Lecture 2: Lagrangian discretization of evolution equations using optimal transport

Quentin Mérigot

Joint work with Jean-Marie Mirebeau, Thomas Gallouët, Hugo Leclerc, Filippo Santambrogio, Federico Stra

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1. Optimal quantization

Optimal transport and optimal quantization

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- Need to compute the squared Wasserstein distance $\mathcal{D}$ (and $\nabla\mathcal{D}$) efficiently...

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Recall: Computing $\mathcal{D}(y_1,\cdots,y_N) \Longleftrightarrow$ Finding $\psi \in \mathbb{R}^N$ s.t. $\forall i,\ \rho(\mathrm{Lag}_i(\psi)) = \frac{1}{N}$.

where $\mathrm{Lag}_i(\psi) = \{x \in \mathbb{R}^d \mid \forall j, \|x-y_i\|^2 + \psi_i \le \|x-y_j\|^2 + \psi_j\}$.

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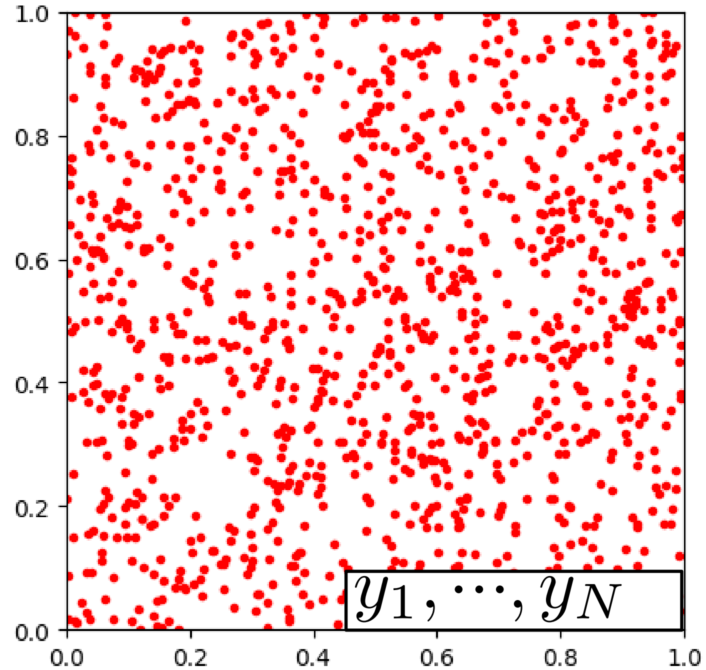
$$\nabla_{y_i}\mathcal{D}(y_1,\cdots,y_N) = y_i - \boxed{\mathrm{bary}(\mathrm{Lag}_i(\psi))}$$

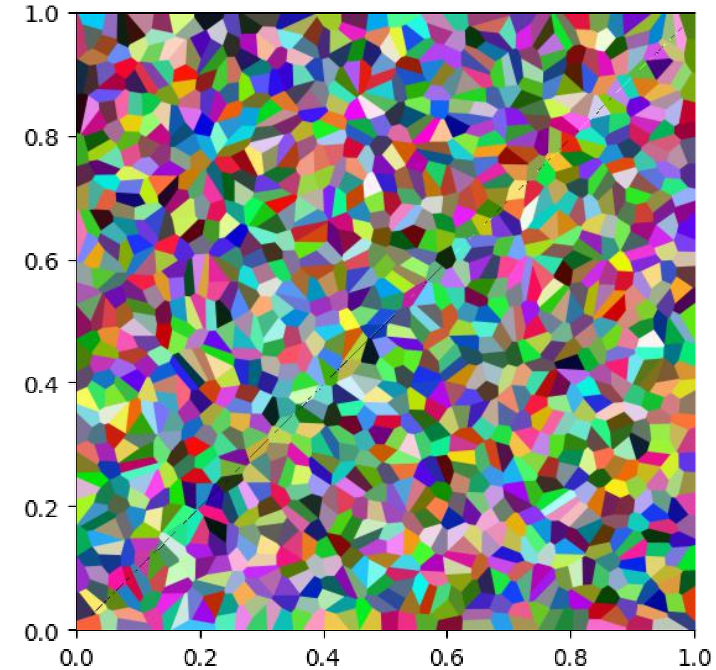
$=: B_i(y_1,\cdots,y_N)$

Computing $\mathcal{D}$ (incompressibility) — example

- **Example 1:** $N = 900$, $\rho_0 = \mathrm{Leb}_{[0,1]^2}$. $\mathcal{D}(y_1, \cdots, y_N) = \frac{N}{2} \mathrm{W}_2^2(\rho_0, \frac{1}{N} \sum_i \delta_{y_i})$



$\frac{1}{N}\mathcal{D} \simeq 0,031$



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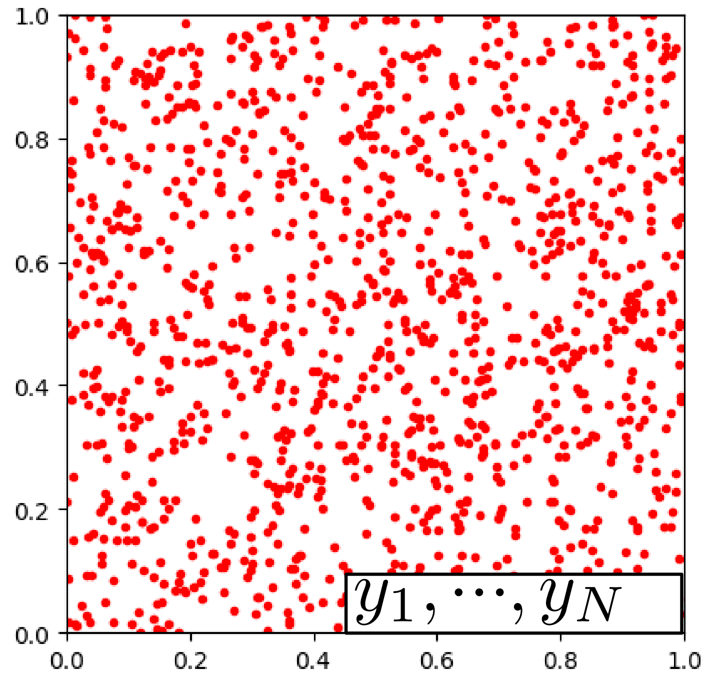

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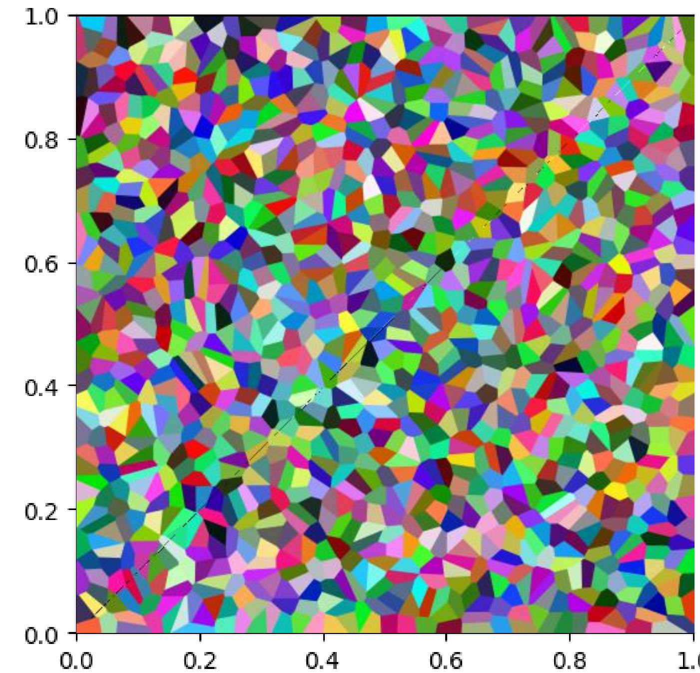

