Entropy dissipation methods for diffusion equations

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**Main references**


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 covered 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

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)
Introduction

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:
  \[ \partial_t h(u) + \partial_x q(u) \leq 0 \]

- 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...)

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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

- $S$ is concave, $\frac{\partial S}{\partial E} > 0$,
- $S$ 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:**
  
  \[
  \begin{align*}
  \partial_t \rho + \text{div}(\rho v) &= 0, \\
  \partial_t (\rho v) + \text{div}(\rho v \otimes v - T) &= 0, \\
  \partial_t (\rho e) + \text{div}(\rho ve + q) &= T : \nabla v
  \end{align*}
  \]

  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
Introduction

Entropies

Fokker-Planck equations
- Bakry-Emery approach
- Extensions

Systematic integration by parts

Cross-diffusion systems
- Examples from physics and biology
- Derivation, gradient flows
- Boundedness-by-entropy method
- Extensions

Uniqueness of weak solutions

Towards discrete entropy methods
- Time-continuous Markov chains
- Time-discrete entropy methods
Example: Heat equation

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

- 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: \( \frac{dH_2}{dt}[u] = 2 \int_{\mathbb{T}^d} (u - u_\infty) \partial_t u \, dx = -2 \int_{\mathbb{T}^d} |\nabla u|^2 \, dx \leq 0 \)
- Poincaré inequality: \( H_2[u] = \| u - u_\infty \|_{L^2}^2 \leq C_P \| \nabla u \|_{L^2}^2 \)
- Combining expressions:

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

- 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**

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

- **Conclusion:** \(\|u(t) - u_\infty\|_{L^2} \leq e^{-C_P^{-1}t}\|u_0 - u_\infty\|_{L^2}\)
- **Same result with spectral theory:** \(C_P^{-1} = \text{first eigenvalue of } -\Delta\)
- **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: \( \partial_t u = -\text{div}(u \nabla \sqrt{\frac{\Delta u}{u}}) \) in \( \mathbb{T}^d \)
- Occurs in quantum semiconductor modeling, \( u \): electron density
- Entropy functional: \( H_1[u] = \int_{\mathbb{T}^d} u \log\left(\frac{u}{u_\infty}\right) dx \)
- Entropy production:
  
  \[
  \frac{dH_1}{dt}[u] = -\int_{\mathbb{T}^d} \text{div}\left(u \nabla \sqrt{\frac{\Delta u}{u}}\right) \log u dx = -\int_{\mathbb{T}^d} \frac{\Delta \sqrt{u}}{\sqrt{u}} \Delta u dx
  \leq -\kappa \int_{\mathbb{T}^d} (\Delta \sqrt{u})^2 dx \leq -\frac{\kappa}{C_P} \int_{\mathbb{T}^d} |\nabla \sqrt{u}|^2 dx \leq -\frac{\kappa}{C_PC_L} H_1[u]
  \]

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

  \[
  H_1[u(t)] \leq e^{-\kappa t/(C_PC_L)} H_1[u_0], \quad t \geq 0
  \]
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: \( H[u] \leq C \langle A(u), H'[u] \rangle \Rightarrow dH/dt \leq -CH \)
- By Gronwall’s inequality, conclude exponential decay: \( H[u(t)] \leq e^{-Ct} H[u_0] \)

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 $\frac{dH}{dt}[u(t)] \leq 0, \; t \geq 0$
- Entropy: $H : D(A) \to \mathbb{R}$ convex Lyapunov functional such that
  - $\exists \Phi \in C^0(\mathbb{R})$: $\Phi(0) = 0$ and
  - $d(u, u_\infty) \leq \Phi(H[u] - H[u_\infty])$ 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

$$H_\alpha[u] = \int_\Omega (u^\alpha - u_\infty^\alpha) dx, \quad F_\alpha[u] = \int_\Omega |\nabla u^\alpha/2|^2 dx, \quad \alpha \geq 1$$
Heat equation revisited

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

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 \( \int_{\mathbb{T}^d} f \, dx = \int_{\mathbb{T}^d} g \, dx = 1 \).

Then, for some \( C_\phi > 0 \),

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

Proof: Taylor expansion of \( \phi \) around 1
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
Linear Fokker-Planck equation

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

- **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

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

**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 ①:** \( \phi(s) = s(\log s - 1) + 1, \quad \phi(s) = s^\alpha - 1 - \alpha(s - 1) \) \( (1 < \alpha \leq 2) \)

**Example ②:** \( \phi(s) = s \log s, \quad V(x) = \frac{1}{2}|x|^2 \) then \( \lambda = 1 \) (optimal!)
Proof: First time derivative

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

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

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

Second time derivative: (key idea!)

\[ \frac{d^2 H_\phi}{dt^2}[u] = - \int_{\mathbb{R}^d} \left( \phi'''(\rho) \partial_t u |\nabla \rho|^2 + 2\phi''(\rho) \nabla \rho \cdot \nabla \partial_t \rho u_\infty \right) \, dx = -l_1 - l_2 \]

First integral:

\[ l_1 = - \int_{\mathbb{R}^d} \nabla (\phi'''(\rho) |\nabla \rho|^2) \cdot (u_\infty \nabla \rho) \, dx \]

\[ = - \int_{\mathbb{R}^d} (\phi'''(\rho) |\nabla \rho|^4 + 2\phi'''(\rho) \nabla \rho \nabla^2 \rho \nabla \rho) u_\infty \, dx \]
Proof: Second time derivative

\[
\frac{d^2 H_\phi}{dt^2} [u] = -l_1 - l_2, \quad l_1 = - \int \phi''''(\rho) |\nabla \rho|^4 + 2 \phi'''(\rho) \nabla \rho \nabla^2 \rho \nabla \rho \, u_\infty \, dx
\]

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

\[
l_2 = 2 \int \phi''(\rho) \nabla \rho \cdot \nabla \partial_t \rho u_\infty \, dx
\]

\[
= 2 \int \phi''(\rho) \left( \nabla \rho \cdot \nabla \Delta \rho - \nabla \rho \nabla^2 \rho \nabla V - \nabla \rho \nabla^2 V \nabla \rho \right) \, dx
\]

\[
\leq 2 \int \phi''(\rho) \left( \text{div}(\nabla^2 \rho \nabla \rho) - |\nabla^2 \rho|^2 - \nabla \rho \nabla^2 \rho \nabla V - \lambda |\nabla \rho|^2 \right) u_\infty \, dx
\]

\[
= 2 \int \left( -\phi''' \nabla \rho \nabla^2 \rho \nabla \rho u_\infty - \phi'' \nabla \rho \nabla^2 \rho \left( \nabla u_\infty + u_\infty \nabla V \right) - \phi'' |\nabla^2 \rho|^2 u_\infty \right) \, dx
\]

\[
- 2\lambda \int \phi''(\rho) |\nabla \rho|^2 u_\infty \, dx, \quad \text{note: } \int \phi''(\rho) |\nabla \rho|^2 u_\infty \, dx = \frac{dH_\phi}{dt}
\]
**Proof: Second time derivative**

