



Weierstrass Institute for
Applied Analysis and Stochastics



Two examples of gradient flows in continuity equation format

Gradient Flows Face to Face
Granada, 18 September 2025

Georg Heinze

based on joint works with

Alexander Mielke, Jan-Frederik Pietschmann, André Schlichting, Artur Stephan

- Gradient systems in continuity equation format
 - Definition and heuristics
 - EDP convergence with embedding
- Example 1: Gradient flows on metric graphs with reservoirs
 - Model and gradient flow formulation
 - Discussion of analytic results
- Example 2: Reaction-diffusion systems
 - Model and gradient flow formulation
 - Discussion of chain rule inequality
- Summary and outlook

Gradient systems in CE format

Gradient systems in continuity equation format

Peletier-Schlichting '23: Gradient system $(X, Y, \nabla, \mathcal{E}, \mathcal{R}^*)$ in CE format:

- Base spaces X, Y and gradient operator $\nabla : C_c^\infty(X) \rightarrow C_c^\infty(Y)$
- Energy $\mathcal{E} : \mathcal{M}_+(X) \rightarrow \mathbb{R}$
- Dual dissipation potential $\mathcal{R}^* : \mathcal{M}_+(X) \times C_c^\infty(Y) \rightarrow [0, \infty]$; convex in 2nd argument
- Gradient flow (GF) equation induced by $(X, Y, \nabla, \mathcal{E}, \mathcal{R}^*)$:

$$\partial_t \mu = -\operatorname{div} D_2 \mathcal{R}^*(\mu, -\nabla D\mathcal{E}(\mu))$$

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- Example: The choices

$$X = Y = \mathbb{R}$$

$$\nabla = \partial_x$$

$$\mathcal{E}(\rho) = \mathcal{H}(\rho|\pi) := \int_{\mathbb{R}} \rho \log(\rho/\pi) - \rho + \pi \, dx$$

$$\mathcal{R}^*(\rho, \xi) = \frac{1}{2} \int_{\mathbb{R}} |\xi|^2 \rho \, dx$$

give us the Fokker-Planck equation

$$\partial_t \rho = \partial_x [\rho \partial_x \log(\rho/\pi)]$$

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Energy dissipation principle (EDP)

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- * Chain rule: $(\mu, j) \in \text{CE}$ s.t. $\operatorname{ess\,sup}_{t \in [0, T]} \mathcal{E}(\mu(t)) < \infty$, $\mathcal{D}(\mu, j) < \infty$, then

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Heuristics:

$$\begin{aligned} \frac{d}{dt} \mathcal{E}(\mu) &= \langle D\mathcal{E}(\mu), \partial_t \mu \rangle = \langle D\mathcal{E}(\mu), -\operatorname{div} j \rangle = -\langle -\nabla D\mathcal{E}(\mu), j \rangle \\ &\geq -\mathcal{R}(\mu, j) - \mathcal{R}^*(\mu, -\nabla D\mathcal{E}(\mu)) \end{aligned}$$

Energy dissipation principle (EDP)

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$$\mathcal{L}(\mu, j) \geq 0$$

- * Energy dissipation principle (EDP):

$$\mathcal{L}(\mu, j) = 0 \iff \begin{cases} (\mu, j) \in \text{CE} \\ j = D_2 \mathcal{R}^*(\mu, -\nabla D\mathcal{E}(\mu)) \end{cases}$$

i.e. $\mathcal{L}(\mu, j) = 0$ if and only if μ is solution of the GF equation

- Next goal: Study limits $(X_\varepsilon, Y_\varepsilon, \nabla_\varepsilon, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon^*) \rightarrow (X_0, Y_0, \nabla_0, \mathcal{E}_0, \mathcal{R}_0^*)$

Convergence of gradient systems

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- Idea: Embed curves satisfying continuity equation in shared space
(cf. Disser-Liero '15, Hraivoronska-Tse '23, Hraivoronska-Schlichting-Tse '24, Esposito-H-Schlichting '24, H-Mielke-Stephan '25)

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Main steps:

- * Compactness: $\exists$ embeddings $\Pi_\varepsilon : \text{CE}_\varepsilon \rightarrow \text{CE}_0$ s.t. for all $(\mu_\varepsilon, j_\varepsilon)_{\varepsilon>0}$ satisfying

$$(\mu_\varepsilon, j_\varepsilon) \in \text{CE}_\varepsilon, \quad \sup_{\varepsilon>0} \text{ess sup}_{t \in [0, T]} \mathcal{E}_\varepsilon(\mu_\varepsilon(t)) < \infty, \quad \sup_{\varepsilon>0} \mathcal{D}_\varepsilon(\mu_\varepsilon, j_\varepsilon) < \infty$$

the family $(\Pi_\varepsilon(\mu_\varepsilon, j_\varepsilon))_{\varepsilon>0}$ is precompact in CE_0