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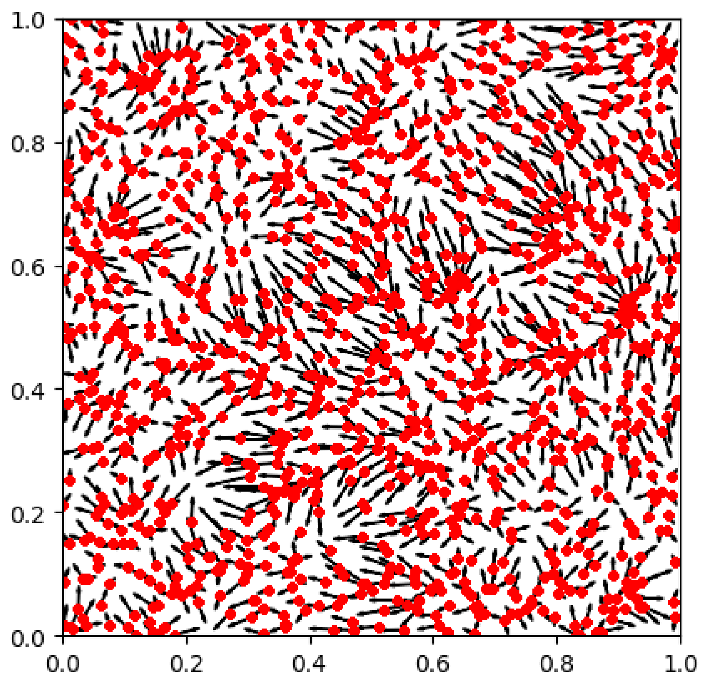
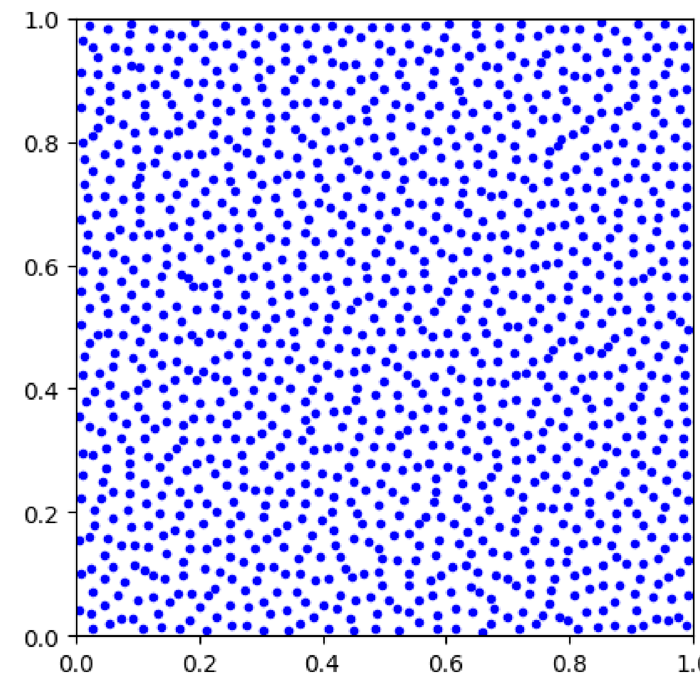


$(-\nabla_{y_i}\mathcal{D})_{1 \le i \le N}$



$(y_i - \nabla_{y_i}\mathcal{D})_{1 \le i \le N}$

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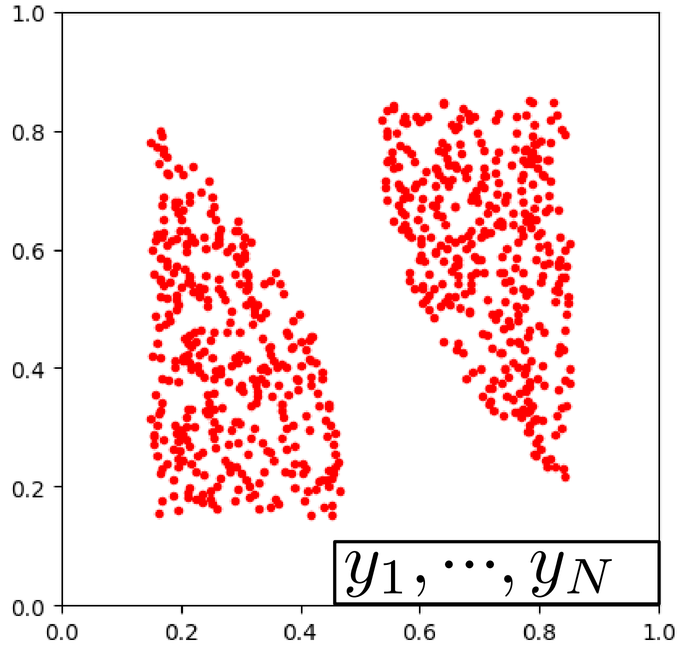
- **Example 2:** $N = 740$, $\rho_0 = \mathrm{Leb}_{[0,1]^2}$. $\mathcal{D}(y_1, \cdots, y_N) = \frac{N}{2} \mathrm{W}_2^2(\rho_0, \frac{1}{N}\sum_i \delta_{y_i})$



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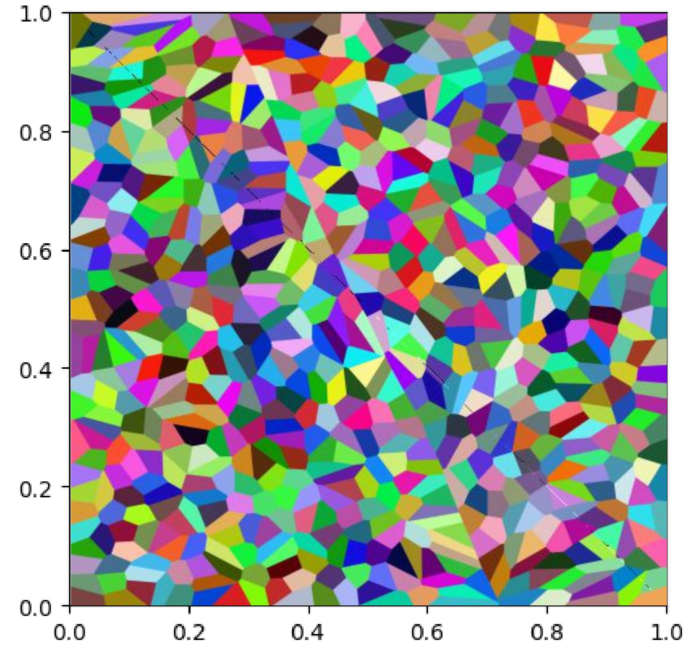

