A gradient flow structure for nonlocal transport equations with nonlinear mobility

KAAS Seminar, Karlstad

November 2023

Oliver Tse

Joint work with **Simone Fagioli**

On gradient flow and entropy solutions for nonlocal transport equations with nonlinear mobility, Nonlinear Analysis, 2022

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The Goal

NTE with nonlinear mobility

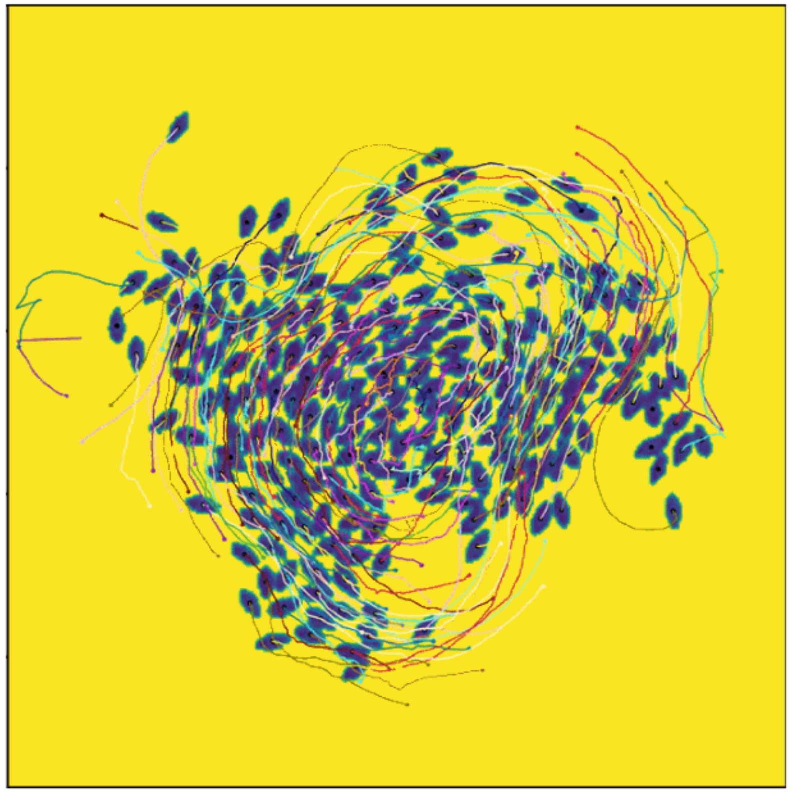
−force

(NTE) $$\partial_t\rho = \partial_x(\,\underbrace{\vartheta(\rho)}_{\text{mobility}}\,\overbrace{\partial_x\mathscr{F}'(\rho)}^{-\text{force}}\,), \qquad \rho(0)=\bar\rho$$

mobility

Free energy:

$$\mathscr{F}(\rho) = \int_{\mathbb{R}} V(x)\,\rho(x)\,dx + \frac{1}{2}\iint_{\mathbb{R}\times\mathbb{R}} W(x-y)\,\rho(x)\,\rho(y)\,dxdy$$



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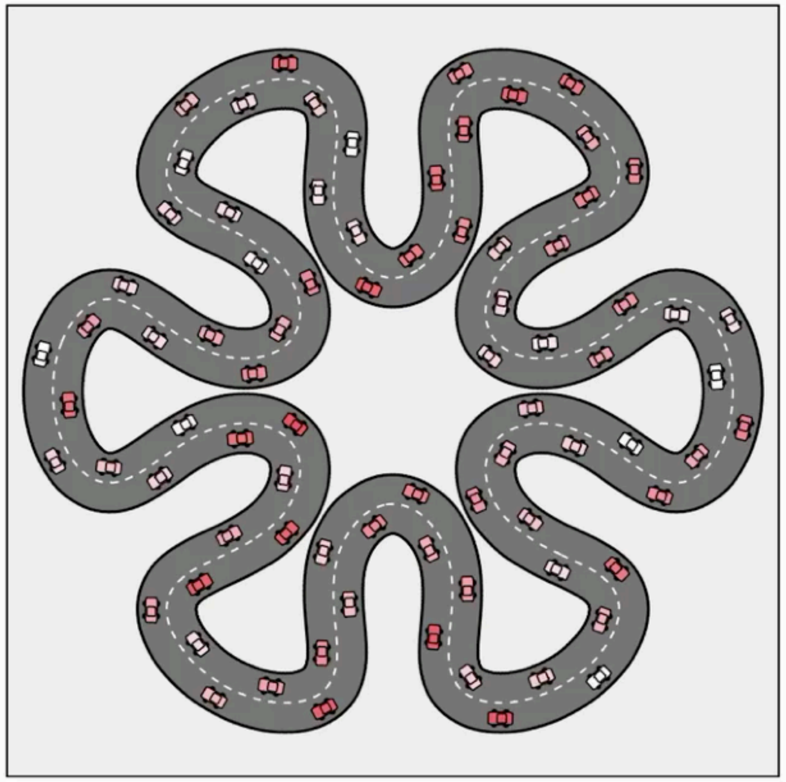


complexity-explorables.org

The Goal

NTE with nonlinear mobility

(NTE)

$$\partial_t \rho = \partial_x \big(\underbrace{\vartheta(\rho)}_{\text{mobility}} \overbrace{\partial_x \mathscr{F}'(\rho)}^{-\text{force}} \big), \qquad \rho(0) = \bar{\rho}$$

