)$

$$\tau^{-1}(u_k - u_{k-1}) = L(u_k), \quad \langle L(u), \phi'(u)\rangle \le 0, \quad \phi \text{ convex}$$

- Example $L = \Delta$ on $\mathbb{R}^d$: $\langle -L(u), \phi'(u)\rangle = \int_{\mathbb{R}^d} \phi''(u)|\nabla u|^2 dx \ge 0$
- Entropy: $H[u_k] = \int_{\mathbb{R}^d} \phi(u_k)dx$
- Multiply equation by $\phi'(u_k)$, assume that $\phi$ is convex:

$$\int_{\mathbb{R}^d}(\phi(u_k)-\phi(u_{k-1}))dx \le \int_{\mathbb{R}^d}(u_k-u_{k-1})\phi'(u_k)dx = \tau\langle L(u_k), \phi'(u_k)\rangle \le 0$$

- Entropy-dissipative scheme: $H[u_k] + \tau\langle -L(u_k), \phi'(u_k)\rangle \le H[u_{k-1}]$

# Time-discrete BDF-2 discretization

Aim: Derive entropy-dissipative higher-order schemes

Continuous equation:

$$\frac{2}{\alpha}u^{1-\alpha/2}\partial_t(u^{\alpha/2}) = \partial_t u = L(u) \text{ in } \Omega, \quad u(0) = u_0, \quad \text{no flux b.c.}$$

- Assume: $\exists$ smooth solution $u(t) \geq 0$
- Entropy: $H[u] = \int_\Omega u^\alpha dx$
- Entropy production: if $\langle L(u), u^{\alpha-1}\rangle \leq 0$,

$$\frac{dH}{dt}[u] = 2\int_\Omega u^{\alpha/2}\partial_t(u^{\alpha/2})dx = \frac{\alpha}{2}\int_\Omega L(u)u^{\alpha-1}dx \leq 0$$

BDF-2 method: BDF = backward differentiation formula

$$\frac{2}{\alpha\tau}v_k^{2/\alpha-1}\left(\frac{3}{2}v_{k+2} - 2v_{k+1} + \frac{1}{2}v_k\right) = L(u_{k+2}), \quad v_k := u_k^{\alpha/2}$$

- Entropy production: $H[u_{k+2}] + \frac{\alpha\tau}{2}\langle -L(u_k), u_k^{\alpha-1}\rangle \leq H[u_0]$
- Only entropy stability, not entropy dissipation

# Time-discrete BDF-2 discretization

$$\frac{2}{\alpha} v_{k+2}^{2/\alpha-1}\left(\frac{3}{2}v_{k+2} - 2v_{k+1} + \frac{1}{2}v_k\right) = L(u_{k+2}), \quad v_k := u_k^{\alpha/2}$$

- Redefine entropy: $H_G[u_{k+2}, u_{k+1}] = \frac{1}{2}\int_\Omega (u_{k+2}^\alpha + (2u_{k+2}^{\alpha/2} - u_{k+1}^{\alpha/2})^2)dx$
- Entropy production: (Bukal-Emmrich-A.J. 2014)

$$H_G[u_{k+2}, u_{k+1}] + \frac{\alpha\tau}{2}\langle -L(u_{k+2}), u_k^{\alpha-1}\rangle \leq H_G[u_{k+1}, u_k]$$

- Questions: ❶ Why is this working? ❷ Can it be generalized?
- Answer ❶: Use inequality

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

- Answer ❷: Yes, use G-stability theory of Dahlquist

# One-leg multistep methods and G-stability

$$\tau^{-1}\rho(E)v_k = L(\sigma(E)v_k), \quad \rho(E)v_k = \sum_{j=0}^{p} \alpha_j v_{k+j}, \; \sigma(E)v_k = \sum_{j=0}^{p} \beta_j v_{k+j}$$