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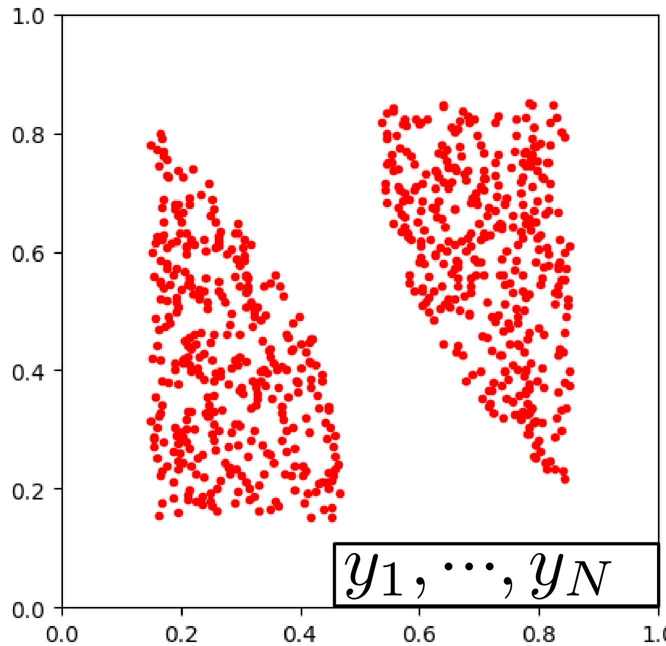

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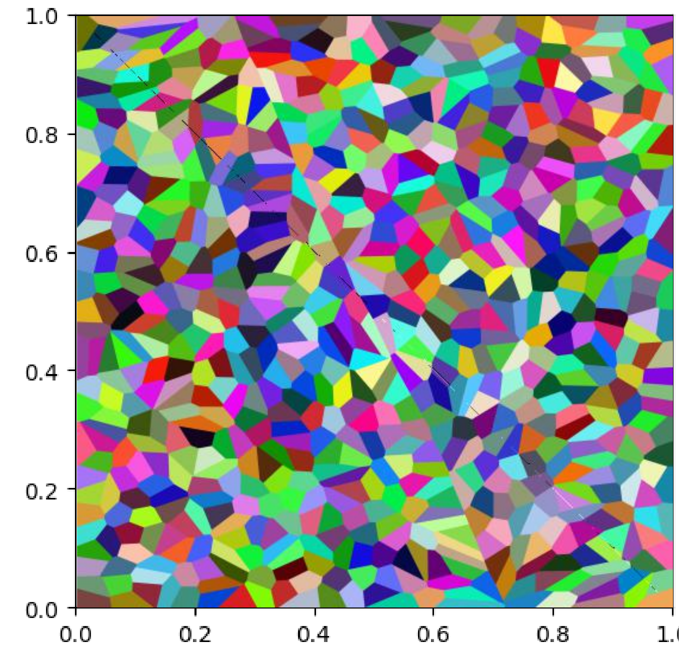

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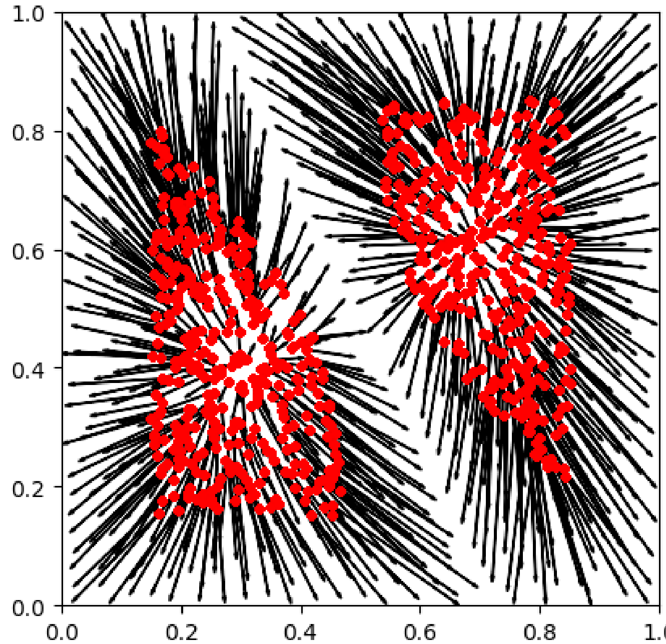

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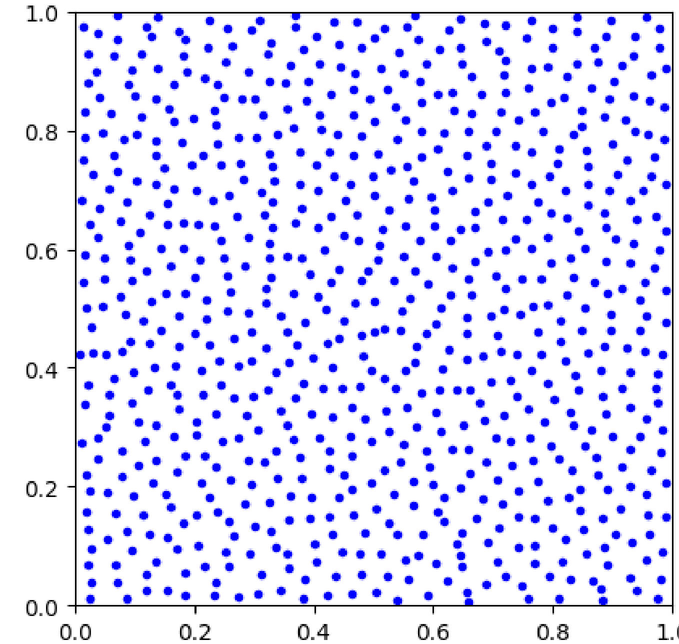

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Optimal quantization as a gradient flow

$\mathcal{D} : y = (y_1, \cdots, y_N) \in \mathbb{R}^{Nd} \mapsto \frac{N}{2} \mathrm{W}_2^2(\rho, \frac{1}{N} \sum_i \delta_{y_i})$

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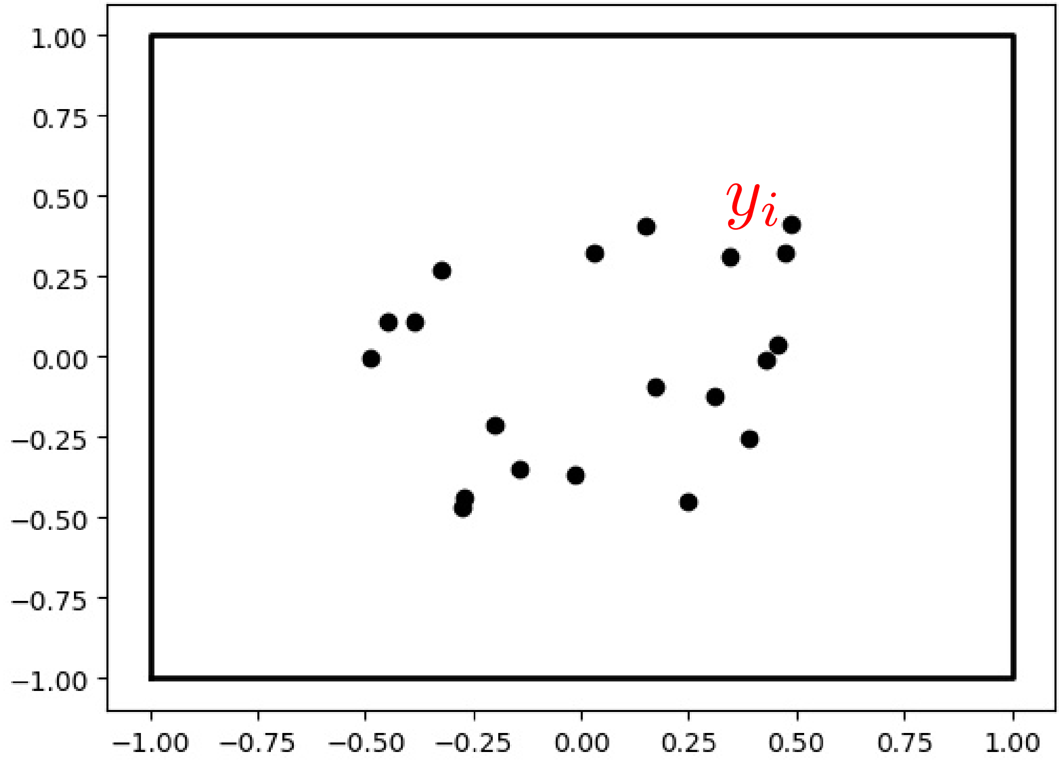
$y_1(0), \cdots, y_N(0)$ iid

