Finite-volume methods for cross-diffusion systems: ideas, techniques, proofs

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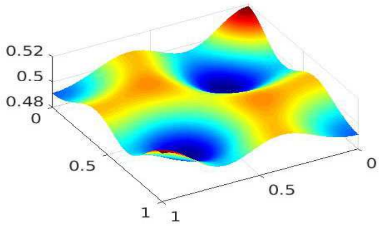
1. Introduction
2. Boundedness-by-entropy method
3. Finite-volume method

Der Wissenschaftsfonds.



Population density in 2D

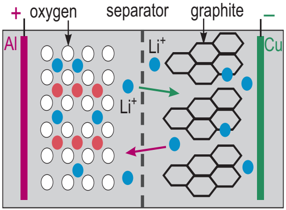
Multi-species systems

Examples:

- Population dynamics: observing, predicting, harvesting
- Fluid mixtures: heliox (diving, asthma), biofilm reactors
- Biology: tumor growth, ion transport through membranes
- Electrolysis: lithium-ion batteries, production of hydrogen from water

Nature is generally composed of multi-species systems!

Modeling: flux depends on gradient of density $\rightarrow$ reaction-diffusion eqs.



http://www.pdfnet.dk

Image: Dr. Cecil Fox

Fick's law for fluid mixtures

- Mass balance equations: density u_i, diffusion flux J_i

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

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

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

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

Problem: uphill diffusion in ternary mixtures (Duncan-Toor 1962)

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

What are cross-diffusion systems?

$$\partial_t u_i - \operatorname{div}\left(\sum_{j=1}^n A_{ij}(u)\nabla u_j\right) = f_i(u) \quad \text{in } \Omega,\ t > 0,\ i = 1, \ldots, n$$

- Systems of quasilinear parabolic equations
- Initial and (no-flux) boundary conditions

What makes these systems special?

- Diffusion/cross-diffusion may lead to pattern formation (Turing 1952)
- Segregation: intersection of supp $u_i(t)$ empty it true initially (Bertsch et al. 1985)
- Generally no maximum principle: How to guarantee that $u_i \geq 0$?
- Generally no regularity theory: $u_i(t)$ may blow-up in Hölder norm in finite time (Stará-John 1995), discontinuous solutions (Bertsch 1985)
- Diffusion matrix $A(u) = (A_{ij}(u))$ often neither symm. nor pos. def.
- Key for analysis: entropy structure

Aim: explain entropy structure, preserve this structure on discrete level

❶ Multicomponent gas mixtures

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

- Volume fractions of gas components u_1, u_2, $u_3 = 1 - u_1 - u_2 \in [0,1]$
- Diffusion matrix: $\delta(u) = d_1 d_2(1 - u_1 - u_2) + d_0(d_1 u_1 + d_2 u_2)$, $d_i > 0$

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

- Application: Patients with airway obstruction inhale Heliox to speed up diffusion
- Proposed by Maxwell 1866 & Stefan 1871
- Derivation from Boltzmann equation: Boudin-Grec-Salvarani 2015
- Problems: $A(u)$ not symmetric, generally not positive def., how to prove that $0 \le u_i \le 1$?

http://cancer.gov, Illu conducting passages.svg

❷ Segregating populations

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

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

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

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

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

Overview

Analysis of cross-diffusion systems

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

Mathematical difficulties:

- Matrix $A(u)$ may be neither symmetric nor positive definite
- Generally no maximum principle, no regularity theory

Idea: Find entropy density $h'(u) =: w$ such that $(*)$ equivalent to

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

Consequences: formal gradient-flow structure

1. $H(u) = \int_\Omega h(u)dx$ (entropy) is Lyapunov functional if $f = 0$:

$$\frac{dH}{dt} = \int_\Omega \partial_t u \cdot \underbrace{h'(u)}_{=w} dx = -\int_\Omega \nabla w^T B \nabla w dx \le 0$$

2. L^∞ bounds for u: $h' : D \to \mathbb{R}^n$ be invertible ($D \subset \mathbb{R}^n$ bounded) $\Rightarrow$ $u(x,t) = (h')^{-1}(w(x,t)) \in D$ (no maximum principle needed!)

Boundedness-by-entropy method

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

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

Assumptions:

1. $\exists$ convex entropy $h \in C^2(D;[0,\infty))$, h' invertible on $D \subset \mathbb{R}^n$
2. "Degenerate" positive definiteness: $\exists\ s > 0$, $\forall\ u \in D$,
   $$z^\top h''(u)A(u)z \geq c\sum_{i=1}^n u_i^{2s-2}z_i^2, \quad \Rightarrow \text{ estimate for } |\nabla u_i^s|^2$$
3. A continuous on D, $\exists C > 0 : \forall u \in D$: $f(u)\cdot h'(u) \leq C(1+h(u))$

Theorem (AJ, Nonlinearity 2015)

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

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

❶ Maxwell-Stefan models

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

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

- Entropy: $H(u) = \int_\Omega h(u)dx$, $u \in D = \{u : u_i > 0,\ u_1 + u_2 < 1\} \subset \mathbb{R}^2$

