Analysis of cross-diffusion systems arising in nonequilibrium thermodynamics

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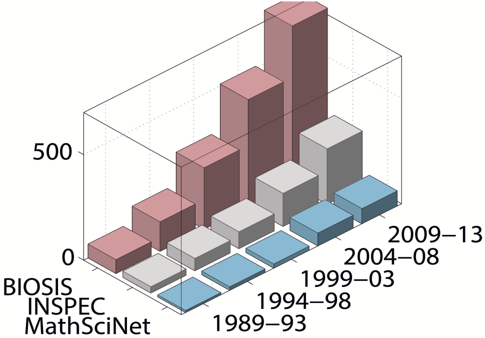
1. Introduction
2. Derivation
3. Entropies and gradient-flow structure
4. Nonstandard examples

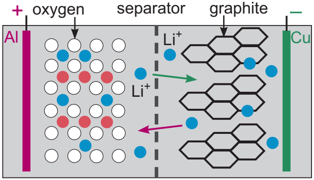
Multi-species systems

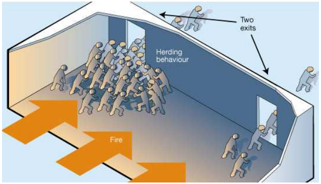
Examples:

- Wildlife populations
- Tumor growth
- Gas mixtures
- Lithium-ion batteries
- Population herding

Nature is composed of multi-species systems



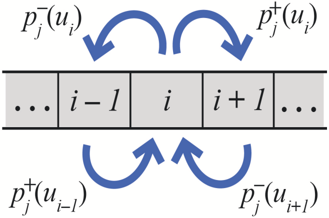




How to model multi-species systems?

Microscopic models:

- Discrete-time Markov chains: matrix-based models
- Continuous-time Markov chains: species move to neighboring cells with transition rate $p_j^{\pm}(u_i)$ ✔
- Particle models: Newton's laws with interactions for each individual



Continuum models:

- Stochastic differential equations: Brownian motion
- Kinetic equations: distribution function depends on phase-space variables (and trait parameters like age, size, maturity)
- Diffusion limit in fluiddynamical equations ✔
- Diffusive equations: deterministic dynamics for particle densities ✔

Overview

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❶ From lattice random walk to cross diffusion

Single species: one space dimension to simplify

- Master equation: time variation = incoming − outgoing

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

- Taylor expansion: (h = grid size)

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

- Diffusion scaling: $t \mapsto t/h^2 \Rightarrow \partial_t \rightsquigarrow h^2\partial_t$

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

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

❶ From lattice random walk to cross diffusion

Multiple species:

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

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

- Transition rates: $p^\pm_{j,i} = p_i(u(x_j)) q_i(u_n(x_{j\pm 1}))$
- Taylor expansion, diffusion scaling and limit $h \to 0$ leads to system of diffusion equations

$$\partial_t u_j = \partial_x \left(\sum_{k=1}^n A_{jk}(u) \partial_x u_k \right), \quad j = 1, \ldots, n$$

- Multi-dimensional case analogous

Examples:

- $q_i = 1$: $A_{ij}(u) = \frac{\partial}{\partial u_j}(u_i pi(u))$ gives population dynamics models
- $p_i = 1$: $A_{ij}(u) = \delta_{ij} q_i(u) + u_i \frac{d}{du_n} q(u_n)$ gives volume-filling models

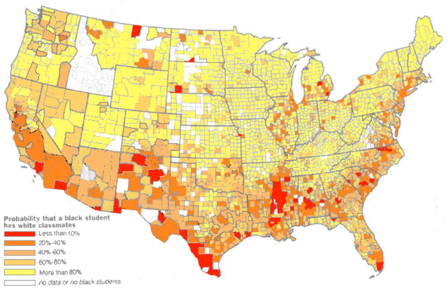
Population dynamics model

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

- $u = (u_1, \ldots, u_n)$ and u_i models population density of ith species
- Diffusion coefficients for $p_i(u) = a_{i0} + a_{i1}u_1 + \cdots + a_{in}u_n$:

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

- Suggested by Shigesada-Kawasaki-Teramoto 1979 for $n = 2$ to model segregation
- Lotka-Volterra functions: $f_i(u) = (b_{i0} - b_{i1}u_1 - b_{i2}u_2)u_i$
- Existence analysis: Kim 1984, Amann 1989, Chen-A.J. 2004, Chen-Daus-A.J. 2016



Source: adapted from the New York Times, April 2, 2000, p. A5.