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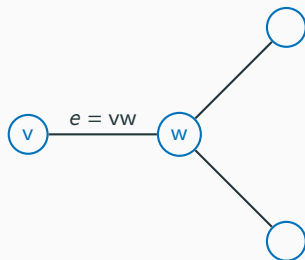
- Immediate consequence: Solutions converge to solutions, i.e.,
if $\mathcal{L}_\varepsilon(\mu_\varepsilon, j_\varepsilon) = 0$ and $\mathcal{L}_0 \geq 0$, then $\mathcal{L}_0(\mu_0, j_0) = 0$

Metric graphs with reservoirs
(GH, J-F Pietschmann, A Schlichting)

Setup

Undirected irreducible simple finite graph:

- Finite set of vertices V
- Set of edges $E \subset V \times V$



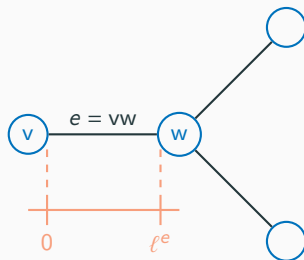
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- Finite set of **vertices** V
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Metric Graph:

- Orientation: $e = vw \in E$ has starting vertex v and end vertex w
- Associate to each $e \in E$ an **intervall** $[0, \ell^e]$



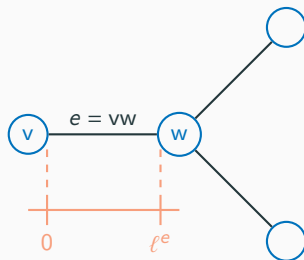
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Dynamics:

- Drift-diffusion along metric edges coupled with reservoirs on vertices

$$\begin{aligned}\partial_t \rho^e &= d^e \partial_x (\partial_x \rho^e + \rho^e \partial_x V^e) \\ -d^e [\partial_x \rho^e + \rho^e \partial_x V^e]_v n_v^e &= r(e, v) \rho^e|_v - r(v, e) \gamma_v \\ \partial_t \gamma_v &= \sum_{e \in E(v)} (r(e, v) \rho^e|_v - r(v, e) \gamma_v)\end{aligned}$$

for potentials $V^e \in \text{Lip}$, diffusivity constants $d^e > 0$, and jump rates $r > 0$

- Freidlin-Wentzell '93: Diffusion on metric intervall obtained as vanishing-diameter limit of diffusion narrow tube using probabilistic approach
- Erbar-Forkert-Maas-Mugnolo '22: McKean-Vlasov-type equations on metric graphs with Kirchhoff-type conditions at vertices identified as GFs w.r.t. suitable dynamic Wasserstein distance
- Fazeny-Burger-Pietschmann '25: “Overdamped isothermal model 3” for gas transport in networks formally understood as dynamic 3-Wasserstein GF
- Burger-Humpert-Pietschmann '23: Dynamic Wasserstein-type distance defined on metric graphs with mass reservoirs at vertices exchanging mass with edges
- Mugnolo-Romanelli '07: Asymptotic behaviour and regularity of solutions studied for similar model to ours using semigroup techniques

$$\partial_t \rho^e = d^e \partial_x (\partial_x \rho^e + \rho^e \partial_x V^e)$$

$$-d^e [\partial_x \rho^e + \rho^e \partial_x V^e]_v n_v^e = r(e, v) \rho^e|_v - r(v, e) \gamma_v$$

$$\partial_t \gamma_v = \sum_{e \in E(v)} (r(e, v) \rho^e|_v - r(v, e) \gamma_v)$$

- Introduce edge reference measures $d\pi^e := \exp(-V^e) dx$
(abuse notation to also write π^e for its density)
- Assume detailed balance condition: $\exists \omega = (\omega_v)_{v \in V} \in \mathcal{M}_{\geq 0}(V)$ s.t.

$$r(e, v) \pi^e|_v = r(v, e) \omega_v \quad \forall e \in E, v \in V$$

$$\partial_t \rho^e = d^e \partial_x (\partial_x \rho^e + \rho^e \partial_x V^e)$$

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- Denote $\mathcal{K}_v^e := r(e, v) \sqrt{\frac{\pi^e|_v}{\omega_v}} = r(v, e) \sqrt{\frac{\omega_v}{\pi^e|_v}}$

► Equations rewritten:

$$\partial_t \rho^e = d^e \partial_x \left(\rho^e \partial_x \log \frac{\rho^e}{\pi^e} \right)$$

$$-d^e \left[\rho^e \partial_x \log \frac{\rho^e}{\pi^e} \right]_v n_v^e = \mathcal{K}_v^e \sqrt{\pi^e|_v \omega_v} \left(\frac{\rho^e}{\pi^e} \Big|_v - \frac{\gamma_v}{\omega_v} \right)$$

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Analytic results:

- * Well-posedness
- * Kirchhoff-type limit: Vanishing reservoirs without cutting dynamics (cf. Erbar-Forkert-Maas-Mugnolo '22)
- * Fast-diffusion limit: Acceleration of edge dynamics (combinatorial graph)

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Strategy:

- Write as gradient flow in CE format
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Numerical simulations:

- Based on finite volume discretization
- Comparison to analytic results
- Highlighting further aspects beyond analysis

