Analysis of entropic cross-diffusion systems of hyperbolic-parabolic type

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Thermodynamic framework

$$\dot{z} = -\mathcal{K}(z)D\mathcal{E}(z)$$

- State variable z = z(t)
- **b** Driving functional $\mathcal{E} = \mathcal{E}(\mathbf{z})$
- Onsager operator \mathcal{K} such that $\mathcal{K}(z)$ is symmetric and positive semi-definite for all z

Example (multi-component diffusion)

 $\pmb{z} = u, \ u = (u_1, \dots, u_n);$ $\mathcal{E} = H$ with $H(u) = \int h(u) \, \mathrm{d}x$ with $h \in C^2$ locally strongly convex

 $\mathcal{K}(u)\Box = -\operatorname{div}(\mathsf{M}(u)\nabla\Box), \qquad \mathsf{M}(u) \in \mathbb{R}^{n \times n}_{\operatorname{sym}}, \quad \mathsf{M}(u) \ge \mathsf{O}$

 \implies Evolution equation $\partial_t u = \operatorname{div}(A(u)\nabla u)$ with $A(u) = M(u)D^2h(u)$

If rank(A(u)) = n, then σ (A(u)) $\subset \mathbb{R}_+ \rightsquigarrow$ parabolic.

Focus of this talk: rank M(u) < n

Outline

Population dynamics

- Hyperbolic-parabolic normal form
- Young measure framework

2 Viscoelastic phase separation

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Directed motion to avoid crowding / Contact inhibition

System of *n* species with partial densities $u = (u_1, \ldots, u_n)$ and partial velocity fields $\mathbf{v}_1, \ldots, \mathbf{v}_n$.

$$\partial_t u_i + \operatorname{div}(u_i \mathbf{v}_i) = 0, \qquad i=1,\ldots,n,$$

for $t > 0, x \in \Omega \subseteq \mathbb{R}^d$.

Phenomenological closure Gurtin, Pipkin (1984), Busenberg, Travis (1983):

$$\mathbf{v}_i = -k_i \nabla p, \qquad p := \sum_{i=1}^n u_i,$$

where $k_i > 0, i = 1, ..., n$.

- ▶ If k_i = k for all i: Globally WP Bertsch, Hilhorst, Mimura, Izuhara (2012) linear transport eq.
- For **unequal k**_i only few results on the initial-value problem:
 - Bertsch et al. (1985), segregated, 1D: Global existence and uniqueness
 - ▶ Lorenzi, Lorz, Perthame (2017), segregated, source: Instabilities in 2D sim. and 1D travelling wave
 - Kim, Tong (2021), segregated, 2D, incompressible with source: LWP for nearly radial interface.
 - Druet, H, Jüngel (2023), mixed data: Local Cauchy theory H, Jüngel: Global measure-valued solutions

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Cauchy theory for mixed initial data

Write PDE system as

 $\partial_t u - \operatorname{div}((\vec{\kappa}(u) \otimes \mathbf{1}) \nabla u) = 0,$

where $\vec{\kappa}(u) = (k_1 u_1, \dots, k_n u_n)^T$, $\mathbf{1} = (1, \dots, 1)^T$. Space domain \mathbb{T}^d , for simplicity.

- Kawashima–Shizuta theory **not** applicable (ker M(u) depends on u)
- Ad hoc strategy': cancel 2nd order spatial derivatives in (n-1) components by suitable change of variables w = Φ(u), where Φ: (ℝ₊)ⁿ → Φ((ℝ₊)ⁿ). For n = 2, obtain with w =: (z, p),

$$\partial_t \mathbf{z} - c(\mathbf{w}) \nabla \mathbf{p} \cdot \nabla \mathbf{z} = -\frac{(k_2 - k_1)}{\mathfrak{a}(\mathbf{w})} |\nabla \mathbf{p}|^2, \qquad \partial_t \mathbf{p} = \operatorname{div}(\mathfrak{a}(\mathbf{w}) \nabla \mathbf{p}).$$

where $c(w) = k_1 + (k_2 - k_1) \frac{k_1 u_1}{a(w)} > 0$, $a(w) = \sum_{i=1}^2 k_i u_i$