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

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

\[
= \int_{\mathbb{R}^d} \left( 2\phi'' |\nabla^2 \rho + \frac{\phi'''}{\phi''} \nabla \rho \otimes \nabla \rho |^2 + \left( \phi'''' - 2\left( \frac{\phi'''}{\phi''} \right)^2 \right) |\nabla \rho|^4 \right) u_\infty dx \geq 0
\]

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

Integrate over $(t, \infty)$:

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

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 decay 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 $\rho = u/u_\infty$: $\int_{\mathbb{R}^d} \rho \, d\pi = \int_{\mathbb{R}^d} u \, dx$
- Relation to previous convex Sobolev inequality:
\[
\int_{\mathbb{R}^d} \phi(\rho) \, d\pi - \phi\left(\int_{\mathbb{R}^d} \rho \, d\pi\right) \leq \frac{1}{\lambda} \int_{\mathbb{R}^d} \phi''(\rho) \, \Gamma(\rho, \rho) \, d\pi
\]

Example 1: $\phi(s) = s(\log s - 1)$ 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 2: $\phi(s) = s^2$ gives Poincaré inequality
\[
\int_{\mathbb{R}^d} \left(\rho - \int_{\mathbb{R}^d} u \, dx\right)^2 \, d\pi \leq \frac{1}{\lambda} \int_{\mathbb{R}^d} \Gamma(\rho, \rho) \, d\pi
\]

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
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

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

- \( \alpha \to 1 \) 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 (Latała/Oleszkiewicz 2000)
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 \(u\), \(N[u] I[u] \geq 2\pi ed\).

- Equivalent formulation: \(4\pi \exp\left(\frac{2}{d} H[u]\right) \leq \frac{8}{ed} \int_{\mathbb{R}^d} |\nabla u^{1/2}|^2 \, dx\)
- 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:

\[
\frac{2}{d} \int_{\mathbb{R}^d} u \log u \, dx = \frac{2}{d} H[u] \leq \frac{2}{\pi ed} \int_{\mathbb{R}^d} |\nabla u^{1/2}|^2 \, dx
\]
Isoperimetric inequality for entropy

**Theorem (Isoperimetric inequality for entropy)**

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

**Proof:**

- $N[u]$ is concave (Costa 1985, Villani 2000) since
  \[ \frac{d^2 N}{dt^2} = \left( \frac{2}{d} \right)^2 N \left( \left( \frac{dH}{dt} \right)^2 - \frac{d}{2} \frac{d^2 H}{dt^2} \right) \leq 0 \]

- Let $v$ solve $\partial_t v = \Delta v$, $v(0) = u$:
  \[ \frac{d}{dt} \left( N[v]I[v] \right) = \frac{2}{d} N \left( I^2 + \frac{d}{2} \frac{dI}{dt} \right) = \frac{2}{d} N \left( \left( \frac{dH}{dt} \right)^2 - \frac{d}{2} \frac{d^2 H}{dt^2} \right) \leq 0 \]

- $N[v(t)]I[v(t)]$ reaches minimum as $t \to \infty \Rightarrow N[v(t)]I[v(t)] \geq m$

- Scaling argument: $m = N[M]I[M]$, where $M(x) = \frac{1}{(2\pi t)^{d/2}} \exp(-|x|^2/2t)$

- Conclusion: $N[u]I[u] = N[v(0)]I[v(0)] \geq N[M]I[M] = 2\pi \varepsilon d$
3 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:
  \[ u(x, t) = (4\pi t)^{-d/2} \int_{\mathbb{R}^d} \exp\left(-\frac{|x - y|^2}{4t}\right) u_0(y) \, dy, \]  thus \( u(t) \to 0 \) in \( L^\infty \) as \( t \to \infty \)

- Entropy is decreasing but
  \[ H_1[u(t)] = \int_{\mathbb{R}^d} u \log u \, dx \leq \int_{\mathbb{R}^d} u(t) \, dx \log \left\| u(t) \right\|_{L^\infty} \to -\infty \quad (t \to \infty) \]

- 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 \( \nu(y, s) = e^{ds} u(e^s y, \frac{1}{2}(e^{2s} - 1)) \)
Relaxation to self-similarity

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

- Function \( v \) solves \( \partial_s v = \text{div}_y(\nabla_y v + yv) \) 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:
  \[ \| v(s) - M \|_{L^1}^2 \leq 2e^{-2s} H_1[u_0], \quad s > 0 \]
- 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

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

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

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

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

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

- \( D(x) = \text{const.}, \quad \nabla^2 V \geq \lambda D^{-1} \) or
- \( D(x) = a(x)I, \quad \left(\frac{1}{2} - \frac{d}{4}\right) \frac{1}{a} \nabla a \otimes \nabla a + \frac{1}{2}(\Delta a - \nabla a \cdot \nabla V)I \)
  \[ + a \nabla^2 V + \frac{1}{2}(\nabla V \otimes \nabla a + \nabla a \otimes \nabla D) \geq \lambda I \]

Then

\[ H[u(t)] \leq e^{-2\lambda t} H[u(0)], \quad t \geq 0 \]
Nonsymmetric Fokker-Planck equations

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

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

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

- 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 \( \text{div}(DFu_\infty) = 0 \) not necessary
Degenerate Fokker-Planck equations

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

- Matrix \( D \in \mathbb{R}^{d \times d} \) constant and degenerate, \( C \in \mathbb{R}^{d \times d} \)
- Assumption 1: \( \forall v: C^\top v = \lambda_C v \Rightarrow v \notin \text{ker}(D) \)
  Consequence: \( u_0 \in L^1 \Rightarrow u \in C^\infty(\mathbb{R}_+ \times \mathbb{R}^d) \) (hypoellipticity)
- Assumption 2: \( \forall \lambda_C \) eigenvalues of \( C^\top \): \( \text{Re}(\lambda_C) > 0 \)
  Consequence: Drift towards \( x = 0 \) due to confinement potential

**Theorem (Erb/Arnold 2014)**

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

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

if all \( \lambda \in \sigma(C) \) with \( \text{Re}(\lambda) = \mu \) 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

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

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

- Valid for $u^\alpha/2 \in H^1(\mathbb{R}^d; \mu) \cap L^{2/\alpha}(\mathbb{R}^d; \mu)$, $1 < \alpha \leq 2$
- If $\mu(x) = e^{-|x|^2/2}$, $D(x) = 1$ then $\lambda = 1$ for all $1 < \alpha \leq 2$
- **Question:** Determine $\lambda$ for $D(x) \neq \text{const}$? (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 $(\Gamma_2 \geq \lambda \Gamma)$ does not work
- **Idea:** Use integral expressions
- **Figure:** $p = 2/\alpha$, $C_p = 2/(\alpha \lambda)$
Nonlinear Fokker-Planck equations

Aim: Extend Bakry-Emery method to

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

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

- $f \in C^3$ strictly increasing, $f(0) = 0$, $f(s) \leq \frac{d}{d-1} sf'(s)$, $f''(0) > 0$
- $\Omega$ 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 \( t > 0 \), \( \| u(t) - u_\infty \|_{L^1} \leq e^{-\lambda t} C(H^*[u_0]) \).