Gradient flow formulation

Drift-diffusion terms:

$$d^e \partial_x \left(\rho^e \partial_x \log \frac{\rho^e}{\pi^e} \right)$$

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$$d^e \partial_x \left(\rho^e \partial_x \log \frac{\rho^e}{\pi^e} \right)$$

Free energy:

$$\mathcal{E}_E(\rho) := \sum_{e \in E} \mathcal{H}(\rho^e | \pi^e) := \sum_{e \in E} \int_0^{\ell^e} \rho^e \log(\rho^e / \pi^e) - \rho^e + \pi^e \, dx$$

with variational derivatives $D\mathcal{E}_E(\rho)|_e = \log(\rho^e / \pi^e)$

Gradient and divergence: For $\varphi : L \rightarrow \mathbb{R}$ (L disjoint union of metric edges)

$$\nabla \varphi|_e = \partial_x \varphi^e$$

$$\operatorname{div} j|_e = \partial_x j^e$$

Dual dissipation potential:

$$\mathcal{R}_E^*(\rho, \xi) := \sum_{e \in E} \frac{1}{2} d^e \int_0^{\ell^e} |\xi_e|^2 \, d\rho^e$$

Drift-diffusion terms:

$$d^e \partial_x \left(\rho^e \partial_x \log \frac{\rho^e}{\pi^e} \right)$$

Free energy:

$$\mathcal{E}_E(\rho) := \sum_{e \in E} \mathcal{H}(\rho^e | \pi^e) := \sum_{e \in E} \int_0^{\ell^e} \rho^e \log(\rho^e / \pi^e) - \rho^e + \pi^e \, dx$$

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Dual dissipation potential:

$$\mathcal{R}_E^*(\rho, \xi) := \sum_{e \in E} \frac{1}{2} d^e \int_0^{\ell^e} |\xi_e|^2 \, d\rho^e$$

► Drift-diffusion terms rewritten:

$$- \operatorname{div} D_\xi \mathcal{R}_E^*(\rho, -\nabla D\mathcal{E}_E(\rho))|_e$$

Gradient flow formulation – jump terms

Jump terms:

$$\sum_{e \in E(v)} \kappa_v^e \sqrt{\pi^e|_v \omega_v} \left(\frac{\rho^e}{\pi^e} \Big|_v - \frac{\gamma_v}{\omega_v} \right)$$

Free energy (denoting $\mu := (\gamma, \rho) \in \mathcal{P}(V \times L)$):

$$\mathcal{E}(\mu) := \mathcal{E}_V(\gamma) + \mathcal{E}_E(\rho) := \sum_{v \in V} \mathcal{H}(\gamma_v | \omega_v) + \sum_{e \in E} \mathcal{H}(\rho^e | \pi^e)$$

Gradient flow formulation – jump terms

Jump terms:

$$\sum_{e \in E(v)} \kappa_v^e \sqrt{\pi^e|_v \omega_v} \left(\frac{\rho^e}{\pi^e} \Big|_v - \frac{\gamma_v}{\omega_v} \right)$$

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Gradient and divergence: For $\Phi = (\phi, \varphi) : \mathbf{V} \times \mathbf{L} \rightarrow \mathbb{R}$

$$\overline{\nabla} \Phi|_{v,e} = \phi_v - \varphi^e|_v \qquad \overline{\operatorname{div}} \bar{j}|_v = - \sum_{e \in E(v)} \bar{j}_v^e$$

Gradient flow formulation – jump terms

Jump terms:

$$\sum_{e \in E(v)} \kappa_v^e \sqrt{\pi^e|_v \omega_v} \left(\frac{\rho^e}{\pi^e} \Big|_v - \frac{\gamma_v}{\omega_v} \right)$$

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Gradient and divergence: For $\Phi = (\phi, \varphi) : \mathbf{V} \times \mathbf{L} \rightarrow \mathbb{R}$

$$\overline{\nabla} \Phi|_{v,e} = \phi_v - \varphi^e|_v \qquad \overline{\operatorname{div}} \bar{j}|_v = - \sum_{e \in E(v)} \bar{j}_v^e$$

Motivating calculation:

$$\sum_{e \in E} \int_0^{\ell^e} \varphi^e \operatorname{div} j^e dx + \sum_{v \in V} \phi_v \overline{\operatorname{div}} \bar{j}_v = \sum_{e \in E} \int_0^{\ell^e} \varphi^e \partial_x j^e dx + \sum_{v \in V} \phi_v \left(- \sum_{e \in E(v)} \bar{j}_v^e \right)$$

Gradient flow formulation – jump terms

Jump terms:

$$\sum_{e \in E(v)} \ell_v^e \sqrt{\pi^e|_v \omega_v} \left(\frac{\rho^e}{\pi^e} \Big|_v - \frac{\gamma_v}{\omega_v} \right)$$

Free energy (denoting $\mu := (\gamma, \rho) \in \mathcal{P}(V \times L)$):

$$\mathcal{E}(\mu) := \mathcal{E}_V(\gamma) + \mathcal{E}_E(\rho) := \sum_{v \in V} \mathcal{H}(\gamma_v | \omega_v) + \sum_{e \in E} \mathcal{H}(\rho^e | \pi^e)$$