▶ If $n \ge 3$, need to ensure symmetrisability of hyperbolic subsystem

Generalisation to rank-r diffusions

Consider, more generally,

$$\partial_t u_i + \operatorname{div}(u_i \mathbf{v}_i) = 0, \qquad i = 1, \ldots, n,$$

with

$$\mathbf{v}_i = -\nabla \big(\sum_{j=1}^n b_{ij} u_j\big),$$

where $B := (b_{ij}) \in \mathbb{R}^{n \times n}$ is such that $B \operatorname{diag}(\lambda) \in \mathbb{R}_{\mathrm{sym}}^{n \times n}$ is positive semi-definite for some $\lambda \in (0, \infty)^n$.

Let $\mathbf{r} := \operatorname{rank} B \in \{1, ..., n\}.$

Theorem (P.-E. Druet, KH, A. Jüngel, CPDE'23)

There exists a domain $\hat{\mathcal{D}} \subset \mathbb{R}^n$ and a C^{∞} -diffeom. $\Phi : (\mathbb{R}_+)^n \to \hat{\mathcal{D}}$, $u \mapsto w$, such that in the *w*-variables, the cross-diffusion system can be recast in **symmetric hyperbolic-parabolic form**:

$$\begin{split} \mathsf{A}_0^{\mathrm{I}}(w) \partial_t w_{\mathrm{I}} &+ \sum_{\nu=1}^d \mathsf{A}_1^{\mathrm{I}}(w, \partial_{x_{\nu}} w_{\mathrm{II}}) \partial_{x_{\nu}} w_{\mathrm{I}} = f^{\mathrm{I}}(w, \nabla w_{\mathrm{II}}), \\ \mathsf{A}_0^{\mathrm{II}} \partial_t w_{\mathrm{II}} &- \operatorname{div} \left(\mathsf{A}_*^{\mathrm{II}}(w) \nabla w_{\mathrm{II}} \right) = 0, \end{split}$$

where $A_0^{\mathrm{I}}: \mathcal{D} \longrightarrow \mathbb{R}_{\mathrm{spd}}^{(n-r) \times (n-r)}$, and $A_1^{\mathrm{I}}: \mathcal{D} \times \mathbb{R}^r \longrightarrow \mathbb{R}_{\mathrm{sym}}^{(n-r) \times (n-r)}$ is linear in 2^{nd} argument. $A_0^{\mathrm{II}} \in \mathbb{R}_{\mathrm{spd}}^{r \times r}$ is constant, and $A_*^{\mathrm{II}}: \mathcal{D} \longrightarrow \mathbb{R}_{\mathrm{spd}}^{r \times r}$, $f^{\mathrm{I}}: \mathcal{D} \times \mathbb{R}^r \longrightarrow \mathbb{R}^{n-r}$ is quadratic in 2^{nd} argument.

Theorem ("Corollary")

Smooth positive initial data in $H^{s}(\mathbb{T}^{d})$, $s > \frac{d}{2} + 1 \implies$ Exists unique local classical solution.

Remark: Threshold $s > \frac{d}{2} + 1$ is classical for Friedrichs-symmetrisable hyperbolic systems.

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Nonlinear structure

For $t > 0, x \in \mathbb{T}^d$:

$$\partial_t u_i + \operatorname{div}(u_i \mathbf{v}_i) = 0, \qquad \mathbf{v}_i = -\nabla(Bu)_i \qquad \text{for } i = 1, \dots, n$$

for $B = (b_{ij}) \in \mathbb{R}^{n \times n}$ symmetric positive semi-definite with $b_{ij} \ge 0$, $b_{ii} > 0$.