Ion transport model

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

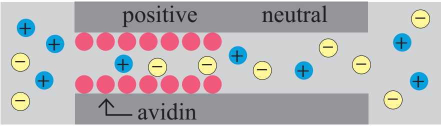
- Central in biological processes such as neural signal transmission and electrical excitability of muscles
- Ion concentration u_i, solvent concentration u_n, $\sum_{j=1}^n u_j = 1$
- Diffusion coefficients for $q_i(u_n) = D_i u_n$:

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

- Derived by Burger-Schlake-Wolfram 2012
- Full model contains electric field V:

$$\partial_t u_i = \operatorname{div} J_i, \quad J_i = D_i u_n \nabla u_i + D_i u_i \nabla u_n + \mu u_i u_n \nabla V$$

- Existence analysis: Burger et al. 2012, A.J. 2015, Zamponi-A.J. 2015



❷ From fluid models to cross diffusion

- Mass and force balance equations:

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

- Force terms: $f_i = \sum_{j=1}^n k_{ij}(v_j - v_i)u_i u_j$
- Properties: $\sum_{i=1}^n u_i = 1$, $\sum_{i=1}^n u_i v_i = 0$, $\sum_{i=1}^n f_i = 0$
- Interphase pressure: $p\nabla u_i$, p: phase pressure (Drew-Segel 1971)
- Assumptions:
  - Inertia approximation: $\varepsilon = 0$
  - Stress tensor: $T_i = -u_i(p\,\mathrm{Id} + P_i)$
  - Pressures: $P_i = P_i(u)$, $P_n = 0$, $k := k_{ij}$

Consequences:

- $k := k_{ij}$ implies that $f_i = -k u_i v_i$
- Pressure: $-\operatorname{div} T_i - p\nabla u_i = u_i \nabla p + \operatorname{div}(u_i P_i)$

$$\partial_t u_i + \operatorname{div}(u_i v_i) = 0, \quad u_i \nabla p + \operatorname{div}(u_i P_i) = -k u_i v_i$$

❷ From fluid models to cross diffusion

$$\partial_t u_i + \operatorname{div}(u_i v_i) = 0, \quad u_i \nabla p + \operatorname{div}(u_i P_i) = -k u_i v_i$$

- Aim: eliminate p and v_i
- Add all force balance equations:

$$0 = -k \sum_{i=1}^{n} u_i v_i = \sum_{i=1}^{n} \big(u_i \nabla p + \operatorname{div}(u_i P_i)\big) = \nabla p + \sum_{i=1}^{n-1} \operatorname{div}(u_i P_i)$$

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

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

- Diffusion coefficients:

$$A_{ii} = (1-u_i)\left(P_i + u_i \frac{\partial P_i}{\partial u_i}\right) - u_i \sum_{j \neq i} u_j \frac{\partial P_j}{\partial u_i},$$

$$A_{ij} = u_i(1-u_i)\frac{\partial P_i}{\partial u_j} - u_i P_j - u_i \sum_{k \neq i} u_k \frac{\partial P_k}{\partial u_j}, \quad j \neq i.$$

Multicomponent gas mixtures

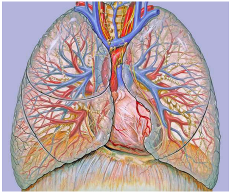
No phase pressure ($p=0$), $P_i=1$ gives Maxwell-Stefan system

$$\partial_t u_i - \operatorname{div} J_i = f_i(u), \quad \nabla u_i = \sum_{j=1}^n d_{ij}(u_j J_i - u_i J_j) =: (CJ)_i, \quad i=1,\ldots,n$$