$N = 20$



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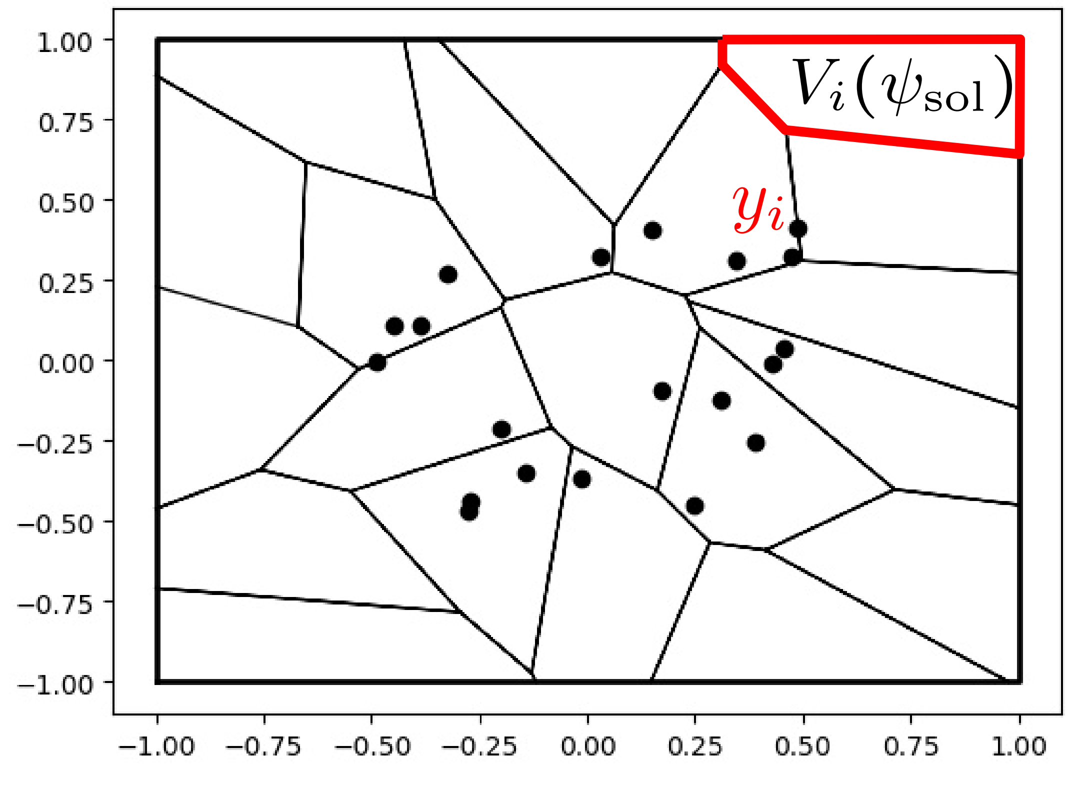

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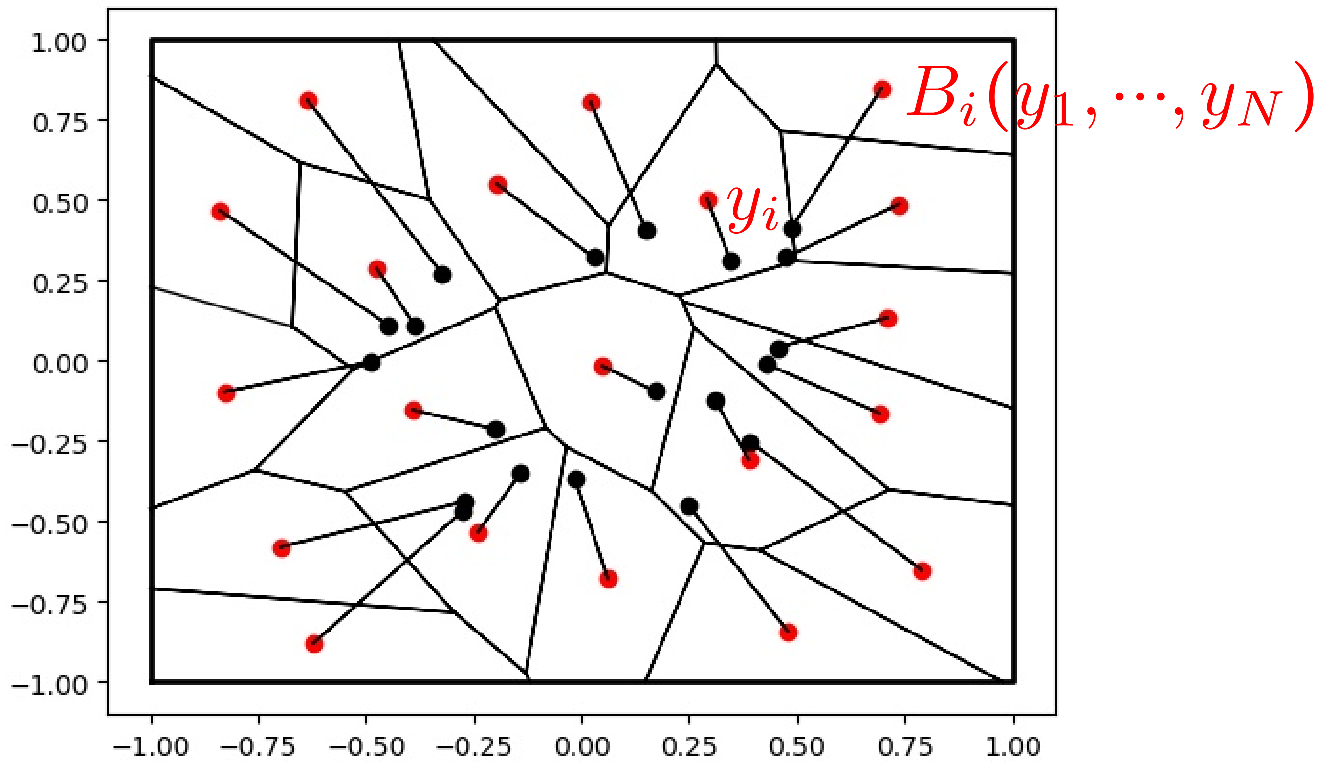