- **Step 1.** First time derivative (entropy production)

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

- **Step 2.** Second time derivative

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

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

  \[
  \Rightarrow \quad \frac{d^2H^*}{dt^2}[u] \geq -2\lambda \frac{dH^*}{dt}[u]
  \]
Proof \((f(u) = u^m, \ V(x) = \frac{\lambda}{2}|x|^2)\)

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

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

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

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

\[
\|u - u_\infty\|_{L^1} \leq \|u - \hat{u}\|_{L^1} + \|\hat{u} - u_\infty\|_{L^1} \leq Ce^{-\lambda t} \\
\leq H^*[u]^{1/2} \leq H^*[u_0]^{1/2} \leq Ce^{-\lambda t}
\]

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

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

Applies to Markov processes (see book of Bakry/Gentil/Ledoux ’14)

Also yields intermediate asymptotics of type $\|u(t) - U(t)\|_{L^1} \leq C t^{-\gamma}$

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 \( \frac{d^2 H}{dt^2} \) requires well chosen integrations by parts.

**Aim:** Make the integrations by parts systematic.

**Motivation:** Consider thin-film equation

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

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

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

  $= \int_\mathbb{T} (u^{\alpha+\beta-1} u_{xxx})_x dx = 0$

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

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

**Question:** How many independent rules of integration by parts?

\[ l_1 = \int_T u^{\alpha+\beta} \left( (\alpha + \beta - 3) \left( \frac{u_x}{u} \right)^4 + 3 \left( \frac{u_x}{u} \right)^2 \frac{u_{xx}}{u} \right) \, dx = 0 \]

\[ l_2 = \int_T u^{\alpha+\beta} \left( (\alpha + \beta - 2) \left( \frac{u_x}{u} \right)^2 \frac{u_{xx}}{u} + \left( \frac{u_{xx}}{u} \right)^2 + \frac{u_x u_{xxx}}{u} \right) \, dx = 0 \]

\[ l_3 = \int_T u^{\alpha+\beta} \left( (\alpha + \beta - 1) \frac{u_x}{u} \frac{u_{xxx}}{u} + \frac{u_{xxxx}}{u} \right) \, dx = 0 \]

**Aim:** Prove that \( \exists c_1, c_2, c_3 \in \mathbb{R} : EP[u] = EP[u] + c_1 l_1 + c_2 l_2 + c_3 l_3 \geq 0 \)

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

- \( EP[u] \) corresponds to \( S(\xi) = -\xi_1 \xi_3 \)
- \( l_1 \) corresponds to \( T_1(\xi) = (\alpha + \beta - 3)\xi_1^4 + 3\xi_1^2 \xi_2 \)
- \( l_2 \) corresponds to \( T_2(\xi) = (\alpha + \beta - 2)\xi_1^2 \xi_2 + \xi_1 \xi_3 + \xi_2^2 \)
- \( l_3 \) corresponds to \( T_3(\xi) = (\alpha + \beta - 1)\xi_1 \xi_3 + \xi_4 \)
Integration-by-parts rules

\[ P[u] \text{ corresponds to } \quad S(\xi) = -\xi_1 \xi_3 \]
\[ l_1 \text{ corresponds to } \quad T_1(\xi) = (\alpha + \beta - 3)\xi_1^4 + 3\xi_1^2 \xi_2 \]
\[ l_2 \text{ corresponds to } \quad T_2(\xi) = (\alpha + \beta - 2)\xi_1^2 \xi_2 + \xi_1 \xi_3 + \xi_2^2 \]
\[ l_3 \text{ corresponds to } \quad T_3(\xi) = (\alpha + \beta - 1)\xi_1 \xi_3 + \xi_4 \]

\( T_i = \text{ integration-by-parts polynomials = shift polynomials } \)

Nonnegativity of entropy production follows . . .

\[ \exists c_1, c_2, c_3 \in \mathbb{R} : \quad P[u] = P[u] + c_1 l_1 + c_2 l_2 + c_3 l_3 \geq 0 \]

. . . from solution of decision problem:

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

- 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 \( \exists \kappa > 0 : \quad EP[u] - \kappa Q[u] \geq 0 \), \( Q[u] \) 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

\[ \partial_t u = \text{div}(\nabla u + u \nabla V) \text{ in } \mathbb{R}^d \]

**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:**
\[
H_\alpha[u] = \frac{\alpha}{4(\alpha - 1)} \left( \int_{\mathbb{R}} \left( \frac{u}{u_\infty} \right)^\alpha u_\infty dx - \left( \int_{\mathbb{R}} u dx \right)^\alpha \right), \quad 1 < \alpha \leq 2
\]

- Set \( w = u^{\alpha/2} \) and compute
\[
\frac{d^2 H_\alpha}{dt^2} = \frac{2}{\alpha} \int_{\mathbb{R}} w^2 \left[ \alpha \left( \frac{w_{xx}}{w} \right)^2 + (2 - \alpha) \left( \frac{w_x}{w} \right)^2 \frac{w_{xx}}{w} \right.
\]
\[
- 2\alpha \frac{w_x}{w} \frac{w_{xx}}{w} V_x - (2 - \alpha) \left( \frac{w_x}{w} \right)^3 V_x + \alpha \left( \frac{w_x}{w} \right)^2 V_x^2 \left] u_\infty dx \right.
\]

- Integrand formulated as polynomial:
\[
S_2(\xi) = \alpha \xi_2^2 + (2 - \alpha) \xi_1 \xi_2 \xi_2 - 2\alpha \xi_1 \xi_2 V_x - (2 - \alpha) \xi_1^3 V_x + \alpha \xi_1^2 V_x^2
\]
Systematic integration by parts

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: \]

\[ S^*(\xi) = (S + c_1 T_1 + c_2 T_2 - c S_1)(\xi) \geq 0 \]
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 \( x = \xi_2^2, \ y = \xi_2 \):

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

- \( S^*(\xi) \geq 0 \) 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 \( \partial_t u = \text{div}(\nabla u + u\nabla V) \) 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

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
Cross-diffusion systems

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

- Meaning: \( \text{div}(A(u) \nabla u)_i = \sum_{j=1}^{n} \text{div}(A_{ij}(u) \nabla u_j), \quad A \in \mathbb{R}^{n \times n}, \quad u \in \mathbb{R}^n \)
- 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 1: Cross-diffusion population dynamics

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

- \( u = (u_1, u_2) \) 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 ②: Ion transport through nano-pores

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

- \((u_1, \ldots, u_N)\) 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 \(0 \leq u_i \leq 1\)
Example 3: Tumor-growth modeling