- Volume fractions of gas components u_i, $\sum_{i=1}^n u_i = 1$
- Invert $\nabla u = CJ$ on $\ker(C)^\perp$, $\ker(C)=\{\mathbf{1}\}$:

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

- Application: Patients with airway obstruction inhale Heliox to speed up diffusion
- Proposed by Maxwell 1866/Stefan 1871
- Duncan-Toor 1962: Fick's law ($J_i \sim \nabla u_i$) not sufficient, include cross-diffusion terms
- Existence analysis: Giovangigli 1999, Bothe 2011, A.J.-Stelzer 2013



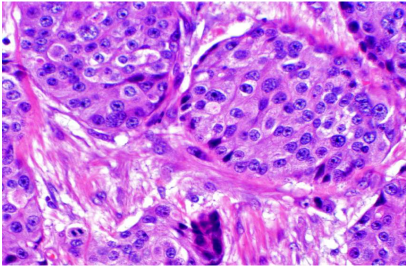
Tumor-growth modeling

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

- Volume fractions of tumor cells u_1, extracellular matrix u_2, nutrients/water $u_3 = 1 - u_1 - u_2$
- Diffusion matrix: pressures $P_1 = u_1$, $P_2 = \beta u_2(1+\theta u_1)$

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

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



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Cross-diffusion systems

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

Main features:

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

Common feature: $\exists\ H(u) = \int_\Omega h(u)dx$ such that $\frac{dH}{dt}(u(t)) \le 0$ for $t > 0$

Physical reason: $H(u)$ is entropy/free energy

Mathematical reason: gradient-flow structure

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

- Example: $\mathbb{R}^d$ with Euclidean structure $\Rightarrow \partial_t u = -H'(u)$
  $H(u)$ is Lyapunov functional since $\partial_t H(u) = -|H'(u)|^2$
- Gradient flow of entropy w.r.t. Wasserstein distance (Otto), entropy $H(u) = \int u \log u dx$: $\partial_t u = \mathrm{div}(u\nabla H'(u)) = \Delta u$

Gradient flows: Cross-diffusion systems

Main assumption

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

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

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

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

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

Consequences:

1. H is Lyapunov functional if $f = 0$:

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

2. L^∞ 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!)

Boundedness-by-entropy method

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

Assumptions:

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

Theorem (A.J., *Nonlinearity* 2015)

Let the above assumptions hold, let $D \subset \mathbb{R}^n$ be bounded, $u^0 \in L^1(\Omega)$, $u^0(x) \in \overline{D}$. 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 Population dynamics model

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

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

- Entropy:

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

$\Rightarrow u = (h')^{-1}(w) = (e^{a_{12}w_1}, e^{a_{21}w_2}) \in D = (0,\infty)^2$
gives automatically nonnegativity of u_i

- Entropy production:

$$\frac{dH}{dt}(u) = -\int_\Omega \left(\frac{4}{a_{12}}(a_{10} + a_{11}u_1)|\nabla\sqrt{u_1}|^2 + \frac{4}{a_{21}}(a_{20} + a_{22}u_2)|\nabla\sqrt{u_2}|^2 + 2|\nabla\sqrt{u_1u_2}|^2 \right) dx \le 0$$

gives global existence of solutions (L. Chen-A.J. 2004-2006)

❷ Ion transport model

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

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

- Entropy:

$$H(u) = \int_\Omega h(u)dx = \int_\Omega \sum_{i=1}^{n} u_i(\log u_i - 1)$$

gives automatically lower and upper bounds:

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

- Entropy production:

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

❸ Tumor-growth models & ❹ Maxwell-Stefan models:

- Same entropy as above
- Gives L^2 estimates for ∇u_i (tumor growth), $\nabla\sqrt{u_i}$ (Maxwell-Stefan)

Relation to nonequilibrium thermodynamics

- Physical entropy s, mathematical entropy $h = -s$
- Chemical potential $= \mu_i = -\frac{\partial s}{\partial u_i} = \frac{\partial h}{\partial u_i} = w_i =$ entropy variable
- Mixture of ideal gases: $\mu_i = \mu_i^0 + \log u_i$, $\mu_i^0 = \text{const.} \Rightarrow$