Gradient and divergence: For $\Phi = (\phi, \varphi) : V \times L \rightarrow \mathbb{R}$

$$\overline{\nabla} \Phi|_{v,e} = \phi_v - \varphi^e|_v \qquad \overline{\operatorname{div}} \bar{j}|_v = - \sum_{e \in E(v)} \bar{j}_v^e$$

Motivating calculation:

$$\begin{aligned} \sum_{e \in E} \int_0^{\ell^e} \varphi^e \operatorname{div} j^e dx + \sum_{v \in V} \phi_v \overline{\operatorname{div}} \bar{j}_v &= \sum_{e \in E} \int_0^{\ell^e} \varphi^e \partial_x j^e dx + \sum_{v \in V} \phi_v \left(- \sum_{e \in E(v)} \bar{j}_v^e \right) \\ &= - \sum_{e \in E} \int_0^{\ell^e} \partial_x \varphi^e j^e dx + \sum_{e \in E} \sum_{v \in V(e)} \varphi^e|_v j^e|_v n_v^e - \sum_{v \in V} \sum_{e \in E(v)} \phi_v \bar{j}_v^e \end{aligned}$$

Gradient flow formulation – jump terms

Jump terms:

$$\sum_{e \in E(v)} \kappa_v^e \sqrt{\pi^e|_v \omega_v} \left(\frac{\rho^e}{\pi^e} \Big|_v - \frac{\gamma_v}{\omega_v} \right)$$

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Gradient and divergence: For $\Phi = (\phi, \varphi) : \mathbf{V} \times \mathbf{L} \rightarrow \mathbb{R}$

$$\overline{\nabla} \Phi|_{v,e} = \phi_v - \varphi^e|_v \qquad \overline{\operatorname{div}} \bar{j}|_v = - \sum_{e \in E(v)} \bar{j}_v^e$$

Motivating calculation:

$$\begin{aligned} \sum_{e \in E} \int_0^{\ell^e} \varphi^e \operatorname{div} j^e dx + \sum_{v \in V} \phi_v \overline{\operatorname{div}} \bar{j}_v &= \sum_{e \in E} \int_0^{\ell^e} \varphi^e \partial_x j^e dx + \sum_{v \in V} \phi_v \left(- \sum_{e \in E(v)} \bar{j}_v^e \right) \\ &= - \sum_{e \in E} \int_0^{\ell^e} \partial_x \varphi^e j^e dx + \sum_{e \in E} \sum_{v \in V(e)} \varphi^e|_v j^e|_v n_v^e - \sum_{v \in V} \sum_{e \in E(v)} \phi_v \bar{j}_v^e \\ &= - \sum_{e \in E} \int_0^{\ell^e} \partial_x \varphi^e j^e dx - \sum_{v \in V} \sum_{e \in E(v)} (\phi_v \bar{j}_v^e - \varphi^e|_v j^e|_v n_v^e) \end{aligned}$$

Gradient flow formulation – jump terms

Jump terms:

$$\sum_{e \in E(v)} \kappa_v^e \sqrt{\pi^e|_v \omega_v} \left(\frac{\rho^e}{\pi^e} \Big|_v - \frac{\gamma_v}{\omega_v} \right)$$

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$$\overline{\nabla} \Phi|_{v,e} = \phi_v - \varphi^e|_v \qquad \overline{\operatorname{div}} \bar{j}|_v = - \sum_{e \in E(v)} \bar{j}_v^e$$

Motivating calculation:

$$\begin{aligned} \sum_{e \in E} \int_0^{\ell^e} \varphi^e \operatorname{div} j^e dx + \sum_{v \in V} \phi_v \overline{\operatorname{div}} \bar{j}_v &= \sum_{e \in E} \int_0^{\ell^e} \varphi^e \partial_x j^e dx + \sum_{v \in V} \phi_v \left(- \sum_{e \in E(v)} \bar{j}_v^e \right) \\ &= - \sum_{e \in E} \int_0^{\ell^e} \partial_x \varphi^e j^e dx + \sum_{e \in E} \sum_{v \in V(e)} \varphi^e|_v j^e|_v n_v^e - \sum_{v \in V} \sum_{e \in E(v)} \phi_v \bar{j}_v^e \\ &= - \sum_{e \in E} \int_0^{\ell^e} \partial_x \varphi^e j^e dx - \sum_{v \in V} \sum_{e \in E(v)} (\phi_v \bar{j}_v^e - \varphi^e|_v j^e|_v n_v^e) \\ &= - \sum_{e \in E} \int_0^{\ell^e} \partial_x \varphi^e j^e dx - \sum_{v \in V} \sum_{e \in E(v)} (\phi_v - \varphi^e|_v) \bar{j}_v^e \end{aligned}$$

Gradient flow formulation – jump terms

Jump terms:

$$\sum_{e \in E(v)} \kappa_v^e \sqrt{\pi^e|_v \omega_v} \left(\frac{\rho^e}{\pi^e} \Big|_v - \frac{\gamma_v}{\omega_v} \right)$$