Free energy:

$$\mathscr{F}(\rho) = \int_{\mathbb{R}} V(x)\,\rho(x)\,dx + \frac{1}{2}\iint_{\mathbb{R}\times\mathbb{R}} W(x-y)\,\rho(x)\,\rho(y)\,dxdy$$

Goal: Provide *gradient flow structure* for **(NTE)**

The Goal

NTE with nonlinear mobility

(NTE) $$\partial_t \rho = \partial_x\big(\rho\beta(\rho)\, \partial_x \mathscr{F}'(\rho) \big), \qquad \rho(0) = \bar\rho$$

Free energy:

$$\mathscr{F}(\rho) = \int_{\mathbb{R}} V(x)\,\rho(x)\,dx + \frac{1}{2}\iint_{\mathbb{R}\times\mathbb{R}} W(x-y)\,\rho(x)\,\rho(y)\,dxdy$$

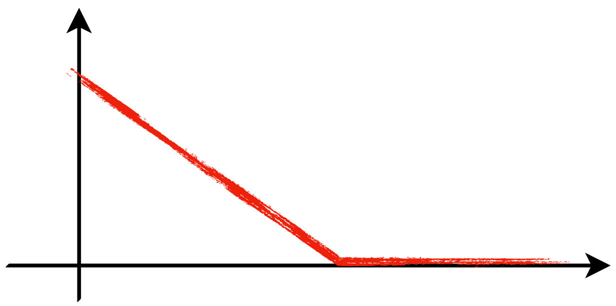
Goal: Provide *gradient flow structure* for **(NTE)**

Assumptions: $\vartheta(\rho) = \rho\beta(\rho)$

(A) $\bar\rho \in \mathrm{BV}_c(\mathbb{R}) \cap L^\infty(\mathbb{R})$ and $\bar\rho \geq \sigma > 0$ on **supp**$(\bar\rho)$

(B) $\beta \in \mathrm{Lip}([0,\infty))$ decreasing, $\beta(0) = \beta_{max} > 0$, $\beta \equiv 0$ on $[M_\beta, +\infty)$ for some $M_\beta > 0$

Eg. $\beta(s) = \big(1-s\big)^+$



The Goal

NTE with nonlinear mobility

(NTE) $$\partial_t \rho = \partial_x(\,\rho\beta(\rho)\,\partial_x \mathscr{F}'(\rho)\,), \qquad \rho(0) = \bar{\rho}$$

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Goal: Provide *gradient flow structure* for **(NTE)**

Assumptions:

(C) $V \in \mathscr{C}^2(\mathbb{R})$ with V' having linear growth

(D) $W \in \mathrm{Lip}_{loc}(\mathbb{R})$ is radially symmetric with $W' \in \mathscr{C}^2(\mathbb{R}\backslash\{0\})$ having linear growth

Eg.

$W(x) = \pm\,|\,x\,|$ **Newtonian/Coloumb potential**

$W(x) = -\,c_A\,e^{-|x|/\ell_A} + c_R\,e^{|x|/\ell_R}$ **Morse-type potential**

Preliminaries

$$\partial_t \rho = \partial_x(\rho\beta(\rho)\, \partial_x \mathscr{F}'(\rho))$$

Goal: Provide *gradient flow structure* for **(NTE)**

Some pre-knowledge:

(CE) $$\partial_t \rho + \partial_x j = 0$$ continuity equation

(KR) $$j = -\vartheta(\rho)\, \partial_x \mathscr{F}'(\rho)$$ kinetic relation

Dual dissipation potential:

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

Preliminaries

$$\partial_t \rho = \partial_x (\rho \beta(\rho)\, \partial_x \mathscr{F}'(\rho))$$

Goal: Provide *gradient flow structure* for **(NTE)**

Some pre-knowledge:

(CE) $$\partial_t \rho + \partial_x j = 0$$ continuity equation

(FF) $$j = D_2 \mathscr{R}^*(\rho, -\partial_x \mathscr{F}'(\rho))$$ force-flux relation

Dual dissipation potential:

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

Legendre-Fenchel duality:

$$\mathscr{R}(\rho, j) + \mathscr{R}^*(\rho, -\partial_x \mathscr{F}'(\rho)) = \langle j, -\partial_x \mathscr{F}'(\rho) \rangle$$

Chain rule:

$$\frac{d}{dt} \mathscr{F}(\rho) = \langle j, \partial_x \mathscr{F}'(\rho) \rangle$$

Preliminaries

$$\partial_t \rho = \partial_x (\rho \beta(\rho) \, \partial_x \mathscr{F}'(\rho))$$

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Chain rule:

$$\frac{d}{dt} \mathscr{F}(\rho) = \langle j, \partial_x \mathscr{F}'(\rho) \rangle$$

Preliminaries

$$\partial_t \rho = \partial_x(\rho \beta(\rho)\, \partial_x \mathscr{F}'(\rho))$$

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Energy-Dissipation balance

(EDB) $$\int_s^t \mathscr{R}(\rho_r, j_r) + \mathscr{R}^*(\rho_r, -\partial_x \mathscr{F}'(\rho_r))\, dr + \mathscr{F}(\rho_t) - \mathscr{F}(\rho_s) = 0$$

Preliminaries

$$\partial_t \rho = \partial_x(\rho\beta(\rho)\, \partial_x \mathscr{F}'(\rho))$$