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

New developments: improved Nernst-Planck model (Druet et al. 2016)

- Mass balance eqs.: $\partial_t u_i + \operatorname{div}(u_i v + J_i) = f_i(u)$, v: mean velocity
- Total mass conservation: $\partial_t u + \operatorname{div}(uv) = 0$, $u = \sum_{i=1}^n u_i$
- Momentum balance equation: $\partial_t(uv) + \operatorname{div}(uv \otimes v - T) = ub$
- Fluxes: $J_i = -\sum_{j=1}^n D_{ij} \nabla \mu_j$, stress tensor: $T = -p\,\mathrm{Id} + T_{\mathrm{visc}}$
- Idea: derive constitutive equations from free energy $\psi(u_1, \ldots, u_n)$

$$\mu_i = \frac{\partial \psi}{\partial u_i}, \quad p = -\psi + \sum_{i=1}^n u_i \mu_i$$

$\rightarrow$ in progress with M. Pokorný et al.

Question: Does entropy structure hold in nonstandard models?

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Van der Waals fluids (A.J.-Mikyška-Zamponi 2016)

- Flow of chemical concentrations u_i in “porous” domain (porosity $= 1$)

$$\partial_t u_i + \operatorname{div}\left(u_i v + \varepsilon \sum_{j=1}^n D_{ij} \nabla \mu_i\right) = 0, \quad i = 1, \dots, n, \quad u_{\text{tot}} = \sum_{i=1}^n u_i$$

$$h(u) = \sum_{i=1}^n u_i(\log u_i - 1) - u_{\text{tot}} \log\left(1 - \sum_{j=1}^n b_j c_j\right) - \sum_{i,j=1}^n a_{ij} u_i u_j$$

- Chemical potential:

$$\mu_i = \frac{\partial h}{\partial u_i} = -\log\left(1 - \sum_{j=1}^n b_j u_j\right) + \frac{b_i u_{\text{tot}}}{1 - \sum_{j=1}^2 b_j u_j} + \log u_i - 2\sum_{j=1}^n a_{ij} u_j$$

- Darcy’s law: $v = -\nabla p$, Gibbs-Duhem relation: $p = \sum_{i=1}^n u_i \mu_i - h(u)$

$$p = \frac{u_{\text{tot}}}{1 - \sum_{j=1}^2 b_j u_j} - \sum_{i,j=1}^2 a_{ij} u_i u_j \quad \text{(van der Waals pressure)}$$

- Cross-diffusion system: $\partial_t u_i = \operatorname{div}\left(\sum_{j=1}^n (u_i u_j + \varepsilon D_{ij}) \nabla \mu_j\right)$

Van der Waals fluids

$$\partial_t u_i = \operatorname{div}\left(\sum_{j=1}^n (u_i u_j + \varepsilon D_{ij})\nabla\mu_j\right)$$

- Entropy:
$$H(u) = \int_\Omega \left\{ \sum_{i=1}^n u_i(\log u_i - 1) - u_{\rm tot}\log\left(1 - \sum_{j=1}^n b_j c_j\right) - \sum_{i,j=1}^n a_{ij}u_i u_j \right\} dx$$
- Entropy production:
$$\frac{dH}{dt} + \int_\Omega |\nabla p|^2 dx + \varepsilon\int_\Omega \textstyle\sum_{i,j=1}^n D_{ij}\nabla\mu_i\cdot\nabla\mu_j dx = 0$$

Assumptions:

- Max. eigenvalue of (a_{ij}) “small” $\Rightarrow h''(u)$ pos. def., $u \leftrightarrow \mu$ invertible
- $\varepsilon > 0 \Rightarrow H^1$ estimates, global existence (A.J.-Mikyška-Zamponi 2016)

What about $\varepsilon = 0$?