Free energy (denoting $\mu := (\gamma, \rho) \in \mathcal{P}(\mathbf{V} \times \mathbf{L})$):

$$\mathcal{E}(\mu) := \mathcal{E}_V(\gamma) + \mathcal{E}_E(\rho) := \sum_{v \in V} \mathcal{H}(\gamma_v | \omega_v) + \sum_{e \in E} \mathcal{H}(\rho^e | \pi^e)$$

Gradient and divergence: For $\Phi = (\phi, \varphi) : \mathbf{V} \times \mathbf{L} \rightarrow \mathbb{R}$

$$\overline{\nabla} \Phi|_{v,e} = \phi_v - \varphi^e|_v \qquad \overline{\operatorname{div}} \bar{j}|_v = - \sum_{e \in E(v)} \bar{j}_v^e$$

Problem: Missing logarithms to rewrite in terms of energy

Gradient flow formulation – jump terms

Jump terms:

$$\sum_{e \in E(v)} \kappa_v^e \sqrt{\pi^e|_v \omega_v} \left(\frac{\rho^e}{\pi^e} \Big|_v - \frac{\gamma_v}{\omega_v} \right)$$

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$$\mathcal{E}(\mu) := \mathcal{E}_{\mathbf{V}}(\gamma) + \mathcal{E}_{\mathbf{E}}(\rho) := \sum_{v \in \mathbf{V}} \mathcal{H}(\gamma_v | \omega_v) + \sum_{e \in \mathbf{E}} \mathcal{H}(\rho^e | \pi^e)$$

Gradient and divergence: For $\Phi = (\phi, \varphi) : \mathbf{V} \times \mathbf{L} \rightarrow \mathbb{R}$

$$\overline{\nabla} \Phi|_{v,e} = \phi_v - \varphi^e|_v \qquad \overline{\operatorname{div}} \bar{j}|_v = - \sum_{e \in E(v)} \bar{j}_v^e$$

Nonlinear transformation: $C^*(r) := 4(\cosh(r/2) - 1)$ has derivative

$(C^*)'(r) = 2 \sinh(r/2)$ which satisfies

$$r - s = \sqrt{rs} (C^*)'(\log r - \log s)$$

Gradient flow formulation – jump terms

Jump terms:

$$\sum_{e \in E(v)} \kappa_v^e \sqrt{\pi^e|_v \omega_v} \left(\frac{\rho^e}{\pi^e} \Big|_v - \frac{\gamma_v}{\omega_v} \right)$$

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$$\mathcal{E}(\mu) := \mathcal{E}_{\mathbf{V}}(\gamma) + \mathcal{E}_{\mathbf{E}}(\rho) := \sum_{v \in \mathbf{V}} \mathcal{H}(\gamma_v | \omega_v) + \sum_{e \in \mathbf{E}} \mathcal{H}(\rho^e | \pi^e)$$

Gradient and divergence: For $\Phi = (\phi, \varphi) : \mathbf{V} \times \mathbf{L} \rightarrow \mathbb{R}$

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$$r - s = \sqrt{rs} (C^*)'(\log r - \log s)$$

► Jump terms rewritten:

$$\sum_{e \in E(v)} \kappa_v^e \sqrt{\rho^e|_v \gamma_v} (C^*)' \left(\log \frac{\rho^e}{\pi^e} \Big|_v - \log \frac{\gamma_v}{\omega_v} \right)$$

Gradient flow formulation – jump terms

Jump terms:

$$\sum_{e \in E(v)} \kappa_v^e \sqrt{\pi^e|_v \omega_v} \left(\frac{\rho^e}{\pi^e} \Big|_v - \frac{\gamma_v}{\omega_v} \right)$$

Free energy (denoting $\mu := (\gamma, \rho) \in \mathcal{P}(\mathbf{V} \times \mathbf{L})$):

$$\mathcal{E}(\mu) := \mathcal{E}_V(\gamma) + \mathcal{E}_E(\rho) := \sum_{v \in V} \mathcal{H}(\gamma_v | \omega_v) + \sum_{e \in E} \mathcal{H}(\rho^e | \pi^e)$$

Gradient and divergence: For $\Phi = (\phi, \varphi) : \mathbf{V} \times \mathbf{L} \rightarrow \mathbb{R}$

$$\overline{\nabla} \Phi|_{v,e} = \phi_v - \varphi^e|_v \qquad \overline{\operatorname{div}} \bar{J}|_v = - \sum_{e \in E(v)} \bar{J}_v^e$$

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$(C^*)'(r) = 2 \sinh(r/2)$ which satisfies

$$r - s = \sqrt{rs} (C^*)'(\log r - \log s)$$

► Jump terms rewritten:

$$\sum_{e \in E(v)} \kappa_v^e \sqrt{\rho^e|_v \gamma_v} (C^*)'(-\overline{\nabla} D\mathcal{E}(\mu)|_{v,e})$$