Goal: Provide *gradient flow structure* for **(NTE)**

(CE) $$\partial_t \rho + \partial_x j = 0$$

(EDB) $$\underbrace{\int_s^t \mathscr{R}(\rho_r, j_r) + \mathscr{R}^*(\rho_r, -\partial_x \mathscr{F}'(\rho_r))\, dr + \mathscr{F}(\rho_t) - \mathscr{F}(\rho_s)}_{=:\ \mathscr{I}(\rho, j)} = 0$$

Gradient flow solution (ρ, j) satisfying **(CE)** is an $(\mathscr{F}, \mathscr{R}, \mathscr{R}^*)$-gradient flow solution of **(NTE)** with initial datum $\bar{\rho} \in \mathscr{M}_c^+(\mathbb{R})$ if

(i) $\rho_t \rightharpoonup^* \bar{\rho}$ weakly-$*$ in $\mathscr{M}^+(\mathbb{R})$ as $t \to 0$;

(ii) **(EDB)** is satisfied for any interval $[s, t] \subset [0,T]$;

(iii) The chain rule holds for almost every $t \in (0,T)$.

GF solution $\rightsquigarrow$ weak solution

Variational Principle **GF solutions are minimizers of $\mathscr{I}$**

Preliminaries

$$\partial_t \rho = \partial_x(\rho\beta(\rho)\,\partial_x \mathscr{F}'(\rho))$$

Goal: Provide *gradient flow structure* for **(NTE)**

non-concave ϑ
irregular interaction forces

(CE) $$\partial_t \rho + \partial_x j = 0$$

(EDB) $$\int_s^t \mathscr{R}(\rho_r, j_r) + \mathscr{R}^*(\rho_r, -\partial_x \mathscr{F}'(\rho_r))\, dr + \mathscr{F}(\rho_t) - \mathscr{F}(\rho_s) = 0$$

Comments:

(i) If $\vartheta(\rho) = \rho$, **(NTE)** has a W_2-GF structure — Carrillo, Di Francesco, Figalli, Laurent, Slepčev '11

(ii) If ϑ concave, $\mathscr{R}$ gives rise to a transport distance — Dolbeault, Nazaret, Savaré '09; Lisini, Marigonda '10

(iii) $\mathscr{F}$ "cannot be λ-convex along geodesics if ϑ is not linear" — Carrillo, Lisini, Savaré, Slepčev '10

(iv) Convergence of discrete JKO to continuous JKO — Di Marino, Portinale, Radici, '22 Arxiv

Preliminaries

$$\partial_t \rho = \partial_x (\rho \beta(\rho) \, \partial_x \mathscr{F}'(\rho))$$

Goal: Provide *gradient flow structure* for **(NTE)**

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(CE) $$\partial_t \rho + \partial_x j = 0$$

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Strategy/Outline:

(i) Construct discrete particle approximation (**DPA**)

(ii) Derive gradient structure for **DPA**

(iii) Deduce limit gradient structure + existence of gradient flow solution

Particle Approximations

$$\partial_t \rho = \partial_x(\rho \beta(\rho)\, \partial_x \mathscr{F}'(\rho))$$

Pseudo-inverse equation $\mathsf{X}(z) := \inf_{x \in \mathbb{R}} \left\{ \rho\, \textbf{Leb}\, ((-\infty, x)) > z \right\}, \quad z \in (0,1)$

$$\partial_t \mathsf{X} = -\, \beta \left(\frac{1}{\partial_z \mathsf{X}} \right) \mathsf{F}_\rho(\mathsf{X})$$

$$\mathsf{F}_\rho(\mathsf{X}(z)) = V'(\mathsf{X}(z)) + \int_0^1 W'(\mathsf{X}(z) - \mathsf{X}(\zeta))\, d\zeta$$

Di Francesco-Rosini (2015)

Particle Approximations

$$\partial_t \rho = \partial_x(\rho \beta(\rho)\, \partial_x \mathscr{F}'(\rho))$$

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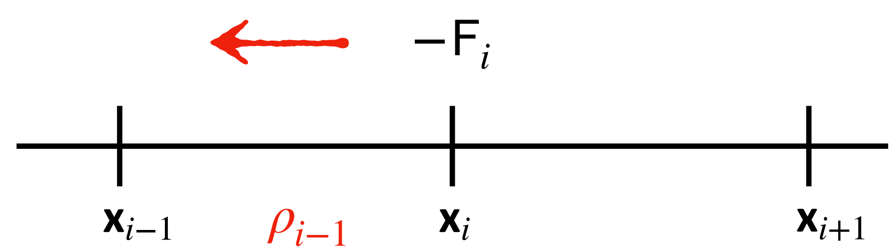
$$\partial_t \mathsf{X} = -\beta\left(\frac{1}{\partial_z \mathsf{X}}\right)\mathsf{F}_\rho(\mathsf{X}) \qquad \mathsf{F}_\rho(\mathsf{X}(z)) = V'(\mathsf{X}(z)) + \int_0^1 W'(\mathsf{X}(z) - \mathsf{X}(\zeta))\, d\zeta$$