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

- Volume fractions of tumor cells \( u_1 \), extracellular matrix \( u_2 \), nutrients/water \( u_3 = 1 - u_1 - u_2 \)
- Diffusion matrix: \((\beta, \theta): \text{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 \( 0 \leq u_i \leq 1 \)
Examples from physics and biology

Example 4: Multicomponent gas mixtures

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

- 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

1 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: \( h = \text{grid size} \)

\[
u(x_{i\pm1}) - u(x_i) = \pm h \partial_x u(x_i) + \frac{1}{2} h^2 \partial_x^2 u(x_i) + O(h^3)
\]
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:** \( t \mapsto t/h^2 \Rightarrow \partial_t \sim h^2 \partial_t \)

\[
    h^2 \partial_t u(x_i) = p(u(x_{i-1}) - u(x_i)) + p(u(x_{i+1}) - u(x_i))
    = ph^2 \partial_x^2 u(x_i) + O(h^3)
\]

- **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 $A = (A_{jk}(u)) \sim$ population model

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

2. Continuum fluid model:

- Mass and force balance equations:

$$\partial_t \rho_i + \text{div}(\rho_i \mathbf{v}_i) = 0, \quad \varepsilon(\partial_t (\rho_i \mathbf{v}_i) + \text{div}(\rho_i \mathbf{v}_i \otimes \mathbf{v}_i)) - \text{div} \mathbf{T}_i - p \nabla \rho_i = f_i$$

$$f_i = \sum_{j=1}^N k_{ij}(\mathbf{v}_j - \mathbf{v}_i)\rho_i \rho_j, \quad i = 1, \ldots, N$$

- Properties: $\sum_{i=1}^N \rho_i = 1$, $\sum_{i=1}^N \rho_i \mathbf{v}_i = 0$, $\sum_{i=1}^N f_i = 0$
- Interphase pressure: $p \nabla \rho_i$, $p$: phase pressure (Drew/Segel 1971)
- Assumptions: inertia approximation ($\varepsilon = 0$), $k := k_{ij}$, stress tensor:

$$\mathbf{T}_i = -\rho_i (p \mathbf{I} \mathbf{d} + \mathbf{P}_i), \quad \mathbf{P}_i: \text{isotropic pressures}, \quad P_N = 0$$
Derivation from continuum fluid model

\[ \partial_t \rho_i + \text{div}(\rho_i \nu_i) = 0, \quad -\text{div} T_i - p \nabla \rho_i = f_i = \sum_{j=1}^{N} k_{ij} (\nu_j - \nu_i) \rho_i \rho_j \]

- Consequence of \( k := k_{ij} \): \( f_i = -k \rho_i \nu_i \)
- Consequence of pressure: \( -\text{div} T_i - p \nabla \rho_i = \rho_i \nabla p + \text{div}(\rho_i P_i) \)
- Add all force balance equations:
  \[ 0 = \sum_{i=1}^{N} f_i = \sum_{i=1}^{N} (\rho_i \nabla p + \text{div}(\rho_i P_i)) = \nabla p + \sum_{i=1}^{N-1} \text{div}(\rho_i P_i) \]
- Replace \( \nabla p \) and expand \( \text{div} P_i = \sum_{j=1}^{N-1} \frac{\partial P_i}{\partial \rho_j} \nabla \rho_j \):
  \[ \partial_t \rho_i + \sum_{j=1}^{N-1} \text{div}(A_{ij}(\rho) \nabla \rho_j) = 0, \quad i = 1, \ldots, N - 1 \]

Example: \( N = 3, P_1 = \rho_1, P_2 = \beta \rho_2(1 + \theta \rho_1) \sim \) 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

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

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
Cross-diffusion systems

Derivation, gradient flows

Previous results

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

Global existence if . . .

- Growth conditions on nonlinearities (Ladyženskaya ... 1988)
- Control on \( L^\infty \) and Hölder norms (Amann 1989)
- Invariance principle holds (Redlinger 1989, Kufner 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, \( \partial_t u = -\nabla H(u), \ H : \mathbb{R}^n \rightarrow \mathbb{R} \)

\[
\frac{d}{dt} H(u) = \nabla H(u) \cdot \partial_t u = -|\nabla H(u)|^2 \implies H \text{ is Lyapunov functional}
\]

- 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 \( L^2(\mathbb{R}^d) \):

\[
\operatorname{grad} H(u) \xi = \int_{\mathbb{R}^d} \nabla u \cdot \nabla \xi \, dx = -\int_{\mathbb{R}^d} \Delta u \xi \, dx \implies \partial_t u = \Delta u
\]

- 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
\[
\partial_t u - \text{div}(A(u) \nabla u) = f(u) \quad \text{possesses formal gradient-flow structure}
\]
\[
\partial_t u - \text{div} \left( B \nabla \text{grad} H(u) \right) = f(u),
\]
where \( B \) is positive semi-definite, \( H(u) = \int_\Omega h(u)dx \) entropy

Equivalent formulation: \( \text{grad} H(u) \simeq h'(u) =: w \) (entropy variable)
\[
\partial_t u - \text{div}(B \nabla w) = f(u), \quad B = A(u) h''(u)^{-1}
\]

Consequences:
- \( H \) is Lyapunov functional if \( f = 0 \):
  \[
  \frac{dH}{dt} = \int_\Omega \partial_t u \cdot h'(u) \, dx = - \int_\Omega \nabla w : B \nabla w \, dx \leq 0
  \]
- \( L^\infty \) 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 1: Population-dynamics model

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

- \( u = (u_1, u_2) \) 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:
  \[ \frac{dH}{dt}[u] = \int_{\Omega} \left( \frac{\log u_1}{a_{12}} \partial_t u_1 + \frac{\log u_2}{a_{21}} \partial_t u_2 \right) \, dx \]
  \[ = -2 \int_{\Omega} \left( \frac{2}{a_{12}}(a_{10} + a_{11}u_1)|\nabla \sqrt{u_1}|^2 + \frac{2}{a_{21}}(a_{20} + a_{22}u_2)|\nabla \sqrt{u_2}|^2 \right. \]
  \[ + \left. |\nabla \sqrt{u_1u_2}|^2 \right) \, dx \leq 0 \]
Example 1: 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?

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

Answer: Yes!

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

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

- 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 2: Ion-transport model

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

- \( u = (u_1, u_2, u_3) \) 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: \( H[u] = \int_{\Omega} h(u) dx, \quad u_4 = 1 - \sum_{i=1}^{3} u_i \)

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

- 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 ②: 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:

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

\[ \leq -C \int_{\Omega} \left( u_4^2 \sum_{i=1}^{3} |\nabla \sqrt{u_i}|^2 + |\nabla \sqrt{u_4}|^2 \right) dx \]

Difficulty: degeneracy at \( u_4 = 0! \)

New diffusion matrix:

\[ B(w) = u_4 \text{diag}(D_1 u_1, D_2 u_2, D_3 u_3) \]

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

\[ u_i = \frac{e^{w_i}}{1 + e^{w_1} + e^{w_2} + e^{w_3}} \in (0, 1) \Rightarrow L^\infty \text{ bounds!} \]
Cross-diffusion systems
Derivation, gradient flows

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: \( \mu_i = \mu_i^0 + \log \rho_i \), \( \mu_i^0 = \text{const.} \) \( \Rightarrow \)

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

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

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

\( \rightarrow \) exactly the expression for the ion-transport model!