- Implicit Euler $p=1$: $(\alpha_0,\alpha_1)=(-1,1)$, $(\beta_0,\beta_1)=(\frac12,\frac12)$
- BDF-2 $p=2$: $(\alpha_0,\alpha_1,\alpha_2)=(\frac12,-2,\frac32)$, $(\beta_0,\beta_1,\beta_2)=(0,0,1)$
- A-stability: Numer. solution $(v_k)$ of $v'=\lambda v$ decreasing if $\mathrm{Re}(\lambda)<0$
- G-stability: $\exists G \in \mathbb{R}^{p\times p}$ symmetric, positive definite: $\forall (v_k)\in\mathbb{R}^p$:

$$\big(\rho(E)v_k, \sigma(E)v_k\big)_2 \geq \frac12\|V_{k+1}\|_G^2 - \frac12\|V_k\|_G^2$$

  where $(\cdot,\cdot)_2$ scalar product on $\mathbb{R}^d$, $\|V_k\|_G^2 = \sum_{i,j=0}^{p-1} G_{ij}(v_{k+1}, v_{k+j})_2$, and $V_k=(v_k,\ldots,v_{k+p-1})$
- Dahlquist 1963: A-stable scheme $(\rho,\sigma)$ is at most of second order
- Dahlquist 1978: $(\rho,\sigma)$ coprime polynomials: A-stable $\Leftrightarrow$ G-stable
- Consequence: G-stable one-leg method is at most of second order!

# One-leg multistep methods and G-stability

$$\rho(E)v_k = \tau B(\sigma(E)v_k), \quad B(u) = \tfrac{\alpha}{2}u^{1-2/\alpha}L(u^{2/\alpha}), \quad v_k = u_k^{\alpha/2}$$

Claim: G-stability implies discrete entropy dissipation

- Assumption: $\langle L(u), u^{\alpha-1}\rangle \le 0 \Rightarrow \langle B(v), v\rangle \le 0$ for $v = u^{\alpha/2}$
- G-stability: $(\rho(E)v_k, \sigma(E)v_k)_2 \ge \frac{1}{2}\|V_{k+1}\|_G^2 - \frac{1}{2}\|V_k\|_G^2$
- Multiply discrete scheme by $\sigma(E)v_k$:

$$\begin{aligned}\frac{1}{2}\|V_{k+1}\|_G^2 - \frac{1}{2}\|V_k\|_G^2 &\le (\rho(E)v_k, \sigma(E)v_k)_2 \\ &= \tau\langle B(\sigma(E)v_k), \sigma(E)v_k\rangle \le 0\end{aligned}$$

- Entropy dissipation: G-stable scheme dissipates $H[V_k] = \frac{1}{2}\|V_k\|_G^2$
- Remark: $H[V_k] \sim V_k^2 \sim U_k^\alpha$
- Convergence rate: Let $(\rho, \sigma)$ be G-stable, of second order, $p = 2$, $B + \kappa\,\mathrm{Id} \ge 0$ $(\kappa > 0) \Rightarrow \|v_k - u(t_k)^{\alpha/2}\| \le C\tau^2$

# Runge-Kutta methods

Question: Re-definition of $H[u]$ unsatisfactory – Can we do better?
Answer: Use Runge-Kutta methods

$$\partial_t u = L[u], \quad H[u] = \int_\Omega \phi(u)dx$$

- Runge-Kutta discretization (uniform time step $\tau$):

$$u_{k+1} = u_k + \tau \sum_{i=1}^{s} b_i K_i, \quad K_i = L\Big[u_k + \tau \sum_{j=1}^{s} a_{ij} K_j\Big]$$

- Goal: $H[u_k] - H[u_{k-1}] \le 0$
- Idea: Fix $u := u_k$, interpret $v(\tau) := u_{k-1}$ as function of $\tau$
- Define $G(\tau) = H[u] - H[v(\tau)]$

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

- To show: $G'(0) \le 0$ and $G''(0) < 0$ (then $G''(\xi) \le 0$ for $\tau \ll 1$)

# Runge-Kutta methods

$$\int_\Omega (\phi(u_k) - \phi(u_{k-1}))dx = H[u] - H[v(\tau)] = G(\tau) = \tau G'(0) + \tfrac{1}{2}\tau^2 G''(\xi)$$