An upwind-type scheme: $\quad \mathbf{x}_i := \mathsf{X}(z_i)$



$$\dot{\mathbf{x}}_i = \beta(\rho_{i-1})\big(-\mathsf{F}_\rho(\mathbf{x}_i)\big)^- + \beta(\rho_i)\big(-\mathsf{F}_\rho(\mathbf{x}_i)\big)^+$$

$$\rho_i = \frac{h}{\mathbf{x}_{i+1} - \mathbf{x}_i}$$

Particle Approximations

$$\partial_t \rho = \partial_x(\, \rho \beta(\rho)\, \partial_x \mathscr{F}'(\rho)\,)$$

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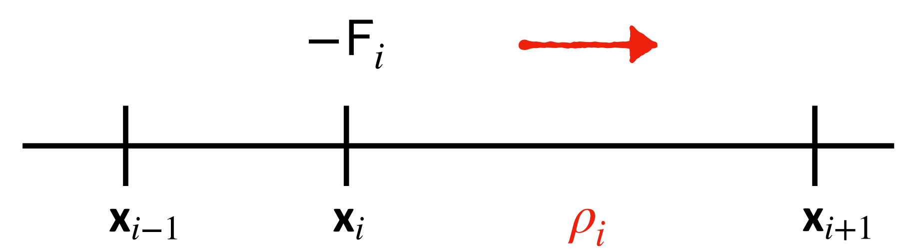

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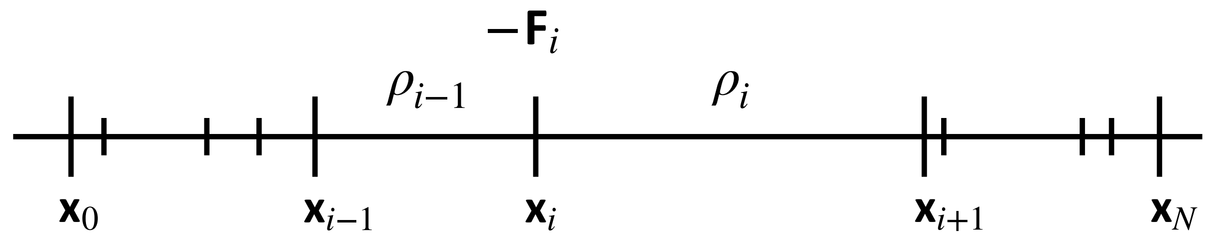

(DPA)

$$\begin{aligned}
\dot{\mathbf{x}}_0 &= \beta_{max}\,(-\mathbf{F}_0)^- + \beta(\rho_0)\,(-\mathbf{F}_0)^+ \\
\dot{\mathbf{x}}_i &= \beta(\rho_{i-1})\,(-\mathbf{F}_i)^- + \beta(\rho_i)\,(-\mathbf{F}_i)^+ \\
\dot{\mathbf{x}}_N &= \beta(\rho_{N-1})\,(-\mathbf{F}_N)^- + \beta_{max}\,(-\mathbf{F}_N)^+
\end{aligned}$$

$$\mathbf{F}_i = V'(\mathbf{x}_i) + \sum_{j\neq i} hW'(\mathbf{x}_i - \mathbf{x}_j)$$

$$\rho_i = \frac{h}{\mathbf{x}_{i+1} - \mathbf{x}_i}$$

Results:

(1) Unique solution $\mathbf{x}$ exists, and $\exists \mu > 0$, independent of h, such that

$$\sigma e^{-\mu T} \leq \rho_i \leq M := \max\{M_\beta\,, \|\bar{\rho}\|_{L^\infty}\}\,;$$

$$\sup_{t\in[0,T]} |\,\mathrm{x}_N(t) - \mathrm{x}_0(t)\,| < \infty$$

(2) **(DPA)** possesses a gradient flow structure!

GF Structure for DPA

$$\dot{\mathbf{x}}_0 = \beta_{max}\,(-\mathbf{F}_0)^- + \beta(\rho_0)\,(-\mathbf{F}_0)^+$$
$$\dot{\mathbf{x}}_i = \beta(\rho_{i-1})\,(-\mathbf{F}_i)^- + \beta(\rho_i)\,(-\mathbf{F}_i)^+$$
$$\dot{\mathbf{x}}_N = \beta(\rho_{N-1})\,(-\mathbf{F}_N)^- + \beta_{max}\,(-\mathbf{F}_N)^+$$

Task: Find $\mathscr{F}_h$ and $\mathscr{R}_h^*$ such that **(DPA)** takes the form

$$\begin{cases} \dot{\mathbf{x}} = \mathbf{j} \\ \mathbf{j} = D_2\mathscr{R}_h^*(\mathbf{x}, -\mathscr{F}_h'(\mathbf{x})) \end{cases}$$

Free energy:

$$\mathbf{F}_i = V'(\mathbf{x}_i) + \sum_{j\neq i} hW'(\mathbf{x}_i - \mathbf{x}_j)$$

$$\mathscr{F}_h(\mathbf{x}) = \sum_i V(\mathbf{x}_i) + \frac{1}{2}\sum_{i,j\neq i} hW(\mathbf{x}_i - \mathbf{x}_j)$$

Dual dissipation potential:

$$\mathscr{R}_h^*(\mathbf{x}, \xi) = \frac{1}{2}\sum_i \beta(\rho_{i-1})\big(\xi_i^-\big)^2 + \beta(\rho_i)\big(\xi_i^+\big)^2$$