- Open problem: Include nonconstant temperature
Cross-diffusion systems

Boundedness-by-entropy method

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

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

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

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

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

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

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

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

**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 \( \text{div}(B(w)\nabla w) \) 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 \( u(w^k) \in D \implies u \in \overline{D} \)

**Strategy:** Problem in \( u \to \) Solve in \( w \to \) Limit gives problem in \( u \)
Proof of existence theorem

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

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

\[
\frac{1}{\tau} \int_{\Omega} (u(w^k) - u(w^{k-1})) \cdot \phi \, dx + \int_{\Omega} \nabla \phi : B(w^k) \nabla w^k \, dx \\
+ \varepsilon \int_{\Omega} \left( \sum_{|\alpha|=m} D^\alpha w^k \cdot D^\alpha \phi + w^k \cdot \phi \right) \, dx = \int_{\Omega} f(u(w^k)) \cdot \phi \, dx
\]
Step ➊: Lax-Milgram argument

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

$$a(w^k, \phi) = \int_\Omega \nabla \phi : B(y) \nabla w^k \, dx + \varepsilon \int_\Omega \left( \sum_{|\alpha| = m} D^\alpha w^k \cdot D^\alpha \phi + w^k \cdot \phi \right) \, dx$$

$$= -\frac{\delta}{\tau} \int_\Omega (u(y) - u(w^{k-1})) \cdot \phi \, dx + \delta \int_\Omega f(u(y)) \cdot \phi \, dx = F(\phi)$$

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

Then $S(\cdot, 1)$ has a fixed point.
Step 2: Leray-Schauder argument

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

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

- 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):

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

- Idea: Derive estimates for $u = u(w)$, not for $w$
Step 3: Uniform estimates

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

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

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

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

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

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

Then exists subsequence \(u^{(\tau)} \rightarrow u\) 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
**Cross-diffusion systems**

**Boundedness-by-entropy method**

### Step 4: Limit $(\tau, \varepsilon) \to 0$

\[
\frac{1}{\tau} \int_0^T \int_\Omega (u^{(\tau)}(t) - u^{(\tau)}(t - \tau)) \cdot \phi \, dx \, dt + \int_0^T \int_\Omega \nabla \phi : A(u^{(\tau)}) \nabla u^{(\tau)} \, dx \, dt \\
+ \varepsilon \int_0^T \int_\Omega \left( \sum_{|\alpha|=m} D^\alpha \omega^{(\tau)} \cdot D^\alpha \phi + \omega^{(\tau)} \cdot \phi \right) \, dx \, dt = \int_0^T \int_\Omega f(u^{(\tau)}) \cdot \phi \, dx \, dt
\]

- **Nonlinear Aubin-Lions lemma:**
  \[
  u^{(\tau)} \to u \quad \text{strongly in } L^2(0, T; L^2) \\
  \varepsilon \omega^{(\tau)} \to 0 \quad \text{strongly in } L^2(0, T; H^m) \\
  A(u^{(\tau)}) \nabla u^{(\tau)} \rightharpoonup A(u) \nabla u \quad \text{weakly in } L^2(0, T; L^2)
  \]

- **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 there exists a global weak solution such that $u(x, t) \in \overline{D}$ and

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

**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 $h''(u)A(u)$
Population model of Shigesada-Kawasaki-Teramoto

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

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

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

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

- Population model of Shigesada-Kawasaki-Teramoto:
  \[ p_i(u) = a_{i0} + a_{i1} u^1 + a_{i2} u^2, \quad i = 1, 2 \]

- Nonlinear transition rates: \( p_i(u) = a_{i0} + a_{i1} u^s_1 + a_{i2} u^s_2, \quad s > 0 \)

- Desvillettes/Lepoutre/Moussa 2014: \( 0 < s < 1 \)

- A.J. 2014: \( 0 < s < 4, (1 - \frac{1}{s})a_{12} a_{21} \leq a_{11} a_{22} \) (weak cross-diffusion)

- Desvillettes/Lepoutre/Moussa/Trescases 2015: \( s > 1 \) and 
  \[ (\frac{s-1}{s+1})^2 a_{12} a_{21} \leq a_{11} a_{22} \] (less restrictive than above)

- Key idea: Exploit extra regularity using duality method for \( \Delta(u_i p_i(u)) \)

Further generalization: \( n \geq 3 \) equations
Existence result only under conditions on \( a_{ij} \), related to detailed balance principle (Daus/A.J., in progress)
Ion-transport model

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

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

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

- Consequence 1:

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

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

- Consequence 2: By nonlinear Aubin-Lions lemma,

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

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

- Consequence 3: $L^\infty$ 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 $L^1$
2 Ion-transport model

\[ w_i^{(\tau)} := (u_4^{(\tau)})^{1/2} u_i^{(\tau)} \to u_4^{1/2} u_i \quad \text{weakly in } L^2(0, T; H^1) \]
\[ y^{(\tau)} := (u_4^{(\tau)})^{1/2} \to u_4^{1/2} \quad \text{strongly in } L^2(0, T; L^2) \]
\[ \nabla(u_4^{(\tau)})^{1/2} \to \nabla u_4^{1/2} \quad \text{weakly in } L^2(0, T; L^2) \]

- **Aim:** Perform limit in

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

- **Problem:** weak $\times$ weak $\nRightarrow$ 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 \(L^2(0, T; L^2)\),

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

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?
3 Tumor-growth model

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

- 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)
  \[
  A(u) = \begin{pmatrix}
  2u_1(1 - u_1) - \beta \theta u_1 u_2^2 & -2\beta u_1 u_2(1 + \theta u_1) \\
  -2u_1 u_2 + \beta \theta u_2^2(1 - u_2) & 2\beta u_2(1 - u_2)(1 + \theta u_1)
  \end{pmatrix}
  \]
- 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:
  \[
  \frac{dH}{dt}[u] + C_\theta \int_{\Omega} \left( (\partial_x u_1)^2 + (\partial_x u_2)^2 \right) dx \leq C(f)
  \]
  and \( C_\theta > 0 \) if and only if \( \theta < \theta^* := 4/\sqrt{\beta} \)
3 Tumor-growth model

Theorem (A.J./Stelzer 2012)

Let $\theta < 4/\sqrt{\beta}$, $H[u_0] < \infty \Rightarrow \exists$ bounded weak solution with

$0 \leq u_1, u_2 \leq 1$

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)
4 Multicomponent gas mixtures

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

- 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 \( \sigma(C) \subset \{0\} \cap \{ z \in \mathbb{C} : \text{Re}(\lambda) < 0 \} \)
Matrix analysis