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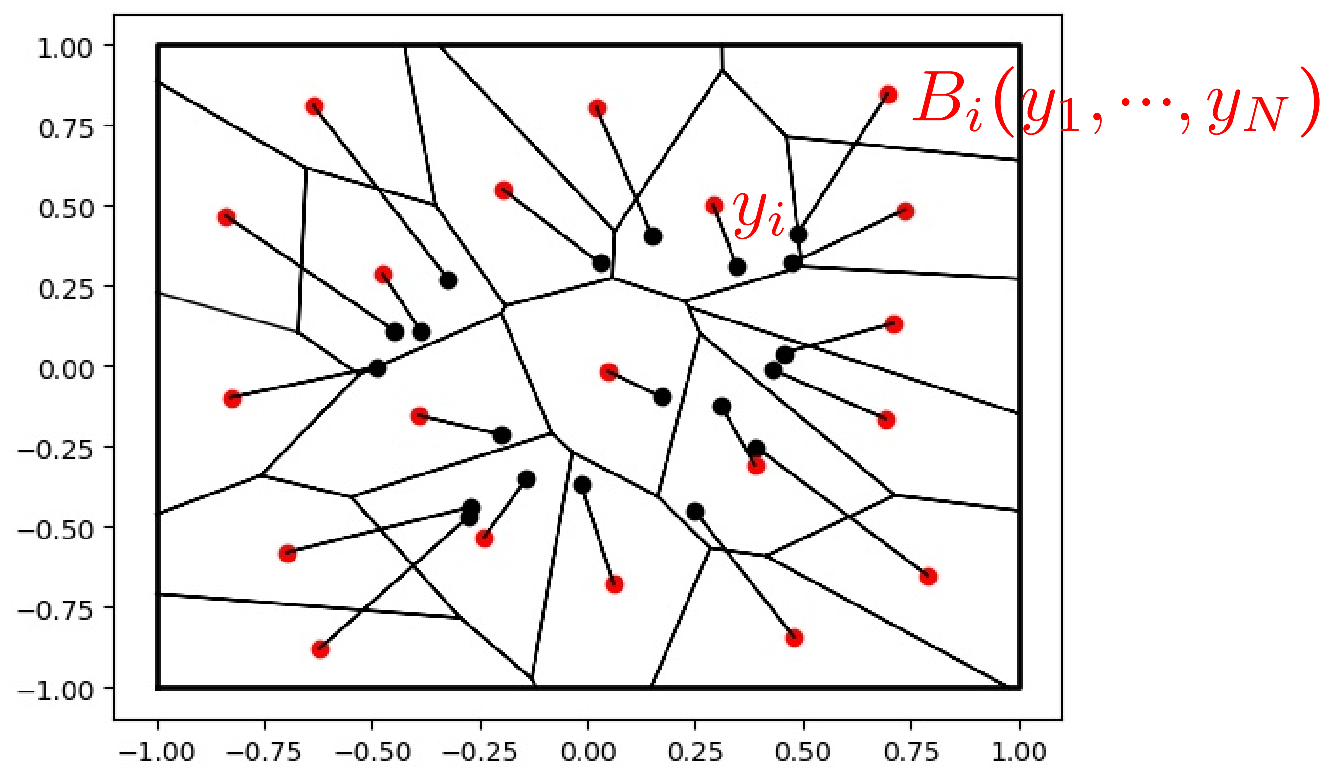


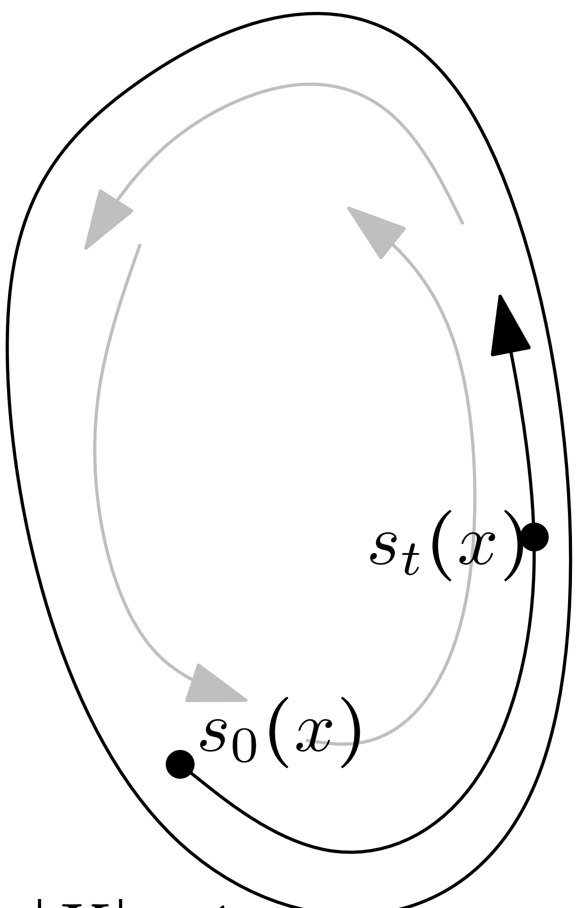
2. Incompressible Euler equations

Joint works with JM Mirebeau and Thomas Gallouët

Solutions to Euler's equations as geodesics in $\mathbb{S}\mathrm{Diff}$

$\mathbb{S}\mathrm{Diff} = \{s : X \to X$ diffeomorphism $\mid \det(\mathrm{D}s) = 1\} \subseteq \mathrm{L}^2(X, \mathbb{R}^d)$ [Arnold 1966]

$X \subseteq \mathbb{R}^d$ bounded



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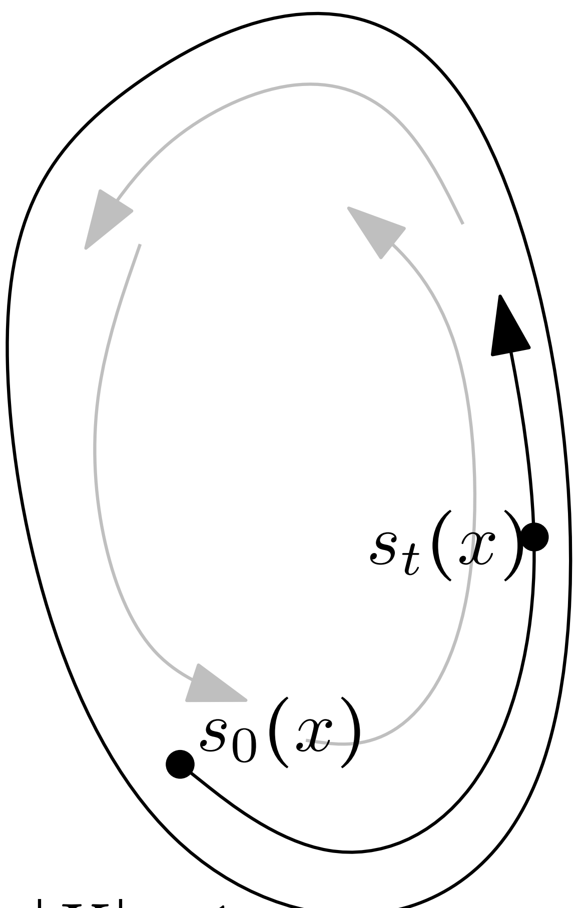