Gradient flow formulation – jump terms

Jump terms:

$$\sum_{e \in E(v)} \kappa_v^e \sqrt{\pi^e|_v \omega_v} \left(\frac{\rho^e}{\pi^e} \Big|_v - \frac{\gamma_v}{\omega_v} \right)$$

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$(C^*)'(r) = 2 \sinh(r/2)$ which satisfies

$$r - s = \sqrt{rs} (C^*)'(\log r - \log s)$$

Dual dissipation potential:

$$\mathcal{R}_{V,E}^*(\mu, \zeta) := \sum_{v \in V} \sum_{e \in E(v)} \kappa_v^e \sqrt{\rho^e|_v \gamma_v} C^*(\zeta_v^e)$$

► Jump terms rewritten:

$$\sum_{e \in E(v)} \kappa_v^e \sqrt{\rho^e|_v \gamma_v} (C^*)'(-\overline{\nabla} D\mathcal{E}(\mu)|_{v,e})$$

Gradient flow formulation – jump terms

Jump terms:

$$\sum_{e \in E(v)} \kappa_v^e \sqrt{\pi^e|_v \omega_v} \left(\frac{\rho^e}{\pi^e} \Big|_v - \frac{\gamma_v}{\omega_v} \right)$$

Free energy (denoting $\mu := (\gamma, \rho) \in \mathcal{P}(\mathbf{V} \times \mathbf{L})$):

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Gradient and divergence: For $\Phi = (\phi, \varphi) : \mathbf{V} \times \mathbf{L} \rightarrow \mathbb{R}$

$$\overline{\nabla} \Phi|_{v,e} = \phi_v - \varphi^e|_v \qquad \overline{\operatorname{div}} \bar{J}|_v = - \sum_{e \in E(v)} \bar{J}_v^e$$

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$$\mathcal{R}_{V,E}^*(\mu, \zeta) := \sum_{v \in V} \sum_{e \in E(v)} \kappa_v^e \sqrt{\rho^e|_v \gamma_v} C^*(\zeta_v^e)$$

► Jump terms rewritten:

$$\sum_{e \in E(v)} D_{\zeta} \mathcal{R}_{V,E}^*(\mu, -\overline{\nabla} D \mathcal{E}(\mu))|_{e,v}$$

Gradient flow formulation – jump terms

Jump terms:

$$\sum_{e \in E(v)} \kappa_v^e \sqrt{\pi^e|_v \omega_v} \left(\frac{\rho^e}{\pi^e} \Big|_v - \frac{\gamma_v}{\omega_v} \right)$$

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Gradient and divergence: For $\Phi = (\phi, \varphi) : \mathbf{V} \times \mathbf{L} \rightarrow \mathbb{R}$

$$\overline{\nabla} \Phi|_{v,e} = \phi_v - \varphi^e|_v \qquad \overline{\operatorname{div}} \bar{J}|_v = - \sum_{e \in E(v)} \bar{J}_v^e$$

Nonlinear transformation: $C^*(r) := 4(\cosh(r/2) - 1)$ has derivative

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Dual dissipation potential:

$$\mathcal{R}_{V,E}^*(\mu, \zeta) := \sum_{v \in V} \sum_{e \in E(v)} \kappa_v^e \sqrt{\rho^e|_v \gamma_v} C^*(\zeta_v^e)$$

► Jump terms rewritten:

$$-\overline{\operatorname{div}} D_\zeta \mathcal{R}_{V,E}^*(\mu, -\overline{\nabla} D \mathcal{E}(\mu))|_v$$

Gradient flow formulation – full system

System in gradient flow form:

$$\begin{aligned}\partial_t \rho^e &= -\operatorname{div} D_\xi \mathcal{R}_E^*(\rho, -\nabla D\mathcal{E}_E(\rho))|_e \\ D_\xi \mathcal{R}_E^*(\rho, -\nabla D\mathcal{E}_E(\rho))|_{e,v} n_v^e &= D_\zeta \mathcal{R}_{V,E}^*(\mu, -\overline{\nabla} D\mathcal{E}(\mu))|_{e,v} \\ \partial_t \gamma_v &= -\overline{\operatorname{div}} D_\zeta \mathcal{R}_{V,E}^*(\mu, -\overline{\nabla} D\mathcal{E}(\mu))|_v\end{aligned}$$

Free energy (denoting $\mu := (\gamma, \rho) \in \mathcal{P}(\mathbf{V} \times \mathbf{L})$):

$$\mathcal{E}(\mu) := \sum_{v \in \mathbf{V}} \gamma_v \log\left(\frac{\gamma_v}{\omega_v}\right) - \gamma_v + \omega_v + \sum_{e \in \mathbf{E}} \int_0^{\ell^e} \rho^e \log\left(\frac{\rho^e}{\pi^e}\right) - \rho^e + \pi^e \, dx$$

Dual dissipation potential:

$$\begin{aligned}\mathcal{R}_E^*(\rho, \xi) &:= \sum_{e \in \mathbf{E}} \frac{1}{2} d^e \int_0^{\ell^e} |\xi_e|^2 \, d\rho^e \\ \mathcal{R}_{V,E}^*(\mu, \zeta) &:= \sum_{v \in \mathbf{V}} \sum_{e \in \mathbf{E}(v)} 4\kappa_v^e \sqrt{\rho^e|_v \gamma_v} (\cosh(\zeta_v^e/2) - 1)\end{aligned}$$