- Solvability for $v(\tau) = u_{k-1}$, given $u = u_k$: implicit function theorem
- To show:

$$G'(0) = \int_\Omega \phi'(u)L[u]dx \le 0, \quad C_{\mathrm{RK}} = 2\sum_{i=1}^s b_i \Big(1 - \sum_{j=1}^s a_{ij}\Big)$$

$$G''(0) = -\int_\Omega \big(C_{\mathrm{RK}}\phi'(u)DL[u](L[u]) + \phi''(u)L[u]^2\big)dx < 0$$

where $DL[u]$: Fréchet derivative of $L$ at $u$

- Runge-Kutta constant $C_{\mathrm{RK}}$:

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

# Example ❶: Diffusion equation

$$\partial_t u = L[u] = \operatorname{div}(a(u)\nabla u) \quad \text{in } \Omega, \quad a(u)\nabla u \cdot \nu = 0 \quad \text{on } \partial\Omega$$

- Entropy: $H[u] = \int_\Omega \phi(u)dx$, $\phi(u) = \frac{1}{\alpha(\alpha+1)}u^{\alpha+1}$, $\alpha > 0$
- Derivative: $DL[u](w) = \operatorname{div}(a'(u)w\nabla u + a(u)\nabla w) = \Delta(a(u)w)$

$$G'(0) = \int_\Omega \phi'(u)\operatorname{div}(a(u)\nabla u)dx = -\int_\Omega \phi''(u)a(u)|\nabla u|^2 dx \le 0$$

$$G''(0) = \int_\Omega \big(C_{\mathrm{RK}}\phi'(u)\Delta(a(u)L[u]) - \phi''(u)L[u]^2\big)dx$$

$$= -\int_\Omega \bigg((C_{\mathrm{RK}}+1)\phi''(u)\mu(u)^2\xi_L^2 + (C_{\mathrm{RK}}+2)\mu'(u)\mu(u)\xi_L\xi_G^2 + \frac{\mu(u)^2}{\phi''(u)}\xi_G^4\bigg)dx, \qquad \mu(u) = \frac{a(u)}{\phi''(u)}$$

- Polynomial variables: $\xi_L = \Delta\phi'(u)$, $\xi_G = |\nabla\phi'(u)|$
- Solve by systematic integration by parts

# Example ❶: Diffusion equation

- Integration-by-parts formulas:

$$0 \le \int_\Omega \operatorname{div}\Big(A(u)(\nabla^2\phi'(u) - \Delta\phi'(u)I)\cdot\nabla\phi'(u)\Big)dx, \ \text{since } \Omega \text{ convex}$$

$$0 = \int_\Omega \operatorname{div}\big(B(u)|\nabla\phi'(u)|^2\nabla\phi'(u)\big)dx$$

- How to find $A(u)$ and $B(u)$? Leads to nonlinear ODE system
- Idea: Special solutions or more specific diffusion equations
- Choose $A'(u) = -\frac{2}{3}(C_{\mathrm{RK}}+2)\mu(u)\mu'(u)\phi''(u)$, $B(u) = \frac{1}{3}(C_{\mathrm{RK}}+2)\mu(u)\mu'(u)$ to cancel mixed terms
- Discrete entropy dissipation if $A(u) \ge 0$ and

$$\left(1-\frac{1}{d}\right)A(u) + (C_{\mathrm{RK}}+1)\phi''(u)\mu(u)^2 \le 0$$

$$(C_{\mathrm{RK}}+2)\mu(u)\mu''(u) + (C_{\mathrm{RK}}-1)\mu'(u)^2 < 0$$

# Example ❶: Diffusion equation

**Theorem (A.J./Schuchnigg 2015)**

*Let $\Omega$ be convex, $k \in \mathbb{N}$, $u_k$ Runge-Kutta solution ($\neq$ steady state). Let*

$$A(u) = \frac{2}{3}(C_{RK}+2)\int_{u_0}^{u} \mu(s)\mu'(s)\phi''(s)ds \geq 0,$$
$$\left(1-\tfrac{1}{d}\right) A(u) + (C_{RK}+1)\phi''(u)\mu(u)^2 \leq 0$$
$$(C_{RK}+2)\mu(u)\mu''(u) + (C_{RK}-1)\mu'(u)^2 < 0$$