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

- Entropy production:

$$\frac{dH}{dt} + c\int_\Omega \sum_{i=1}^{2} |\nabla\sqrt{u_i}|^2 dx \le C_f(1 + H)$$

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

$$w_i = \frac{\partial h}{\partial u_i} = \log\frac{u_i}{u_3}, \qquad u_i = \frac{e^{w_i}}{1 + e^{w_1} + e^{w_2}} \in D$$

Boundedness-by-entropy theorem: $\exists$ global-in-time weak solution

❷ SKT population model

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

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

- Entropy: $h(u) = a_{21}u_1(\log u_1 - 1) + a_{12}u_2(\log u_2 - 1)$, $D=(0,\infty)^2$
- Entropy production:

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

- Entropy variables: $w_i = \partial h/\partial u_i = \log u_i \Rightarrow u_i = \exp(w_i) > 0$

Boundedness-by-entropy method not applicable but technique applies

Theorem (L. Chen-AJ, SIMA 2004)

Let $a_{ii}>0$. Then $\exists$ nonnegative weak solution u such that

$$u_i \in L^2(0,T;H^1(\Omega)),\ \partial_t u_i \in L^q(0,T;W^{1,q}(\Omega)'), \quad q=2(d+1)$$

Discrete entropy structure

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

- Choose test function $h'(u)$:

$$\frac{d}{dt}\int_\Omega h(u)dx + \int_\Omega \nabla h'(u)^T A(u)\nabla u dx = 0$$

- Apply chain rule $\nabla h'(u) = h''(u)\nabla u$ and use symmetry of $h''(u)$:

$$\frac{d}{dt}\int_\Omega h(u)dx + \int_\Omega \nabla u^T \underbrace{h''(u)A(u)}_{\text{pos. def.}}\nabla u dx = 0$$

Question: How to formulate discrete chain rule? E.g. finite differences:

- Scalar case $h : \mathbb{R} \to \mathbb{R}$: mean-value theorem

$$\exists \widetilde{u}: \quad h''(\widetilde{u})(u - v) = h'(u) - h'(v)$$

- Vector case $h : \mathbb{R}^n \to \mathbb{R}$: vector-valued mean-value theorem

$$\left(\int_0^1 h''(su + (1-s)v)ds\right)(u - v) = h'(u) - h'(v)$$

- Problem: Existence of $\widetilde{u}$ for vector-valued case unclear!

Overview

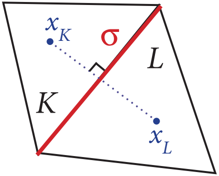
1. Introduction
2. Boundedness-by-entropy method
3. Finite-volume method
4. Existence and convergence

Finite-volume method

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

Admissible mesh:

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



Idea of method: integrate over K and integrate by parts

$$\partial_t \int_K u_i dx - \int_\sigma \underbrace{(A(u)\nabla u)_i}_{=-F_i} \cdot \nu ds = \int_K f_i(u) dx$$

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

$$\mathrm{m}(K)\frac{u^k_{i,K} - u^{k-1}_{i,K}}{\Delta t} + \sum_{\sigma\in\mathcal{E}_K} F^k_{i,K,\sigma} = \mathrm{m}(K) f_i(u^k_K)$$

Numerical flux

Definitions and assumption:

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

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

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

Example: scalar case with $h(u) = u(\log u - 1)$

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

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

Numerical flux: scalar case

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

General scalar case: $h:\mathbb{R}\to\mathbb{R}$, h'' invertible

- Define $\widetilde{u}_\sigma^k$ by $h''(\widetilde{u}_\sigma^k)(u_L^k - u_K^k) = h'(u_L^k) - h'(u_K^k)$
- Multiply scheme by $h'(u_K^k)$, sum over $K\in\mathcal{T}$:

$$\sum_{K\in\mathcal{T}} \frac{\mathrm{m}(K)}{\Delta t} \underbrace{(u_K^k - u_K^{k-1})h'(u_K^k)}_{\geq h(u_K^k) - h(u_K^{k-1})\ (h \text{ convex})}$$

$$+ \sum_{\sigma\in\mathcal{E}} \tau_\sigma \underbrace{\mathrm{D}_{K,\sigma} h'(u^k)}_{= h''(\widetilde{u}_\sigma^k)\mathrm{D}_{K,\sigma} u^k} A(\widetilde{u}_\sigma^k)\mathrm{D}_{K,\sigma} u^k = \sum_{K\in\mathcal{T}} \mathrm{m}(K) \underbrace{f(u_K^k)h'(u_K^k)}_{\leq C_f}$$

- Discrete entropy inequality: $H(u^k) = \sum_{K\in\mathcal{T}} \mathrm{m}(K) h(u_K^k)$

$$H(u_K^k) - H(u_K^{k-1}) + \Delta t \sum_{\sigma\in\mathcal{E}} \tau_\sigma \underbrace{A(\widetilde{u}_\sigma^k)h''(\widetilde{u}_\sigma^k)}_{\geq 0}(\mathrm{D}_{K,\sigma} u^k)^2 \leq C\Delta t$$

Numerical flux: vector-valued case

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

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

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

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

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

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

- What happens if h'' is not diagonal? See second talk!