Gradient and divergence:

$$\begin{aligned}\nabla \varphi|_e &= \partial_x \varphi^e & \operatorname{div} j|_e &= \partial_x j^e \\ \overline{\nabla} \Phi|_{v,e} &= \phi_v - \varphi^e|_v & \overline{\operatorname{div}} \bar{j}|_v &= - \sum_{e \in \mathbf{E}(v)} \bar{j}_v^e\end{aligned}$$

- Free energy functional (denoting $\mu := (\gamma, \rho) \in \mathcal{P}(\mathcal{V} \times \mathcal{L})$):

$$\mathcal{E}(\mu) := \sum_{v \in \mathcal{V}} \mathcal{H}(\gamma_v | \omega_v) + \sum_{e \in \mathcal{E}} \mathcal{H}(\rho^e | \pi^e)$$

- Free energy functional (denoting $\mu := (\gamma, \rho) \in \mathcal{P}(\mathbf{V} \times \mathbf{L})$):

$$\mathcal{E}(\mu) := \sum_{v \in \mathbf{V}} \mathcal{H}(\gamma_v | \omega_v) + \sum_{e \in \mathbf{E}} \mathcal{H}(\rho^e | \pi^e)$$

- Dissipation functional (denoting $j := (\bar{j}, j) \in \mathcal{M}((\mathbf{V} \times \mathbf{E}) \times \mathbf{L})$):

$$\begin{aligned} \mathcal{D}(\mu, j) = & \sum_{e \in \mathbf{E}} \int_0^T \frac{1}{2d^e} \int_0^{\ell^e} \frac{|j^e|^2}{\rho^e} dx dt \\ & + \sum_{e \in \mathbf{E}} \int_0^T \int_0^{\ell^e} 2d^e \left| \partial_x \sqrt{\frac{\rho^e}{\pi^e}} \right|^2 \pi^e dx dt \\ & + \sum_{v \in \mathbf{V}} \sum_{e \in \mathbf{E}(v)} \int_0^T \kappa_v^e \sqrt{\rho^e|_v} \gamma_v C(\bar{j}_v^e / \kappa_v^e \sqrt{\rho^e|_v}, \gamma_v) dt \\ & + \sum_{v \in \mathbf{V}} \sum_{e \in \mathbf{E}(v)} \int_0^T 2\kappa_v^e \sqrt{\pi^e|_v, \omega_v} \left| \sqrt{\frac{\rho^e}{\pi^e}} \Big|_v - \sqrt{\frac{\gamma_v}{\omega_v}} \right|^2 dt \end{aligned}$$

- Free energy functional (denoting $\mu := (\gamma, \rho) \in \mathcal{P}(\mathbf{V} \times \mathbf{L})$):

$$\mathcal{E}(\mu) := \sum_{v \in \mathbf{V}} \mathcal{H}(\gamma_v | \omega_v) + \sum_{e \in \mathbf{E}} \mathcal{H}(\rho^e | \pi^e)$$

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$$\begin{aligned} \mathcal{D}(\mu, j) = & \sum_{e \in \mathbf{E}} \int_0^T \frac{1}{2d^e} \int_0^{\ell^e} \frac{|j^e|^2}{\rho^e} dx dt \\ & + \sum_{e \in \mathbf{E}} \int_0^T \int_0^{\ell^e} 2d^e \left| \partial_x \sqrt{\frac{\rho^e}{\pi^e}} \right|^2 \pi^e dx dt \\ & + \sum_{v \in \mathbf{V}} \sum_{e \in \mathbf{E}(v)} \int_0^T \kappa_v^e \sqrt{\rho^e|_v} \gamma_v C(\bar{j}_v^e / \kappa_v^e \sqrt{\rho^e|_v} \gamma_v) dt \\ & + \sum_{v \in \mathbf{V}} \sum_{e \in \mathbf{E}(v)} \int_0^T 2\kappa_v^e \sqrt{\pi^e|_v, \omega_v} \left| \sqrt{\frac{\rho^e}{\pi^e}} \Big|_v - \sqrt{\frac{\gamma_v}{\omega_v}} \right|^2 dt \end{aligned}$$

- Continuity equation: $(\mu, j) \in \text{CE}$ if for all $\Phi = (\phi, \varphi) \in C^1(\mathbf{V} \times \mathbf{L})$ and a.e. time

$$\frac{d}{dt} \left[\sum_{v \in \mathbf{V}} \phi_v \gamma_v + \sum_{e \in \mathbf{E}} \int_0^{\ell^e} \varphi^e d\rho^e \right] = \sum_{e \in \mathbf{E}} \int_0^{\ell^e} \partial_x \varphi^e dj^e + \sum_{v \in \mathbf{V}} \sum_{e \in \mathbf{E}(v)} (\phi_v - \varphi^e|_v) \bar{j}_v^e$$