*Then there exists $\tau_k > 0$ such that for all $0 < \tau \leq \tau_k$,*

$$H[u_k] + \tau \int_\Omega \phi''(u_k)a(u_k)|\nabla u_k|^2 dx \leq H[u_{k-1}]$$

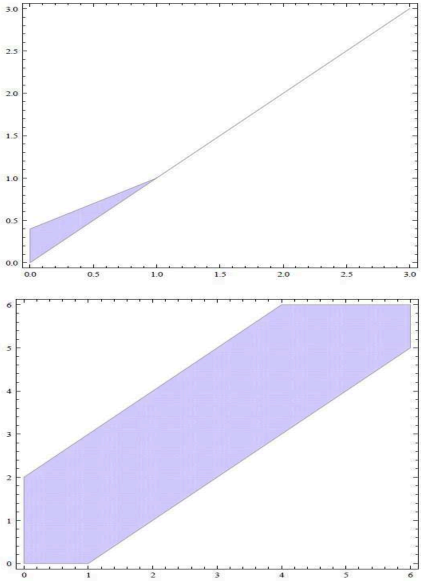
- Same conditions as in Liero-Mielke 2013
- Gives local entropy-dissipation estimate, possibly $\tau_k \to 0$ as $k \to \infty$
- Numerical experiments indicate that $\exists\ \tau^*$: $\tau_k \geq \tau^* > 0$
- If $\int_\Omega \phi''(u)a(u)|\nabla u|^2 dx \geq \kappa H[u]$ then $H[u_k] \leq (1+\tau^*\kappa)^{-k} H[u_0]$

# Example ❷: Porous-medium equation

$$\partial_t u = \Delta(u^\beta) \quad \text{in } \Omega$$

- Compute $A(u)$ and $B(u)$ for $a(u) = \beta u^{\beta-1}$, $\phi(u) = \frac{u^\alpha}{\alpha(\alpha+1)}$
- Top figure: Admissible region $(\alpha, \beta)$ for $d = 2$
- Yields entropy dissipation
- Admissible region not optimal

- Ansatz: $A(u) = c_A u^{2\beta-\alpha-1}$, $B(u) = c_B u^{2\beta-2\alpha-1}$
- Solve decision problem by computer algebra system
- Bottom figure: Admissible region $(\alpha, \beta)$ for $d = 2$



# Summary

Time-continuous Markov chains

- Entropy dissipation for logarithmic entropy
- Exponential decay for special cases: Caputo/Dai Pra/Posta 2009 (discrete Bochner identity) and Mielke 2013 (matrix analysis)
- Heavy computations, so far only for linear situations

Space-discrete diffusion equations:

- Only one result by Mielke 2013 for linear Fokker-Planck equation
- Porous-medium equation: work in progress (A.J.-Yue)

Time-discrete diffusion equations:

- One-leg multistep: Entropy stability for BDF-2, entropy dissipation for schemes of order $p \leq 2$, but only for G-matrix entropy
- Runge-Kutta: entropy dissipation using systematic integr. by parts

Many open problems for discrete entropy methods!

# Total summary

## Bakry-Emery approach

- Exponential time decay for diffusion equations, very flexible method, applicable to nonlinear equations, non-constant coefficients etc.
- Yields convex Sobolev inequalities, sometimes with optimal constants
- Systematic integration by parts by solving polynomial decision problems

## Cross-diffusion systems

- Formal gradient-flow or entropy structure
- Global existence analysis, $L^\infty$ bounds, uniqueness of weak solutions

## Discrete entropy methods

- Spatial discretization: Markov-chain approach of Caputo et al., Mielke
- Time discretization: BDF methods, Runge-Kutta methods

# Open problems

Around Fokker-Planck:

- Large-time asymptotics for nonsymmetric Fokker-Planck-type eqs.
- Exploiting techniques from information theory (entropy power)
- Optimality of systematic integration by parts

Around cross-diffusion:

- Bakry-Emery approach for (cross-) diffusion systems
- Finding entropies for general cross-diffusion systems
- Entropy structure for diffusion systems with temperature
- Coupling Maxwell-Stefan and Navier-Stokes models
- Uniqueness of weak solutions to cross-diffusion systems

Around discrete methods:

- Discrete analogue to Bakry-Emery approach
- Field is widely open for nonlinear equations

# Thank you for your attention!