Formal gradient-flow structure $\dot{u} = -\mathcal{K}(u)D\mathcal{E}(u)$, $\mathcal{K}(u)\Box = -\operatorname{div}(\mathsf{M}(u)\nabla\Box)$. Two options:

Driving functional	$\mathcal{E}(u)$		Mobility $M(u)$	
Boltzmann	$H(u) = \int_{\mathbb{T}^d} h(u) \mathrm{d}x$	$h(u) = \sum_i u_i \log u_i$	$M_{ik}(u) = u_i b_{ik} u_k$	
Rao	$Q(u) = \frac{1}{2} \int_{\mathbb{T}^d} u^T B u \mathrm{d} x$		$M_{ik}(u) = u_i \delta_{ik}$	"Otto"

Thus, along smooth positive solutions

$$\frac{\mathrm{d}}{\mathrm{d}t}H(u) = -\int_{\mathbb{T}^d} |\nabla \sqrt{B}u|^2 \,\mathrm{d}x, \qquad \frac{\mathrm{d}}{\mathrm{d}t}Q(u) = -\int_{\mathbb{T}^d} \sum_{i=1}^n u_i |\mathsf{v}_i|^2 \,\mathrm{d}x.$$

A priori estimates ... and the problem of compactness

Suppose $(u^{(m)})_m$ is sequence of (approximate) solutions with $u_i^{(m)} \ge 0$ for all *i* and

 $\operatorname{essup}_t H(u^{(m)}(t)) \leq C, \qquad \operatorname{essup}_t Q(u^{(m)}(t)) \leq C,$

$$\int_0^\infty \int_{\mathbb{T}^d} |\nabla \sqrt{B} u^{(m)}|^2 \, \mathrm{d} x \mathrm{d} \tau \leq C, \qquad \int_0^\infty \int_{\mathbb{T}^d} \sum_i u_i^{(m)} |\mathsf{v}_i^{(m)}|^2 \, \mathrm{d} x \mathrm{d} \tau \leq C,$$

where $v_i^{(m)} = -\nabla (Bu^{(m)})_i$.

This implies boundedness of $u_i^{(m)}, v_i^{(m)}$, and $u_i^{(m)}v_i^{(m)}$ in suitable $L^p(L^q), p, q > 1$. After passing to a subsequence

$$u^{(m)} \stackrel{*}{\rightharpoonup} u$$
 in $L^{\infty}(L^2)$, $v_i^{(m)} \rightarrow v_i = \nabla(Bu)_i$ in $L^2(L^2)$, and $u_i^{(m)}v_i^{(m)} \rightarrow \overline{u_i^{(m)}v_i^{(m)}}$ in $L^2(L^{4/3})$.

If ker *B* is non-trivial, it is unclear whether $\overline{u_i^{(m)}v_i^{(m)}}$ and u_iv_i coincide.

Young measures (YM)

YM as PDE *solution* concept were first considered by DiPerna (1985) for hyperbolic conservation laws. Associate with each $u^{(m)}$ a parametrised probability measure $\mu^{(m)} = (\mu_{t,x}^{(m)})_{t,x}$ via

$$\mu^{(m)} := \delta_{(u^{(m)}, \nabla \widehat{u}^{(m)})}$$

where $\hat{u}^{(m)} := P_{(\ker B)^{\perp}} u^{(m)}$ and $P_{(\ker B)^{\perp}}$ the projection onto $(\ker B)^{\perp} \subseteq \mathbb{R}^n$. Then

$$u_i^{(m)}\mathsf{v}_i^{(m)} = -\int_W s_i(B\rho)_i \mathrm{d}\mu^{(m)}(s,\rho) =: -\langle \mu^{(m)}, s_i(B\rho)_i \rangle$$

where $W := [0,\infty)^n \times (\ker B^{\perp})^d$. For every T > 0, the sequence

$$(\mu^{(m)})_m \subset L^{\infty}_{w^*}((0,T) \times \mathbb{T}^d; \mathcal{M}(W)) \simeq (L^1((0,T) \times \mathbb{T}^d; C_0(W)))^*$$

is bounded and hence weakly-* convergent along subsequence.