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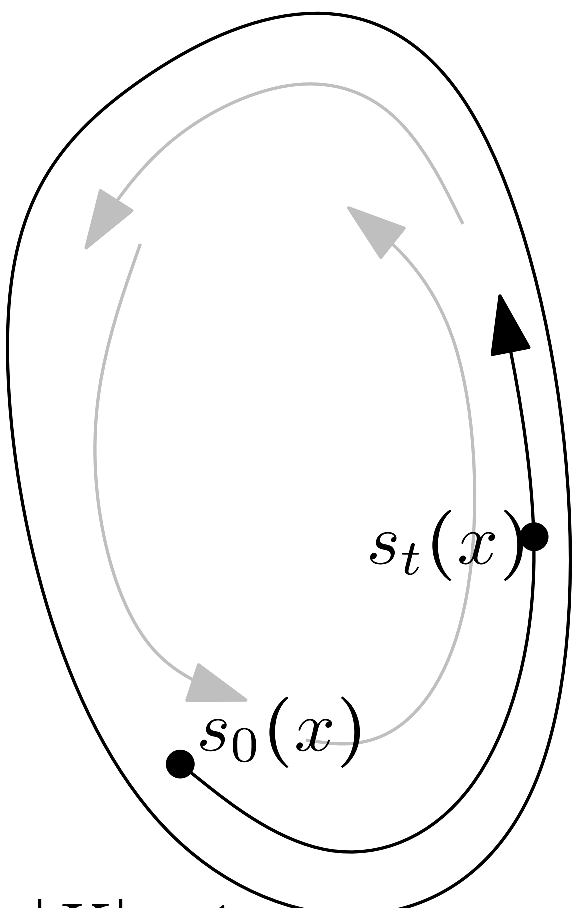

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($\mathrm{T}_{\mathrm{id}}\mathbb{S}\mathrm{Diff}$ = divergence-free vector fields = $\{\nabla p \mid p : X \to \mathbb{R}\}^\perp$)

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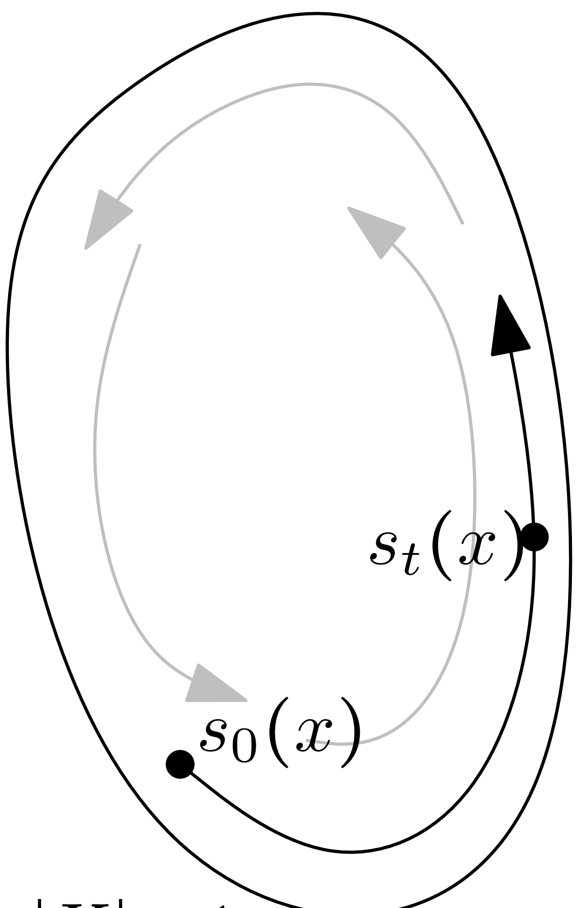

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Solutions to Euler's equations as geodesics in $\mathbb{S}\mathrm{Diff}$

$\mathbb{S}\mathrm{Diff} = \{s : X \to X$ diffeomorphism $\mid \det(\mathrm{D}s) = 1\} \subseteq \mathrm{L}^2(X, \mathbb{R}^d)$ [Arnold 1966]

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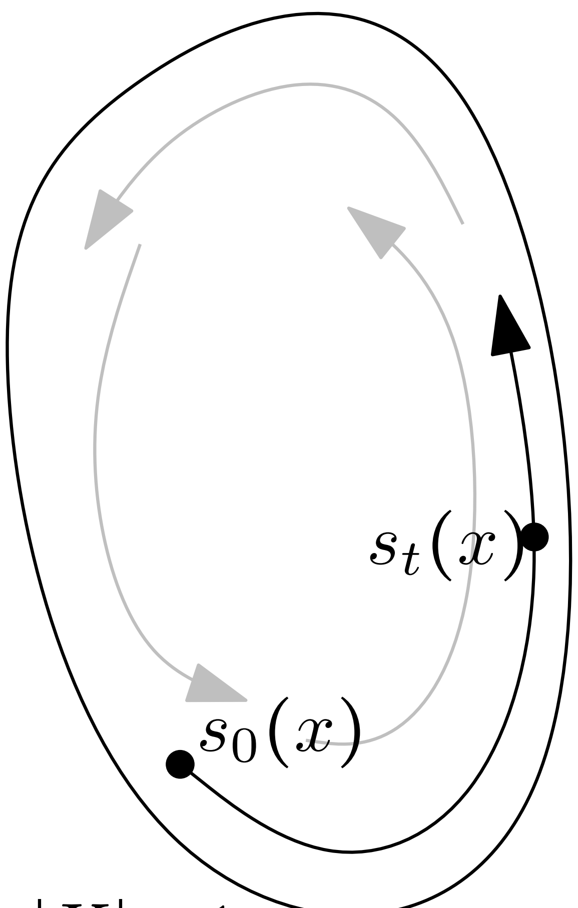

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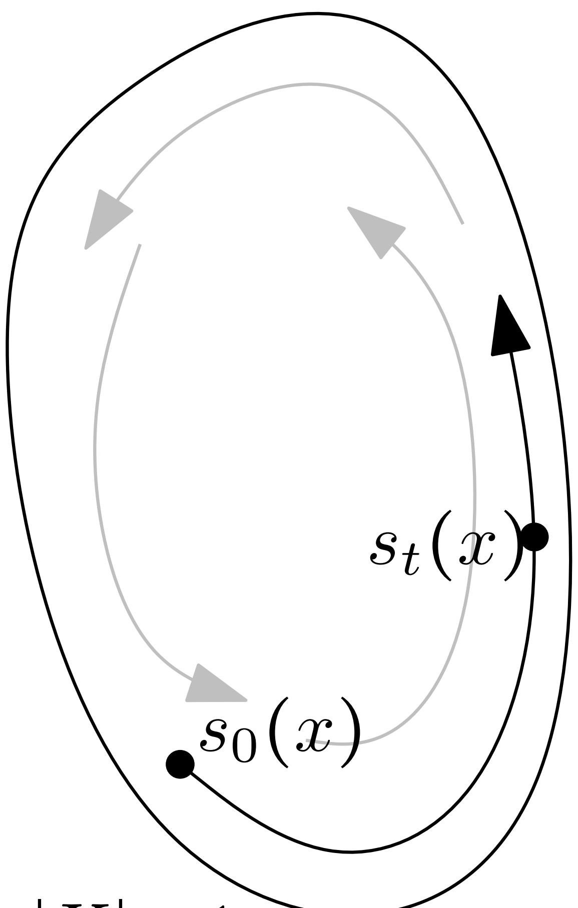

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Can this formulation be used for numerical computations (Brenier) ?
$\longrightarrow$ Minimizing geodesics (with Jean-Marie Mirebeau, 2015)
$\longrightarrow$ Cauchy problem (with Thomas Gallouet, 2016).