GF Structure for DPA

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$$\int_s^t \mathscr{R}_h(\mathbf{x}_r, \mathbf{j}_r) + \mathscr{R}_h^*(\mathbf{x}_r, -\mathscr{F}_h'(\mathbf{x}_r))\,dr + \mathscr{F}_h(\mathbf{x}_t) - \mathscr{F}_h(\mathbf{x}_s) = 0$$

DPA as Numerical Scheme

$$\dot{\mathbf{x}}_0 = \beta_{max}(-\mathbf{F}_0)^- + \beta(\rho_0)(-\mathbf{F}_0)^+$$
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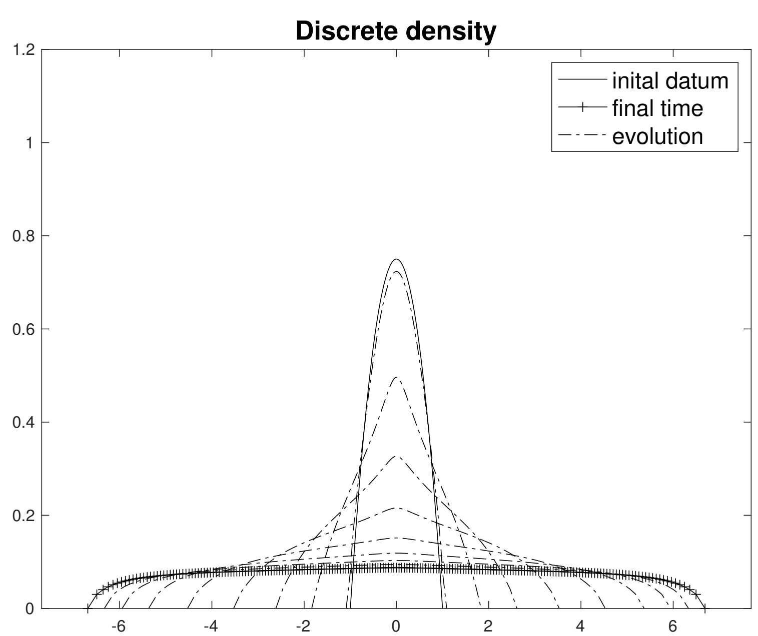
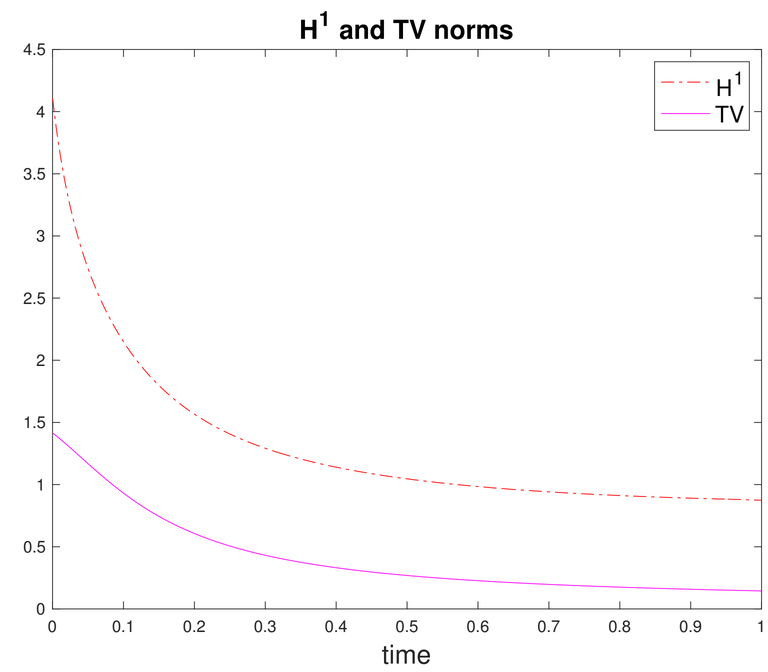
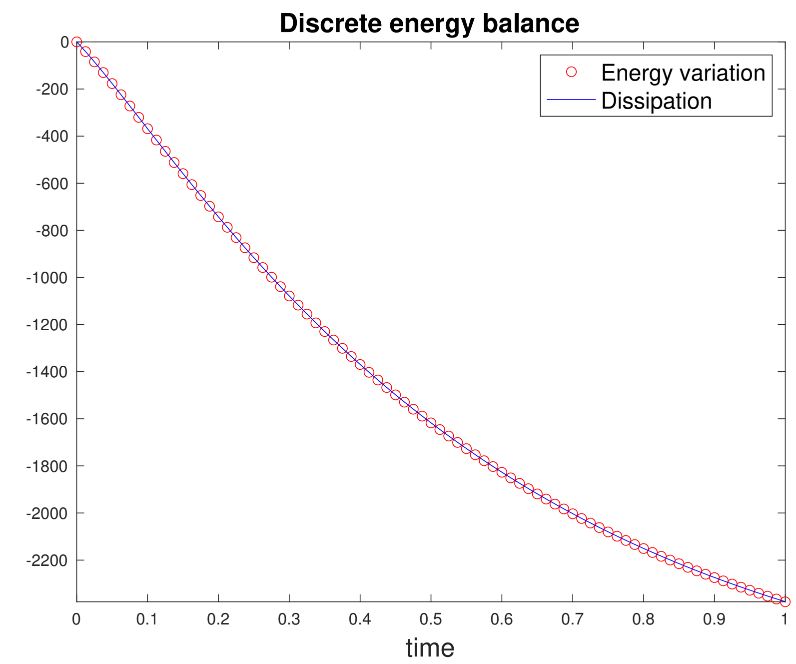
$$W(x) = -|x|, \quad V \equiv \frac{|x|^2}{2}$$