Dissipative measure-valued-strong uniqueness

We call $U \in C^1([0, T] \times \mathbb{T}^d)^n$ a strong solution if it satisfies $\partial_t U_i - \operatorname{div} (U_i \nabla (BU)_i) = 0$ in the weak sense and if it is strictly positive componentwise.

Theorem (KH, A. Jüngel)

Let $U \in C^1([0, T] \times \mathbb{T}^d)^n$ be a strong solution with initial datum $U(0, \cdot) = u^{\text{in}}$, and let μ be a dissipative measure-valued solution. Then

$$\mu_{t,x} = \delta_{U(t,x)} \otimes \delta_{\nabla \widehat{U}(t,x)} \quad \text{for a.e. } (t,x) \in (0,\mathcal{T}) \times \mathbb{T}^d.$$

Remarks:

- Weak-strong uniqueness of measure-valued solutions was first obtained by Brenier, De Lellis, Székelyhidi (2011) for the incompressible Euler equations.
- ▶ The proof is based on the relative entropy technique (Dafermos 1979, DiPerna 1979).

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Viscoelastic phase separation (VPS)

Phase separation in polymer-solvent mixture



► Zhou, Zhang, E (2006): $\mathcal{E}(u,q) = F(u) + \frac{1}{2} \int_{\Omega} q^2 dx$, $F(u) = \int_{\Omega} \left(\frac{\varepsilon^2}{2} |\nabla u|^2 + f(u)\right) dx$, f Flory-Hug. $u = u(t,x) \in [-1,1]$ order parameter; $q = q(t,x) \in \mathbb{R}$ bulk stress variable

$$\begin{split} \partial_t u &= -\operatorname{div}\left((1-u^2)\boldsymbol{j}\right), \qquad \boldsymbol{j} = -[(1-u^2)\nabla\frac{\delta F}{\delta u} - \nabla(A(u)q)], \qquad t > 0, x \in \Omega, \\ \partial_t q &= -\frac{1}{\tau(u)}q + A(u)\operatorname{div}\boldsymbol{j}, \qquad t > 0, x \in \Omega, \\ (1-u^2)\boldsymbol{j} \cdot \nu &= 0, \qquad \nabla u \cdot \nu = 0, \qquad t > 0, x \in \partial\Omega, \end{split}$$

A(u): bulk modulus; $\tau(u)$: relaxation time; $\Omega \subset \mathbb{R}^d$ smooth bounded domain, d ≥ 2. ► Brunk, Lukáčová-Medvid'ová (2022) with hydrodynamics \longrightarrow later today

Entropic structure

$$\dot{\mathbf{z}} = -\mathcal{K}(\mathbf{z})D\mathcal{E}(\mathbf{z})$$

• State $\mathbf{z} = (u, q)$

- Free energy $\mathcal{E}(u,q) = F(u) + \frac{1}{2} \int_{\Omega} q^2 \, \mathrm{d}x$ with $\nabla u \cdot \nu = 0$ on $\partial \Omega$
- ▶ Onsager operator \mathcal{K} : $M(u), L(u) \in \mathbb{R}^{2\times 2}_{sym}$ positive semi-definite, $N_1(u) \in \mathbb{R}^{2\times 2}$

 $\mathcal{K}(u,q)\Box = -N_1(u)^T \operatorname{div} (\mathsf{M}(u)\nabla(N_1(u)\Box)) + \mathsf{L}(u)\Box \quad \text{with no-flux b.c.}$

ZZE model:

$$M(u) = N_2(u)m(u)(\mathbf{1} \otimes \mathbf{1})N_2(u), \text{ where } \mathbf{1} = (1,1)^T, \qquad L(u) = \operatorname{diag}\left(0, \frac{1}{\tau(u)}\right)$$
$$N_1(u) = \operatorname{diag}(1, -A(u)), \quad N_2(u) = \operatorname{diag}\left(1, \frac{1}{n(u)}\right)$$