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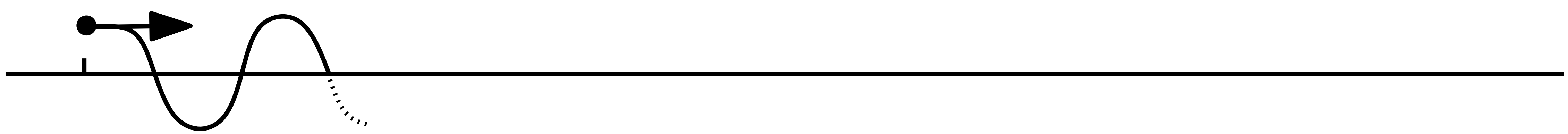

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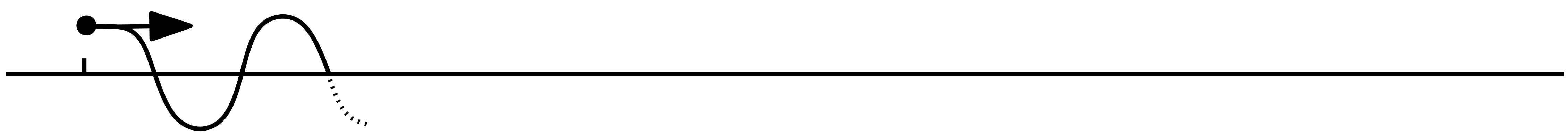

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$\longrightarrow$ $\mathcal{C}^1$ convergence towards the geodesic requires $\boxed{\frac{h}{\varepsilon} \longrightarrow 0.}$

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Leb = restriction of Lebesgue measure to a compact domain X

$\mathbb{S} = \{s : X \to X \mid s_{\#}\mathrm{Leb} = \mathrm{Leb}\} \longrightarrow$ "measure-preserving maps"

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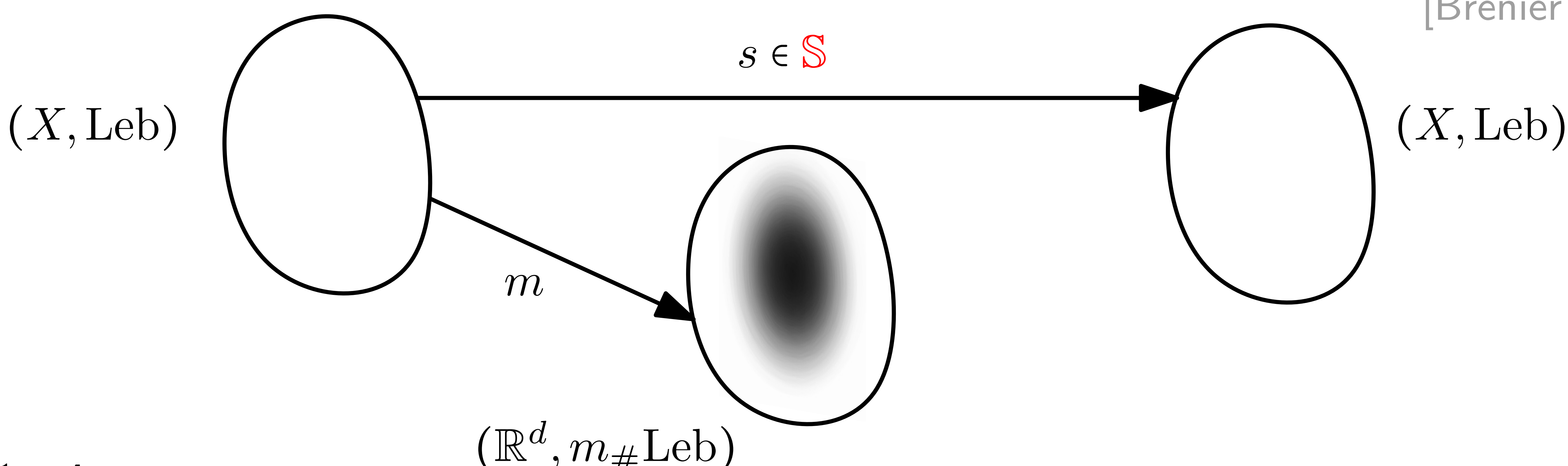

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Let $\bar{T}$ be the quadratic optimal transport map between Leb and $m_{\#}\mathrm{Leb}$. Then,

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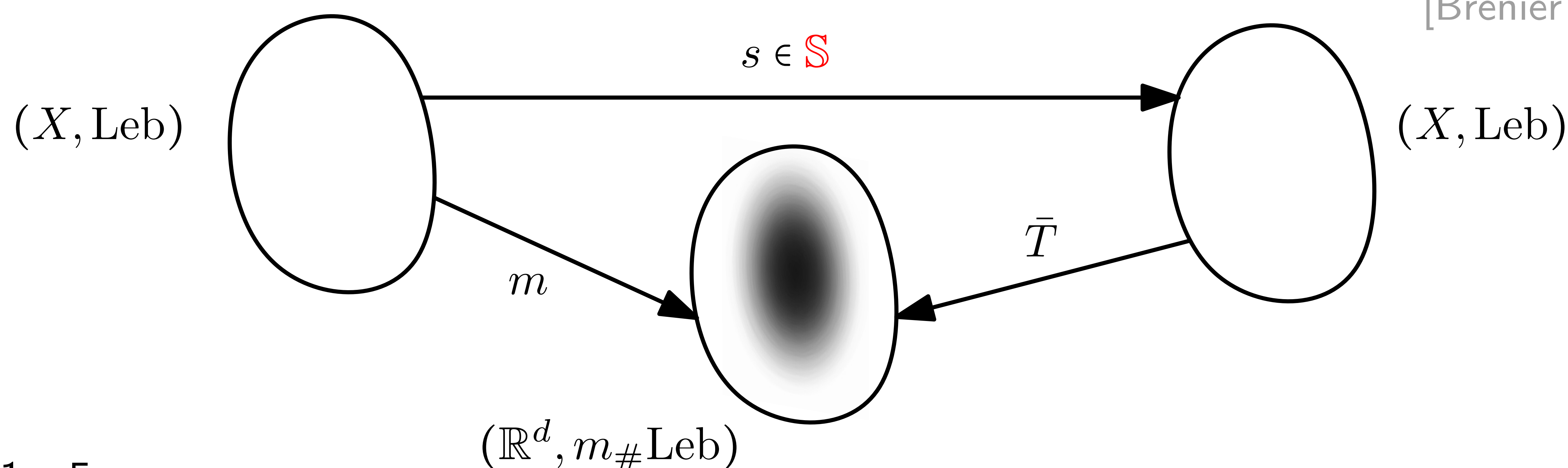

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$\boxed{\text{opt. quant.: } \nabla_{y_i}\mathcal{D} = B_i - y_i}$ $\longrightarrow$