- System is not parabolic in the sense of Petrovskii
- Lack of parabolicity compensated by conserved quantities: for all ϕ

$$\frac{d}{dt}\int_\Omega u_{\rm tot}\phi\left(\frac{u_1}{u_{\rm tot}},\ldots,\frac{u_{n-1}}{u_{\rm tot}}\right)dx = 0,$$

open: physical interpretation

Partial averaging in economics (A.J.-Zamponi 2016)

- Reference: talk of P.L. Lions (Vienna 2015)
- Forward Kolmogorov equation with volatility $\sigma = \mathrm{diag}(\sigma_i)$, zero drift

$$\partial_t f = \frac{1}{2}\sum_{j=1}^{n} \frac{\partial^2}{\partial x_j^2}(\sigma_j^2 f), \quad \text{in } \mathbb{R}^n, \ t > 0$$

  $f(x_1, \ldots, x_n, t)$ is probability density of Ito process
- Assumption: σ_j is function of partial averages

$$u_i(x,t) = \int_{\mathbb{R}} f(x, x_n, t) e^{\lambda_i x_n} dx_n, \quad x = (x_1, \ldots, x_{n-1})$$

- Interpretation: u_i = average with respect to economic parameter x_n
- Simplify: $i = 1, 2$, $\sigma = \sigma_j$, $\mu_i := \lambda_i^2 \sigma_n / 2$:

$$\partial_t u_i = \frac{1}{2}\Delta\big(\sigma(u)^2 u_i\big) + \mu_i u_i \quad \text{in } \mathbb{R}^{n-1}, \ t > 0, \ i = 1, 2$$

- Parabolic in sense of Petrovskii if $\sigma + u_1 \partial_1 \sigma + u_2 \partial_2 \sigma \geq 0$
- Fulfilled if e.g. $\sigma(u)^2 = 2a(u_1/u_2)$ for some function a

Partial averaging in economics

$$\partial_t u_i = \Delta\big(a(u_1/u_2)u_i\big) + \mu_i u_i \quad \text{in } \mathbb{T}^d,\ t>0, \quad u_i(0)=u_i^0$$
or $\partial_t u = \operatorname{div}(A(u)\nabla u)$

- Assumptions: $a \in C^1(\mathbb{R})$, $a(r) \ge r|a'(r)|$, $a(r) \ge a_0/(r^p + r^{-p})$, examples: $a(r) = r^p$ for $0 < p \le 1$, $a(r) = 1/r$
- Nonstandard entropy: $\alpha \ge p+4$

$$H(u) = \int_{\mathbb{T}^d} h(u)dx,\ h(u) = \left(\frac{u_1}{u_2}\right)^{\alpha} u_1^2 + \left(\frac{u_1}{u_2}\right)^{-\alpha} u_2^2 + \sum_{i=1}^2 (u_i - \log u_i)$$

- Entropy production:

$$\frac{dH}{dt} + \int_{\mathbb{T}^d}\left(\left(\frac{u_1}{u_2}\right)^{\alpha-p} + \left(\frac{u_1}{u_2}\right)^{p-\alpha}\right)(|\nabla u_1|^2 + |\nabla u_2|^2)dx \le C(\mu_1,\mu_2)H$$

- Properties: h convex, $h''(u)A(u)$ positive definite
- Yields global existence of weak solutions (A.J.-Zamponi 2016)

Summary

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

- Macroscopic modeling of multi-species systems leads to cross-diffusion systems
- Derivation from lattice, kinetic, fluid, stochastic models
- Many systems possess entropy structure or gradient-flow structure

$$\frac{dH}{dt} + \int_\Omega \nabla u : h''(u)A(u)\nabla u dx = 0, \; H = \int_\Omega h(u)dx, \; w = h'(u)$$

- Benefit: global existence, L^∞ estimates, relation to thermodynamics
- Entropy method very flexible, applicable to nonstandard situations

Perspectives:

- How large is class of diffusion systems having an entropy structure?
- Intertwine thermodynamics and analysis of cross-diffusion systems
- Analysis of complex multicomponent fluids (nonideal, non-isothermal)

Transformation by entropy increase?

Ganesha = elephant head, patron of sciences, kind & jovial & wise