• with $m(u) = (1 - u^2)^2$, $n(u) = 1 - u^2$

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Modified **ZZE model**:

$$\begin{split} \mathsf{M}(u) &= \mathsf{N}_2(u)\mathsf{m}(u)(\mathbf{1}\otimes\mathbf{1})\mathsf{N}_2(u), \quad \text{where } \mathbf{1} = (1,1)^T, \qquad \mathsf{L}(u) = \mathsf{diag}\left(0,\frac{1}{\tau(u)}\right)\\ \mathsf{N}_1(u) &= \mathsf{diag}(1,-\mathsf{A}(u)), \quad \mathsf{N}_2(u) = \mathsf{diag}\left(1,\frac{1}{\mathsf{n}(u)}\right) \end{split}$$

▶ with $m(u) = 1 - u^2$, $u \mapsto n(u)$ monotonic; $\min_{[-1,1]} |n| > 0$; either $n' \equiv 0$ or |n'| > 0 on [-1,1]

. . .

Effect of coupling function n(u)

$$\begin{aligned} \partial_t u &= -\operatorname{div}\left(m(u)\boldsymbol{j}\right), \qquad \boldsymbol{j} = -\left[\nabla w - \frac{1}{n(u)}\nabla(A(u)q)\right], \quad w \in \partial_u F_\varepsilon, \qquad t > 0, x \in \Omega, \\ \partial_t q &= -\frac{1}{\tau(u)}q + A(u)\operatorname{div}\left(\frac{m(u)}{n(u)}\boldsymbol{j}\right), \qquad t > 0, x \in \Omega, \\ m(u)\boldsymbol{j} \cdot \nu &= 0, \qquad \nabla u \cdot \nu = 0, \qquad t > 0, x \in \partial\Omega, \end{aligned}$$

with $F_{\varepsilon}(u) = \int_{\Omega} \left(\frac{\varepsilon^2}{2} |\nabla u|^2 + f(u) \right) \mathrm{d}x.$

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with $F_{\varepsilon}(u) = \int_{\Omega} \left(\frac{\varepsilon^2}{2} |\nabla u|^2 + f(u)\right) \mathrm{d}x.$

Later-stage evolution of Cahn-Hilliard type models

Expect curvature flow:

 $V_{\Gamma} = \mathcal{G}_{\Gamma} \kappa_{\Gamma}, \qquad V_{\Gamma}: \text{ normal velocity}, \quad \kappa_{\Gamma}: \text{ mean curvature of interface } \Gamma.$



Degenerate Cahn–Hilliard equation along $t \mapsto \varepsilon^2 t$ and vanishing temperature θ :

▶ Formal asymptotics by Cahn, Elliott, Novick–Cohen (1996) yield surface diffusion flow:

$$\mathcal{G}_{\mathsf{\Gamma}} = -rac{\sigma}{\delta} \Delta_{\mathsf{\Gamma}}, \qquad rac{\sigma}{\delta} = rac{16}{\pi^2} > 0,$$

[for logarithmic potential with $\theta = O(\varepsilon^{\alpha})$, $\alpha > 0$; resp. double-obstacle potential $f^{(DO)}$] Rigorous limit is open

Interface dynamics in VPS (KH, J. R. King, A. Münch, B. Wagner) (i) If $n \equiv 1$: intermediate surface diffusion flow [Cahn, Taylor (1994)]

$$\mathcal{G}_{\Gamma} = -\sigma (\delta \mathsf{Id} - \omega \Delta_{\Gamma})^{-1} \Delta_{\Gamma}, \qquad \sigma, \delta, \omega > 0.$$