Chain rule and well-posedness

* Chain rule identity:

$$\mathcal{E}(\mu(t)) - \mathcal{E}(\mu(s)) = \int_s^t \left[\langle \nabla D\mathcal{E}_E(\rho(\tau)), j(\tau) \rangle + \langle \bar{\nabla} D\mathcal{E}(\mu(\tau)), \bar{j}(\tau) \rangle \right] d\tau$$

Proof: Exploit decoupling due to CE format

- Metric edge terms: Special case of Erbar-Forkert-Maas-Mugnolo '22
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Chain rule and well-posedness

* Chain rule identity:

$$\mathcal{E}(\mu(t)) - \mathcal{E}(\mu(s)) = \int_s^t \left[\langle \nabla \mathcal{D} \mathcal{E}_E(\rho(\tau)), j(\tau) \rangle + \langle \bar{\nabla} \mathcal{D} \mathcal{E}(\mu(\tau)), \bar{j}(\tau) \rangle \right] d\tau$$

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Proof: Abstract EDP convergence applied with finite volume approximation (similar to Hraivoronska-Tse '23)

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- * Uniqueness of solutions:

Proof: Use that $(\mu, j) \mapsto \mathcal{L}(\mu, j)$ is strictly convex w.r.t. affine interpolations

Kirchhoff limit

Kirchhoff limit

- Kirchhoff means no mass exchange with vertex reservoirs

- Remove mass from reservoirs

$$\pi^\varepsilon := \frac{\pi}{\pi(L) + \varepsilon\omega(V)} \quad \text{and} \quad \omega^\varepsilon := \frac{\varepsilon\omega}{\pi(L) + \varepsilon\omega(V)}$$

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- Limit model coincides with model in Erbar-Forkert-Maas-Mugnolo '23

- Limit model is gradient flow

Fast edge-diffusion limit

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- Rescale diffusivity constant:

$$d^{e,\varepsilon} := \frac{1}{\varepsilon} d^e$$

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- Limit model is graph gradient flow on extended graph $(\hat{V}, \hat{E})$

* Can be further reduced to graph gradient flow on (V, E) by sending $\pi^e \rightarrow 0$ and $\kappa_v^e \rightarrow \infty$ s.t. $\kappa_v^e \sqrt{\pi^e |v \omega_v|} \in O(1)$ (cf. also Peletier-Schlichting '23)

Reaction-diffusion systems
(GH, A Mielke, A Stephan)

Setup and gradient system

- Finitely many species $i \in I$ with concentrations $\rho = (\rho_i)_{i \in I} \in \mathcal{M}_{\geq 0}(\mathbb{T}^d; \mathbb{R}^I)$
- Each species drift-diffuses with diffusion constant $d_i > 0$
- Reactions $r \in R$ with rates $\kappa_r > 0$ and stoichiometric coefficients $\alpha_i^r, \beta_i^r \in [0, \infty)$

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 - Consider mass-action kinetics with detailed balance
- Reaction-diffusion system (RDS):

$$\partial_t \rho_i = d_i \operatorname{div} \left(\rho_i \nabla \log \left(\frac{\rho_i}{\pi_i} \right) \right) + \sum_{r \in R} \kappa_r \pi^{\frac{\alpha^r + \beta^r}{2}} \left(\left(\frac{\rho}{\pi} \right)^{\alpha^r} - \left(\frac{\rho}{\pi} \right)^{\beta^r} \right) (\beta_i^r - \alpha_i^r)$$

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- Gradient system for diffusive part similar to before

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- Finitely many species $i \in I$ with concentrations $\rho = (\rho_i)_{i \in I} \in \mathcal{M}_{\geq 0}(\mathbb{T}^d; \mathbb{R}^I)$
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where $\rho^\lambda = \prod_{i \in I} \rho_i^{\lambda_i}$ and $\pi \in \mathcal{M}_{\geq 0}(\mathbb{T}^d; \mathbb{R}^I)$ are reference concentrations

- Gradient system for **diffusive part** similar to before
- Reaction “gradient” $\Gamma : \mathbb{R}^I \rightarrow \mathbb{R}^R$ defined by $\Gamma_{ir} := \gamma_i^r := \alpha_i^r - \beta_i^r$
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- RDS written as GF in CE format:

$$\partial_t \rho = - \operatorname{div} D_\xi \mathcal{R}_{\text{diff}}^*(\rho, -\nabla D\mathcal{E}(\rho)) + \Gamma^* D_\zeta \mathcal{R}_{\text{react}}^*(\rho, -\Gamma D\mathcal{E}(\rho))$$

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Summary and outlook

H-Pietschmann-Schlichting: GF on metric graph with vertex reservoirs

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Some future perspectives:

- Coupling of metric graph model with dynamics on domains (with J Krautz, J-F Pietschmann)
- GF with other boundary conditions as limits (with A Schlichting)
- PME as GF of Boltzmann entropy: Approximation by spatially discrete reaction systems (with A Mielke, A Stephan)
- Rigorous GF formulation for nonlinear cross-diffusion with exclusion