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

- Formulate: \( \nabla u = -C(u) J, \quad u = (u_1, \ldots, u_n), \quad J = (J_1, \ldots, J_n) \)
  \[ C_{ij} = c_{ij} u_i \text{ for } i \neq j, \quad C_{ii} = -\sum_{j \neq i} c_{ij} u_j, \quad \sum_{i=1}^{n} J_i = 0 \]

- \( \sum_j C_{ij} = 0 \Rightarrow C \) 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
Cross-diffusion systems

Extensions

Entropy structure

\[ \partial_t u - \text{div} \, J = f(u), \quad \nabla u = -C(u)J \]

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

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

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

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

Theorem (A.J./Stelzer 2014)

Let \( (c_{ij}) \) symmetric, \( \sum_{i=1}^{n} f_i(u) \log u_i \leq 0 \). Then \( \exists \) global weak solution
\[ u_i^{1/2} \in L^2_{\text{loc}}(0, \infty; H^1), \quad 0 \leq u_i \leq 1, \quad \sum_{i=1}^{n-1} u_i \leq 1 \]
Extensions of Maxwell-Stefan models

Limitations: zero barycentric velocity, equal molar masses, isothermal

More realistic models: (see Bothe/Dreyer 2015)

- Include barycentric velocity $\nu$:
  \[
  \partial_t \rho_i + \text{div}(\rho_i \nu - J_i) = 0, \quad i = 1, \ldots, n
  \]
  \[
  \partial_t \rho + \text{div}(\rho \nu) = 0, \quad \partial_t (\rho \nu) + \text{div}(\rho \nu \otimes \nu) + \nabla p = \rho f + \nu \Delta \nu
  \]
  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

\begin{align*}
\partial_t \rho &= \Delta (\rho \theta^{1/2-\beta}), \\
\partial_t (\rho \theta) &= \kappa \Delta (\rho \theta^{3/2-\beta}) + \frac{\rho}{\tau} (1 - \theta)
\end{align*}

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 \( C_1, C_2 > 0 \)
  \[ \frac{dH}{dt} + C_1 \int_{\Omega} \theta^{1/2-\beta} (\rho^{-1} |\nabla \rho|^2 + \theta^{-1} |\nabla \theta|^2) \leq C_2 \]

Problem: Estimate is not helpful near \( \theta = 0 \)
Entropy structure

\[ \partial_t \rho = \Delta \left( \rho \theta^{1/2-\beta} \right), \quad \partial_t (\rho \theta) = \kappa \Delta \left( \rho \theta^{3/2-\beta} \right) + \frac{\rho}{T} (1 - \theta) \]

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:
  \[
  \frac{d}{dt} \int_{\Omega} \rho^2 \theta^b \, dx + C_1 \int_{\Omega} \left| \nabla \left( \rho \theta^{2b+1-2\beta}/4 \right) \right|^2 \, dx \leq C_2
  \]
- Special choices of \( b \in \mathbb{R} \) yields estimates
  \[
  \int_{\Omega} \left( |\nabla \rho|^2 + |\nabla u|^2 + |\nabla v|^2 \right) \, dx \leq C_3
  \]
- Implicit Euler scheme \((u^k, v^k)\): apply maximum principle
  \[ u^k \geq m(u^{k-1}, v^{k-1}) > 0, \quad v^k \geq m(u^{k-1}, v^{k-1}) > 0 \]
Global existence

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

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

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

\[ \rho, \rho \theta^b \in L^2_{\text{loc}}(0, \infty; H^1), \quad b \in \{1, \frac{1}{2} - \beta, \frac{3}{2} - \beta\} \]

- **Proof highly technical:** truncate \( \theta^k = v^k / u^k \), show that \( \theta^k \geq m(\theta^{k-1}) > 0 \), include boundary cond., use different entropies

- **Open problem:** Existence with electric field term
  
  \[ \partial_t \rho = \text{div} \left( \nabla (\rho \theta^{1/2-\beta}) + \rho \theta^{-1/2-\beta} \nabla V \right) \]

- **Equilibration to constant steady state \((\rho_D, \theta_D)\):**
  
  \[ \| n(t) - n_D \|_{L^2} + \| \theta(t) - \theta_D \|_{L^2} \leq \frac{C_1}{(1 + C_2 t)^{1/2}} \]

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

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   - Extensions
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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: $\partial_t u = \text{div}(\nabla u + u \nabla V)$ 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 $u_1 - u_2$:

$$\frac{1}{2} \frac{d}{dt} \int_\Omega (u_1 - u_2)^2 \, dx = \int_\Omega \partial_t (u_1 - u_2)(u_1 - u_2) \, dx$$

$$= -\int_\Omega |\nabla (u_1 - u_2)|^2 \, dx - \int_\Omega (u_1 - u_2) \nabla (u_1 - u_2) \cdot \nabla V \, dx$$

$$= \frac{1}{2} \nabla ((u_1 - u_2)^2)$$
Example

**First idea:** Integration by parts

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

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

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

**Second idea:** Cauchy-Schwarz inequality

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

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 \( d(u_1, u_2) \geq \frac{1}{8} \| u_1 - u_2 \|^2_{L^2} \)
- 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 \( \partial_t u_i = \text{div}(\nabla u_i + u_i \nabla V) \)

\[
\frac{d}{dt} d(u_1, u_2) = \sum_{i=1}^2 \int_\Omega \left( \phi'(u_i) - \phi'\left(\frac{u_1 + u_2}{2}\right) \right) \partial_t u_i dx
\]

\[
= -4 \int_\Omega \left( |\nabla u_1^{1/2}|^2 + |\nabla u_2^{1/2}|^2 - |\nabla (u_1 + u_2)^{1/2}|^2 \right) dx \leq 0
\]

- Integrate over \( t \):

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

- Drawback: Possibly not very robust (see Gajewski-Skrypnyk 2004)
A cross-diffusion example

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

- 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:

\[
\partial_t u_i = \text{div}(q(u_n) \nabla u_i - u_i \nabla q(u_n)), \quad i = 1, \ldots, n - 1
\]

**Step ➊**: Uniqueness for \( u_n 

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

\[
\partial_t u_n = \text{div}(q(u_n) \nabla u_n + (1 - u_n) \nabla q(u_n)) = \Delta Q(u_n),
\]

\[
Q'(s) = q(s) + (1 - s) q'(s) \geq 0
\]

- Let \( u_n, v_n \) be two weak solutions with same initial data
Uniqueness of weak solutions

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

\[ \partial_t u_n = \Delta Q(u_n) \text{ in } \Omega, \quad \nabla u_n \cdot \nu = 0 \text{ on } \partial \Omega, \quad u_n(0) = u_0^0 \]