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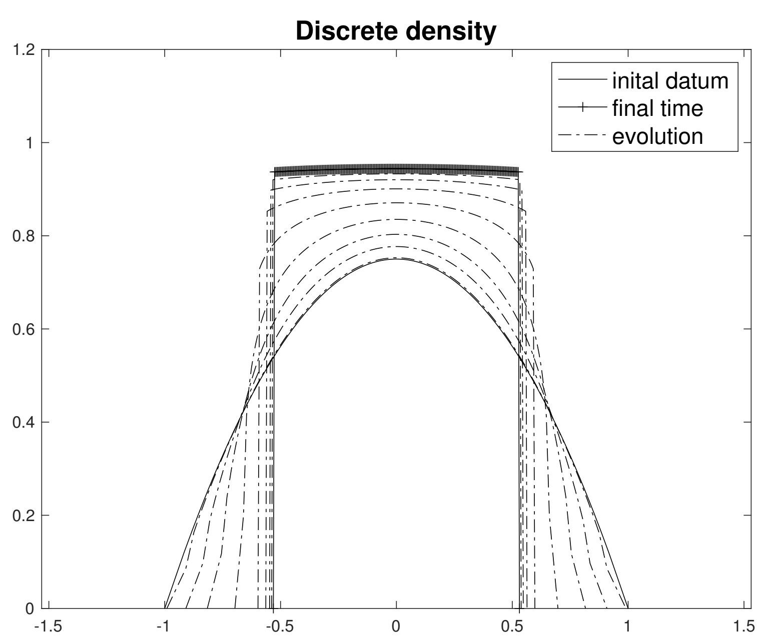
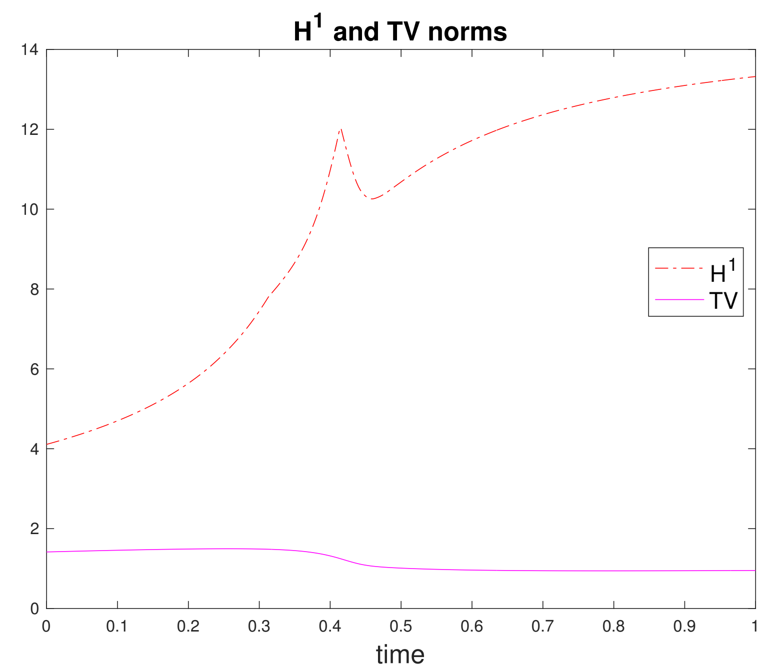
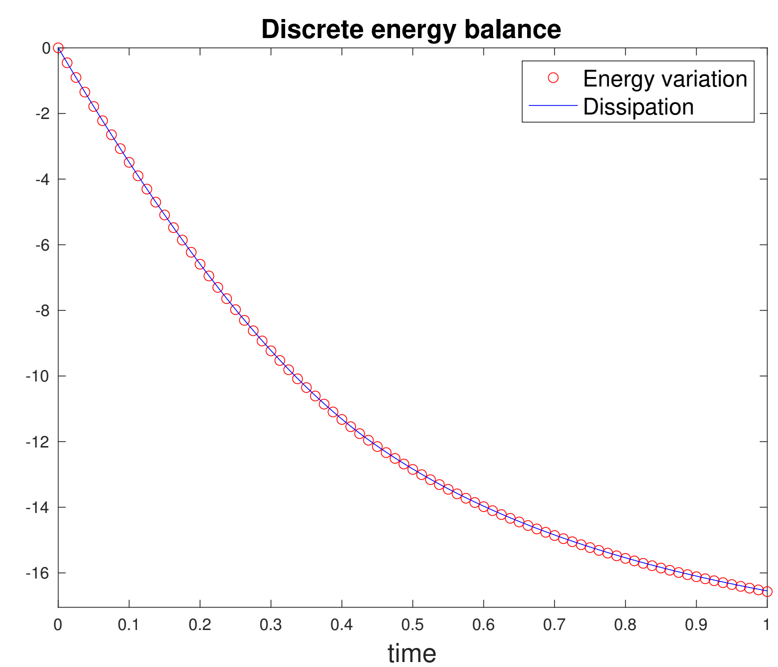
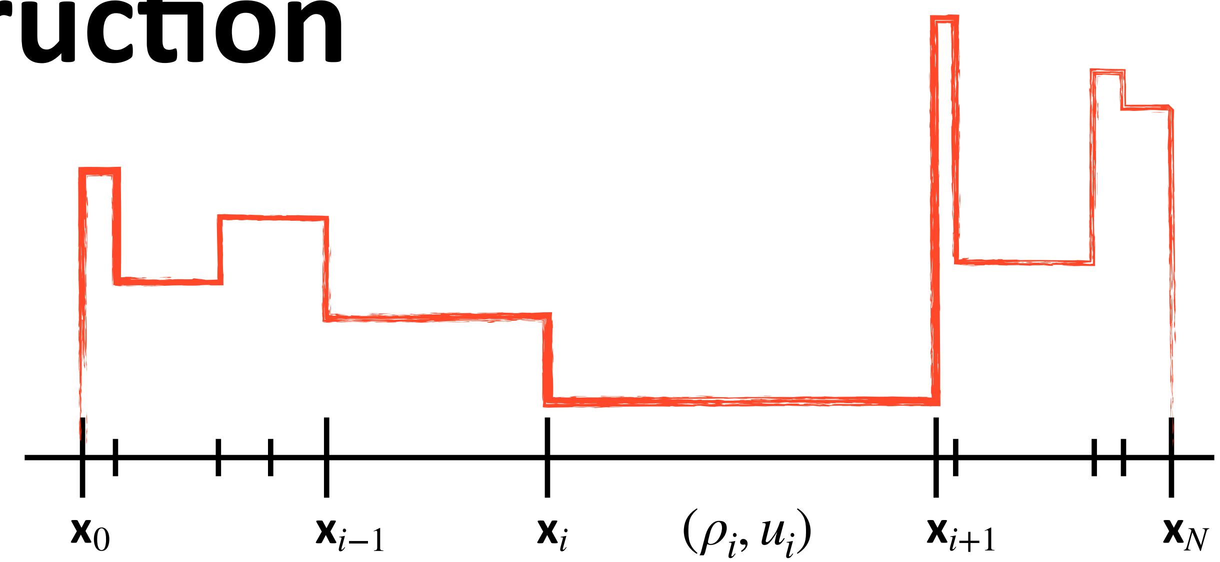
$$W(x) = |x|, \;\; V \equiv 0$$