Overview

Discrete gradient estimate

$$H(u^k) - H(u^{k-1}) + \Delta t \sum_{\sigma=K|L} \tau_\sigma (\mathrm{D}_{K,\sigma} u^k)^T h''(\widetilde{u}_\sigma^k) A_\sigma(\widetilde{u}_\sigma) \mathrm{D}_{K,\sigma} u^k \le C\Delta t$$

Population model:

- Diffusion matrix and Hessian of entropy density:

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

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

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

$$\sum_{\sigma\in\mathcal{E}} \tau_\sigma (\mathrm{D}_{K,\sigma} u^k)^T h''(\widetilde{u}_\sigma^k) A_\sigma(\widetilde{u}_\sigma) \mathrm{D}_{K,\sigma} u^k \ge C \sum_{i=1}^{2} \sum_{\sigma\in\mathcal{E}} a_{ii} \tau_\sigma (\mathrm{D}_{K,\sigma} u_i^k)^2$$

- Gradient estimate not needed for existence but for convergence result

Population model: existence of discrete solutions

$$\mathrm{m}(K)\frac{u_{i,K}^k - u_{i,K}^{k-1}}{\Delta t} + \sum_{\sigma\in\mathcal{E}_K} F_{i,K,\sigma}^k = \mathrm{m}(K) f_i(u_K^k), \quad i = 1,2$$

Theorem (A.J.-Zurek, SINUM 2022)

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

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

- Discrete entropy: $H(u^k) = \sum_{i=1}^2\sum_{K\in\mathcal{T}}\mathrm{m}(K)u_{i,K}(\log u_{i,K}^k - 1)$
- Scheme preserves positivity, mass, and entropy structure
- Can be generalized to n population species (detailed balance needed)
- Valid for general entropy: h convex, h_i' invertible and strictly concave

Population model: ideas of proof

Theorem (A.J.-Zurek, SINUM 2022)

Let $\Omega \subset \mathbb{R}^3$, $a_{ii} > 0$ for $i = 1, 2$, $f(u) \cdot h'(u) \le C_f(1 + h(u))$, and $\Delta t < 1/C_f$. Then $\exists\ u_{i,K}^k \ge 0$ satisfying discrete entropy inequality

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

Ideas of proof:

- Formulation in entropy variable $w_i = \log u_i$ $\to$ yields positivity for $u_i = \exp w_i > 0$
- Regularization by discrete version of $\varepsilon(-\Delta w_i^\varepsilon + w_i^\varepsilon)$ $\to$ yields bounded weak solutions $w_i^\varepsilon \in H^2(\Omega) \hookrightarrow L^\infty(\Omega)$
- Fixed-point problem solved by Brouwer topological degree argument $\to$ only uniform bound for $H(u^\varepsilon)$ (i.e. $L^1(\Omega)$ bound) needed
- Limit $\varepsilon \to 0$: follows from $L^1(\Omega)$ estimate and Bolzano–Weierstraß

Population model: convergence of the scheme

Theorem (A.J.-Zurek, SINUM 2022)

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

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

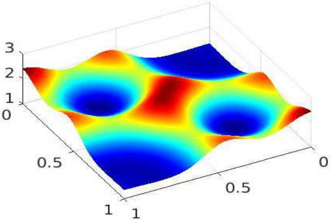
where u solves the population model and ∇^m is the approximate gradient (defined on dual mesh).

Ideas of proof:

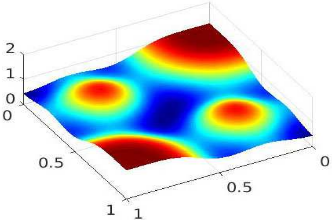
- Discrete entropy inequality gives uniform bounds in (discrete) $L^\infty(0,T;L^1(\Omega))$ and $L^2(0,T;H^1(\Omega))$
- Gagliardo–Nirenberg inequality gives uniform bound in $L^3(\Omega \times (0,T))$
- Discrete time derivative in (discrete) $L^1(0,T;W^{1,6}(\Omega)')$
- Apply discrete Aubin–Lions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

Numerical experiments

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

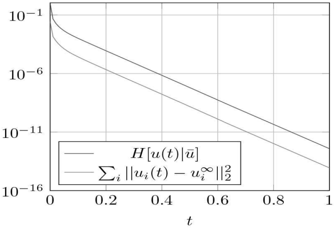


u_1



u_2

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



Summary and perspectives

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

Entropy density: $h(u) = \sum_{i=1}^n h_i(u_i)$

Summary:

- Boundedness-by-entropy provides $L^\infty(\Omega)$ bounds for suitable entropies
- Diagonal Hessian $\Rightarrow$ discrete chain rule from mean approximation
- Finite-volume cheme preserves positivity, mass, and entropy structure
- Existence & convergence proof based on fixed-point argument & discrete compactness

Next lecture:

- Develop discrete boundedness-by-entropy method
- Finite-volume scheme for Maxwell–Stefan systems
- Temporal higher-order finite-volume schemes