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

\[ \frac{1}{2} \frac{d}{dt} \int_{\Omega} |\nabla \xi|^2 dx = \int_{\Omega} \nabla \partial_t \xi \cdot \nabla \xi dx = -\int_{\Omega} \partial_t \Delta(\xi) \xi dx \]

\[ = \int_{\Omega} \partial_t (u_n - v_n) \xi dx = -\int_{\Omega} \nabla (Q(u_n) - Q(v_n)) \cdot \nabla \xi dx \]

\[ = -\int_{\Omega} (Q(u_n) - Q(v_n))(u_n - v_n) dx \leq 0 \]

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

Step 2: Uniqueness for $u_1, \ldots, u_{n-1}$

\[ \partial_t u_i = \text{div}(q(u_n) \nabla u_i - u_i \nabla q(u_n)), \quad i = 1, \ldots, n - 1 \]

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

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

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

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

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

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

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

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

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

\[
\partial_t u - \text{div}(A(u)\nabla u) = 0 \quad \text{in } \Omega,
\]

\[
A_{ij}(u) = \delta_{ij} q_i(u_n) + u_i q_i'(u_n)
\]

*with $\nabla u_i \cdot \nu = 0$ on $\partial \Omega$, $u_i(0) = u_i^0$, $i = 1, \ldots, n$.**
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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 $\Rightarrow$ summation by parts
- Extension of chain rule to discrete case is challenging:

\[
\nabla f(u) = f'(u) \nabla u \Rightarrow f(u_i) - f(u_{i-1}) = \frac{f(u_i) - f(u_{i-1})}{u_i - u_{i-1}} (u_i - u_{i-1})
\]

Problem: many choices for approx. of $f'(u)$, multi-dimensions 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 $S_t$: $(S_tf)(x) = E[f(X_t)|X_0 = x]$ for $f \in L^2(\Sigma)$
- Generator $L$: operator on $L^2(\Sigma)$ such that $S_t = e^{tL}$

Example 1: 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: $(S_tf)(\xi) = \sum_\eta p_t(\xi, \eta)f(\eta)$

Example 2: Let $Lu = \text{div}(\nabla u + xu)$ 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 $\int_{\Sigma} Lfd\pi = 0$ or $\int_{\Sigma} S_t fd\pi = \int_{\Sigma} fd\pi$ 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 $\xi, \eta \in \Sigma \iff L^* = L$ on $L^2(\pi)$

Example 1: ODE system $\partial_t u = Qu$
- Dual semigroup: $S^*_t = e^{tL^*}$, where $L^*$ adjoint to $L = Q$ in $L^2(\pi)$
- Invariant measure:

$$\sum_{\xi} (Lf)(\xi)\pi(\xi) = \sum_{\xi, \eta} Q(\xi, \eta)f(\eta)\pi(\xi) = \sum_{\eta} \left( \sum_{\xi} \pi(\xi)Q(\xi, \eta) \right)f(\eta)$$

$\Rightarrow \pi Q = 0$ 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
  $$\int_\Sigma L f d\pi = 0 \quad \text{or} \quad \int_\Sigma S_t f d\pi = \int_\Sigma f d\pi \quad \text{for all } f$$
- 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 2: Fokker-Planck operator $Lu = \text{div}(\nabla u + xu)$ in $\mathbb{R}^d$
- $L$ symmetric with respect to $d\pi = e^{\frac{|x|^2}{2}} dx$:
  $$\int_{\mathbb{R}^d} Lu v e^{\frac{|x|^2}{2}} dx = - \int_{\mathbb{R}^d} (\nabla u + xu) \cdot (\nabla v + xv) e^{\frac{|x|^2}{2}} dx = \int_{\mathbb{R}^d} u L v e^{\frac{|x|^2}{2}} dx$$
  $\Rightarrow \pi$ is reversible measure
- Invariant measure $d\pi = \rho dx$ solves $0 = \int_{\mathbb{R}^d} L f \rho dx = \int_{\mathbb{R}^d} f L' \rho dx$ $\Rightarrow$
  $$0 = L' \rho = \Delta \rho - x \cdot \nabla \rho \Rightarrow \rho = \text{const.}$$
**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 $f \log f \in L^1(\pi)$,

  $\text{Ent}_\pi[f] = \int_\Sigma f \log fd\pi - \int_\Sigma fd\pi \log \int_\Sigma fd\pi$

  If $f = \frac{d\mu}{d\pi}$ then $\text{Ent}_\pi[f] = H[\mu|\pi]$ ($\pi$ 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 \( \text{Ent}_\pi[f] \leq \kappa^{-1} \mathcal{E}(f, \log f) \) then

\[
\frac{dH}{dt}[S_t^* \mu | \pi] \leq -\kappa \text{Ent}_\pi[S_t f] = -\kappa H[S_t^* \mu | \pi] \Rightarrow H[S_t^* \mu | \pi] \leq e^{-\kappa t} H[\mu | \pi]
\]

- Question: How to prove \( \text{Ent}_\pi[f] \leq \kappa^{-1} \mathcal{E}(f, \log f) \)?

Dai Pra/Posta 2014: Compute second time derivative

\[
\frac{d^2}{dt^2} \text{Ent}_\pi[S_t f] = \int_\Sigma \left( L^2 S_t f \log S_t f + \frac{(LS_t f)^2}{S_t f} \right) d\pi
\]

\[
\geq \kappa \mathcal{E}(S_t f, \log S_t f) = -\kappa \frac{d}{dt} \text{Ent}_\pi[S_t f]
\]

- Integration from 0 to \( \infty \) yields

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

\[
\Rightarrow \text{Desired estimate } \text{Ent}_\pi[S_0 f] = \text{Ent}_\pi[f] \leq \kappa^{-1} \mathcal{E}(f, \log f)
\]
**Verification of inequality**

It remains to prove:

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

- **Generator**: \( Lf(\xi) = \sum_{\eta} Q(\xi, \eta)(f(\xi) - f(\eta)) \), \( Q \): jump rates
- **Under detailed balance**, \( E(f, \log f) = -\frac{1}{2} \sum_{\xi, \eta} Q(\xi, \eta)(f(\xi) - f(\eta))(\log f(\xi) - \log f(\eta)) \geq 0 \)
  
  and thus, \( \frac{dH}{dt}[S^*_t \mu|\pi] = -E(f, \log f) \leq 0, \ f = \frac{d\mu}{d\pi} \)
- **Computation of** \( L^2 f \log f + f^{-1}(Lf)^2 \) much more involved!