Continuous reconstruction



Density: $$\hat{\rho}^h = \sum_i \rho_i \, 1_{(\mathbf{x}_{i+1}, \mathbf{x}_i)}$$

Flux: $$\hat{j}^h = \sum_i \rho_i \, u_i \, 1_{(\mathbf{x}_{i+1}, \mathbf{x}_i)}\,, \qquad u_i(x) = \frac{\mathbf{x}_{i+1} - x}{\mathbf{x}_{i+1} - \mathbf{x}_i} \dot{\mathbf{x}}_i + \frac{x - \mathbf{x}_i}{\mathbf{x}_{i+1} - \mathbf{x}_i} \dot{\mathbf{x}}_{i+1}$$

Results:

$$\|\hat{\rho}^h_t\|_{BV} \leq c_{BV} \, \|\bar{\rho}\|_{BV}$$

$$\sup_{t \in [0,T]} |\,\mathrm{supp}\,(\hat{\rho}^h_t)\,| < \infty$$

(1) The pair $(\hat{\rho}^h, \hat{j}^h)$ satisfies **(CE)** for all $h > 0$;

(2) *Compactness:* $\exists\,(\rho, j)$ satisfying **(CE)** such that $\rho \in L^\infty([0,T] \times \mathbb{R})$, and

$$\hat{\rho}^h_t \to \rho_t \quad \text{in } L^1(\mathbb{R}) \quad \text{for every } t \in [0,T]$$

$$\int_\cdot \hat{j}^h_t \, dt \rightharpoonup^* \int_\cdot j_t \, dt \quad \text{weakly-}* \text{ in } \mathscr{M}([0,T] \times \mathbb{R})$$

Recap

$$\partial_t \rho = \partial_x(\rho\beta(\rho)\, \partial_x \mathscr{F}'(\rho))$$

Continuous world

(NTE)

$$\begin{cases} \partial_t \rho + \partial_x j = 0 \\ j = D_2 \mathscr{R}^*(\rho, -\partial_x \mathscr{F}'(\rho)) \end{cases}$$

$$\mathscr{I}(\rho, j) := \int_s^t \mathscr{R}(\rho_r, j_r) + \mathscr{R}^*(\rho_r, -\partial_x \mathscr{F}'(\rho_r))\, dr + \mathscr{F}(\rho_t) - \mathscr{F}(\rho_s) = 0$$

Discrete world

Evolutionary Γ- convergence!