(ii) If $n \in C^{\infty}(\mathbb{R})$ with $\min_{[-1,1]} |n| > 0$, $\min_{[-1,1]} |n'| > 0$, then $\mathcal{G}_{\Gamma} : \kappa \to V$ is determined by a constrained elliptic equation. Given $\kappa = \kappa(s), s \in \Gamma$, find solution (f, V), f = f(s, u), V = V(s) : $-\partial_u(a\partial_u f) - \tilde{m}\Delta_{\Gamma}f = (1 - \partial_u(\frac{n}{n'}))V$ in $\Gamma \times [-1,1],$ $-a\partial_u f = -\frac{n}{n'}V$ on $\Gamma \times \{\pm 1\},$ $\int_{-1}^{+1} (f + \frac{n}{n'}\partial_u f) du = \sigma \kappa$ on Γ ("solvability condition"; constraint)

For special choice of $m(u), A(u), \tau(u)$:

$$\mathcal{G}_{\Gamma} = \sigma \eta \sqrt{-\Delta_{\Gamma}} + \sigma \mathcal{R}(\sqrt{-\Delta_{\Gamma}}), \quad \mathcal{R} \text{ of lower order}, \qquad \eta = \left(\left(\frac{n(1)}{n'(1)}\right)^2 + \left(\frac{n(-1)}{n'(-1)}\right)^2 \right)^{-1}$$

Order of $\mathcal{R}(\sqrt{-\Delta_{\Gamma}})$ is $-\infty$ if $n = n(u)$ is affine.

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Thank you!

Definition (Dissipative measure-valued dmv solution)

Let $\mu \in L^{\infty}_{w^*}([0,\infty) \times \mathbb{T}^d; \mathcal{P}(W))$ be parametrised measure and define $u := \langle \mu, s \rangle$ and $\mathbf{y} := \langle \mu, \mathbf{p} \rangle$. Then, μ is called a dmv solution if for all T > 0:

Basic regularity: For i = 1, ..., n

$$u_i \in L^{\infty}(0,\infty;L^2), \quad \partial_t u \in L^2(0,\infty;(W^{1,4})^*), \quad \mathbf{y} \in L^2((0,T) \times \mathbb{T}^d;(\ker B^{\perp})^d), \quad \mathbf{y} = \nabla \widehat{u}.$$

Moreover, μ acts trivially on the \hat{s} -component, i.e. for all $f \in C_0(W)$: $\langle \mu, f(s, \mathbf{p}) \rangle = \langle \mu, f(\hat{u} + P_{\ker B}s, \mathbf{p}) \rangle$

Dissipation inequalities: It holds for a.e. t > 0 that

$$\begin{split} & \mathcal{H}^{\mathrm{mv}}(u(t)) + \int_{0}^{t} \int_{\mathbb{T}^{d}} \langle \mu_{\tau,x}, |B^{1/2}\mathbf{p}|^{2} \rangle \mathrm{d}x \mathrm{d}\tau \leq \mathcal{H}(u^{\mathrm{in}}), \quad \text{where } \mathcal{H}^{\mathrm{mv}}(u(t)) := \int_{\mathbb{T}^{d}} \langle \mu_{t,x}, h(s) \rangle \mathrm{d}x, \\ & \mathcal{Q}(u(t)) + \sum_{i=1}^{n} \int_{0}^{t} \int_{\mathbb{T}^{d}} \langle \mu_{\tau,x}, s_{i} | (B\mathbf{p})_{i} |^{2} \rangle \mathrm{d}x \mathrm{d}\tau \leq \mathcal{Q}(u^{\mathrm{in}}). \end{split}$$

Evolution equation: It holds for all i = 1, ..., n and $\phi \in C^1_c([0, T) \times \mathbb{T}^d)$ that

$$\int_0^T \int_{\mathbb{T}^d} u_i \partial_t \phi \mathrm{d}x \mathrm{d}t + \int_{\mathbb{T}^d} u_i^{\mathrm{in}} \phi(0) \mathrm{d}x = \int_0^T \int_{\mathbb{T}^d} \langle \mu_{t,x}, s_i(B\mathbf{p})_i \rangle \cdot \nabla \phi \mathrm{d}x \mathrm{d}t$$