**Approach ➊**: 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 ➋**: 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)

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

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

\[
\partial_t u = -D^\top L D \log \rho, \quad L = \text{diag}(\kappa_i L_i), \quad L_i = \frac{\rho_{i+1} - \rho_i}{\log \rho_{i+1} - \log \rho_i}
\]
→ 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 \( \rho \nabla \log \rho = \nabla \rho \):

\[
(LD \log \rho)_i = \sum_j L_{ij} (D \log \rho)_j = -\kappa_i \frac{\rho_{i+1} - \rho_i}{\log \rho_{i+1} - \log \rho_i} h^{-1} (\log \rho_{i+1} - \log \rho_i) = \kappa_i (D \rho)_i
\]
Discretized Fokker-Planck equation

\[ \partial_t u = -D^\top LD \log \rho \]

- Discrete entropy: \( H[u] = \sum_i u_i \log(u_i/u_\infty,i) =: \langle u, \log \rho \rangle \)
- Discrete entropy production:
  \[ \frac{dH}{dt}[u] = \langle \partial_t u, \log \rho \rangle = -\langle D^\top LD \log \rho, \log \rho \rangle = -\langle D \log \rho, LD \log \rho \rangle \]
- Second time derivative:
  \[ \frac{d^2H}{dt^2}[u] = \langle D \log \rho, MD \log \rho \rangle \]
- Show that \( M \geq 2\mu L \Rightarrow \frac{d^2H}{dt^2} \geq -2\mu \frac{dH}{dt} \Rightarrow \text{exponential decay} \)

**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

\[ \mu = \frac{2}{h^2} \Phi \left( \frac{h^2}{8} \lambda \right) \rightarrow \lambda \text{ as } h \rightarrow 0, \quad \Phi(s) = \frac{3 \text{ Erf}(s^{1/2}) - \text{ Erf}(3s^{1/2})}{2 \text{ Erf}(s^{1/2})} \]

Error function: \( \text{ Erf}(s) = 2\pi^{-1/2} \int_0^s \exp(-t^2)dt \)
Towards discrete entropy methods

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 $u_k = u(t_k)$

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

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

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

- Entropy-dissipative scheme: $H[u_k] + \tau \langle -L(u_k), \phi'(u_k) \rangle \leq H[u_{k-1}]$
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
\[
\frac{2}{\alpha \tau} v_k^{2/\alpha-1} \left( \frac{3}{2} v_{k+2} - 2 v_{k+1} + \frac{1}{2} v_k \right) = L(u_{k+2}), \quad v_k := u_k^{\alpha/2}
\]

- 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: \( H_G[u_{k+2}, u_{k+1}] = \frac{1}{2} \int_\Omega (u_k^\alpha + (2u_{k+2}^{\alpha/2} - u_{k+1}^{\alpha/2})^2) dx \)
- 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: ➊ Why is this working? ➋ Can it be generalized?
- Answer ➊: Use inequality

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

- Answer ➋: Yes, use G-stability theory of Dahlquist
One-leg multistep methods and G-stability

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

- Implicit Euler \( p = 1 \): \((\alpha_0, \alpha_1) = (-1, 1), (\beta_0, \beta_1) = (\frac{1}{2}, \frac{1}{2})\)
- BDF-2 \( p = 2 \): \((\alpha_0, \alpha_1, \alpha_2) = (\frac{1}{2}, -2, \frac{3}{2}), (\beta_0, \beta_1, \beta_2) = (0, 0, 1)\)
- A-stability: Numer. solution \((v_k)\) of \(v' = \lambda v\) decreasing if \(\text{Re}(\lambda) < 0\)
- G-stability: \(\exists G \in \mathbb{R}^{p \times p}\) symmetric, positive definite: \(\forall (v_k) \in \mathbb{R}^p:\)

\[
(\rho(E) v_k, \sigma(E) v_k)_2 \geq \frac{1}{2} \|V_{k+1}\|_G^2 - \frac{1}{2} \|V_k\|_G^2
\]

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 \(\iff\) G-stable
- Consequence: G-stable one-leg method is at most of second order!
One-leg multistep methods and G-stability

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

Claim: G-stability implies discrete entropy dissipation

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

\[
\frac{1}{2} \| V_{k+1} \|_G^2 - \frac{1}{2} \| V_k \|_G^2 \leq (\rho(E)v_k, \sigma(E)v_k)_2 = \tau \langle B(\sigma(E)v_k), \sigma(E)v_k \rangle \leq 0
\]

- **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, \( p = 2 \), \( B + \kappa I \geq 0 \) \( (\kappa > 0) \Rightarrow \| v_k - u(t_k)^{\alpha/2} \| \leq C\tau^2 \)
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 $\tau$):

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

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

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

- To show: $G'(0) \leq 0$ and $G''(0) < 0$ (then $G''(\xi) \leq 0$ for $\tau \ll 1$)
Runge-Kutta methods

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

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

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

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

where \( DL[u] \): Fréchet derivative of \( L \) at \( u \)

- Runge-Kutta constant \( C_{RK} \):

\[ C_{RK} = 2 \) (explicit Euler), 1 (Runge-Kutta \( \geq 2 \)), 0 (implicit Euler) \]
Example 1: Diffusion equation

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

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

\[ G'(0) = \int_{\Omega} \phi'(u) \text{div}(a(u) \nabla u) \, dx = - \int_{\Omega} \phi''(u) a(u) |\nabla u|^2 \, dx \leq 0 \]

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

\[ = - \int_{\Omega} \left( (C_{RK} + 1) \phi''(u) \mu(u)^2 \xi_L^2 + (C_{RK} + 2) \mu'(u) \mu(u) \xi_L \xi_G^2 \right. \]

\[ + \left. \frac{\mu(u)^2}{\phi''(u)} \xi_G^4 \right) \, dx, \quad \mu(u) = \frac{a(u)}{\phi''(u)} \]

- Polynomial variables: \( \xi_L = \Delta \phi'(u), \quad \xi_G = |\nabla \phi'(u)| \)
- Solve by systematic integration by parts
Example 1: Diffusion equation

Integration-by-parts formulas:

\[ 0 \leq \int_{\Omega} \text{div} \left( A(u)(\nabla^2 \phi'(u) - \Delta \phi'(u)) \cdot \nabla \phi'(u) \right) \, dx, \text{ since } \Omega \text{ convex} \]

\[ 0 = \int_{\Omega} \text{div} \left( B(u)|\nabla \phi'(u)|^2 \nabla \phi'(u) \right) \, dx \]

How to find \( A(u) \) and \( B(u) \)? Leads to nonlinear ODE system

Idea: Special solutions or more specific diffusion equations

Choose \( A'(u) = -\frac{2}{3}(C_{RK} + 2)\mu(u)\mu'(u)\phi''(u) \), \( B(u) = \frac{1}{3}(C_{RK} + 2)\mu(u)\mu'(u) \) to cancel mixed terms

Discrete entropy dissipation if \( A(u) \geq 0 \) and

\[
\left( 1 - \frac{1}{d} \right) A(u) + \left( C_{RK} + 1 \right) \phi''(u)\mu(u)^2 \leq 0
\]

\[
(C_{RK} + 2)\mu(u)\mu''(u) + (C_{RK} - 1)\mu'(u)^2 < 0
\]
Example 1: Diffusion equation

Theorem (A.J./Schuchnigg 2015)

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

$$A(u) = \frac{2}{3} (C_{RK} + 2) \int_{u_0}^u \mu(s) \mu'(s) \phi''(s) ds \geq 0,$$

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

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

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 2: Porous-medium equation

\[ \partial_t u = \Delta (u^\beta) \text{ in } \Omega \]

- 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!