(DPA)

$$\begin{cases} \dot{\mathbf{x}} = \mathbf{j} \\ \mathbf{j} = D_2 \mathscr{R}_h^*(\mathbf{x}, -\mathscr{F}_h'(\mathbf{x})) \end{cases}$$

$$\mathscr{I}_h(\mathbf{x}, \mathbf{j}) := \int_s^t \mathscr{R}_h(\mathbf{x}_r, \mathbf{j}_r) + \mathscr{R}_h^*(\mathbf{x}_r, -\mathscr{F}_h'(\mathbf{x}_r))\, dr + \mathscr{F}_h(\mathbf{x}_t) - \mathscr{F}_h(\mathbf{x}_s) = 0$$

Sandier-Serfaty (2004), Mielke (2016), Mielke-Montefusco-Peletier (2021)

Recap

$$\partial_t \rho = \partial_x(\rho\beta(\rho)\, \partial_x \mathscr{F}'(\rho))$$

Continuous world

$$\mathscr{I}(\rho, j) := \int_s^t \mathscr{R}(\rho_r, j_r) + \mathscr{R}^*(\rho_r, -\partial_x \mathscr{F}'(\rho_r))\, dr + \mathscr{F}(\rho_t) - \mathscr{F}(\rho_s) = 0$$

Discrete world

$$\mathscr{I}_h(\mathbf{x}, \mathbf{j}) := \int_s^t \mathscr{R}_h(\mathbf{x}_r, \mathbf{j}_r) + \mathscr{R}_h^*(\mathbf{x}_r, -\mathscr{F}_h'(\mathbf{x}_r))\, dr + \mathscr{F}_h(\mathbf{x}_t) - \mathscr{F}_h(\mathbf{x}_s) = 0$$

Question: If $(\mathbf{x}^h, \mathbf{j}^h)$ satisfies $\mathscr{I}_h(\mathbf{x}^h, \mathbf{j}^h) = 0$ then $\partial_t \hat\rho^h + \partial_x \hat\jmath^h = 0$, but

$$\mathscr{I}(\hat\rho^h, \hat\jmath^h) \approx 0?$$

What do we get for $\mathscr{I}(\rho, j)$?

Final Steps

$$\mathscr{I}(\rho, j) := \int_s^t \mathscr{R}(\rho_r, j_r) + \mathscr{R}^*(\rho_r, -\partial_x \mathscr{F}'(\rho_r))\, dr + \mathscr{F}(\rho_t) - \mathscr{F}(\rho_s)$$

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$$\mathscr{I}(\hat{\rho}^h, \hat{j}^h) \approx 0?$$ ✓

What do we get for $\mathscr{I}(\rho, j)$?

Results:

(1)
$$\mathscr{I}_h(\hat{\rho}^h, \hat{j}^h) \le h \mathscr{I}_h(\mathbf{x}^h, \mathbf{j}^h) + o(h)$$

(2)
$$\begin{cases} \mathscr{F}(\rho_t) = \lim_{h\to 0} \mathscr{F}_h(\hat{\rho}_t^h) \qquad \textbf{for every } t \in [0,T] \\ \int_s^t \mathscr{R}(\rho_r, j_r)\, dr \le \liminf_{h\to 0} \int_s^t \mathscr{R}(\hat{\rho}_r^h, \hat{j}_r^h)\, dr \\ \int_s^t \mathscr{R}^*(\rho_r, -\partial_x \mathscr{F}'(\rho_r))\, dr \le \liminf_{h\to 0} \int_s^t \mathscr{R}^*(\hat{\rho}_r^h, -\partial_x \mathscr{F}'(\hat{\rho}_r^h))\, dr \end{cases}$$

Final Steps

$$\mathscr{I}(\rho, j) := \int_s^t \mathscr{R}(\rho_r, j_r) + \mathscr{R}^*(\rho_r, -\partial_x \mathscr{F}'(\rho_r))\,dr + \mathscr{F}(\rho_t) - \mathscr{F}(\rho_s)$$

Questions: If $(\mathbf{x}^h, \mathbf{j}^h)$ satisfies $\mathscr{I}_h(\mathbf{x}^h, \mathbf{j}^h) = 0$ then $\partial_t \hat{\rho}^h + \partial_x \hat{j}^h = 0$, but

$$\mathscr{I}(\hat{\rho}^h, \hat{j}^h) \approx 0?$$ ✓

What do we get for $\mathscr{I}(\rho, j)$? ✓

Results:

(1) + (2) $\mathscr{I}(\rho, j) \le \liminf_{h \to 0} \mathscr{I}_h(\hat{\rho}^h, \hat{j}^h) \le 0$

\+ **Chain rule** $\rightsquigarrow$ $\mathscr{I}(\rho, j) \ge 0$

} $\mathscr{I}(\rho, j) = 0$ → **Gradient flow solution of (NTE)!**

☹ **Rate of convergence**

1D

Summary

(DPA)
$$\int_s^t \mathscr{R}_h(\mathbf{x}_r, \mathbf{j}_r) + \mathscr{R}_h^*(\mathbf{x}_r, -\mathscr{F}_h'(\mathbf{x}_r))\, dr + \mathscr{F}_h(\mathbf{x}_t) - \mathscr{F}_h(\mathbf{x}_s) = 0$$

Continuous reconstruction $(\hat{\rho}^h, \hat{j}^h)$

$$\mathscr{I}_h(\hat{\rho}^h, \hat{j}^h) = o(h)$$

Compactness $\exists(\rho, j) : \ (\hat{\rho}^h, \hat{j}^h) \to (\rho, j)$

Lower semicontinuity of $\mathscr{R}^*$ **and** $\mathscr{R}^*$

Convergence of $\mathscr{F}(\hat{\rho}_t^h)$ **to** $\mathscr{F}(\rho_t)$

(NTE)
$$\int_s^t \mathscr{R}(\rho_r, j_r) + \mathscr{R}^*(\rho_r, -\partial_x \mathscr{F}'(\rho_r))\, dr + \mathscr{F}(\rho_t) - \mathscr{F}(\rho_s) = 0$$

Thank you!