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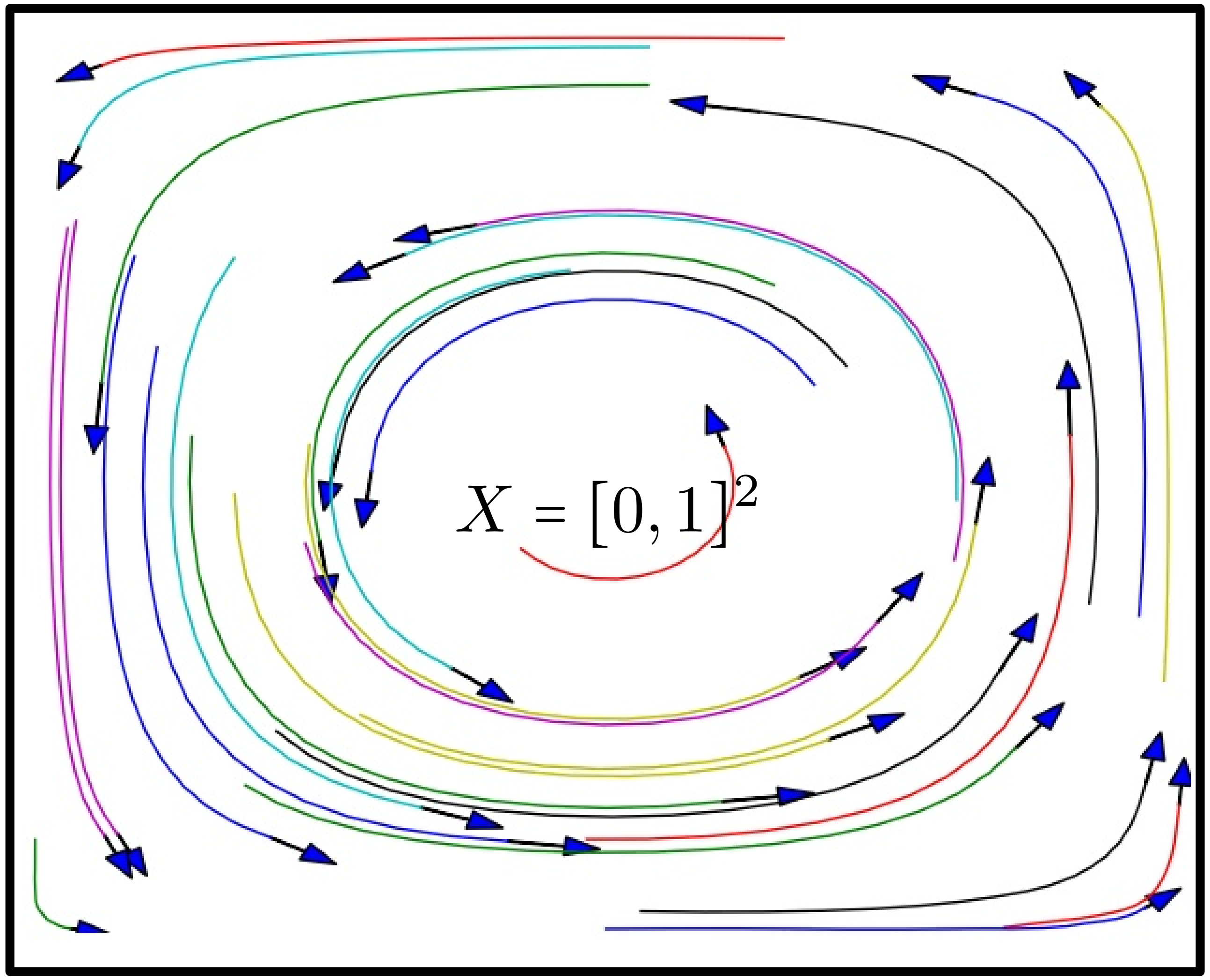
$\longrightarrow$ Convergence of a time-discretization using the symplectic Euler scheme.

Numerical result: Stationary flow on $[0,1]^2$

Stationary flow on $[0,1]^2$: speed: $u(\mathbf{x}) = (\cos(\pi x_1)\sin(\pi x_2), \sin(\pi x_1)\cos(\pi x_2))$

pressure: $p(\mathbf{x}) = \frac{1}{4}(\sin^2(\pi x_1) + \sin^2(\pi x_2))$



Numerical result: Instabilities

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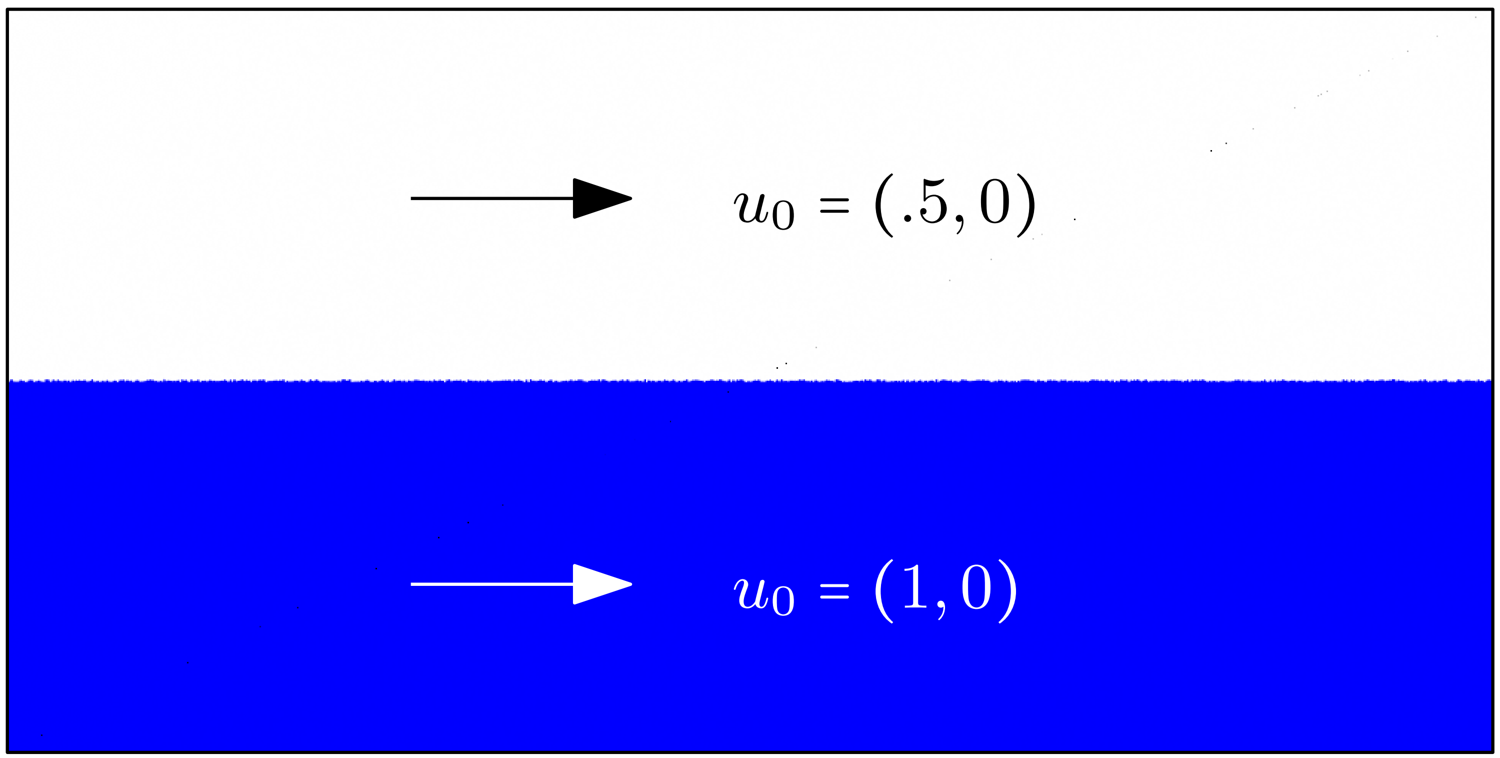

$X = [0,2] \times [-.5,.5]/(x = 0 \sim x = 2)$

200k particles, 2000 timesteps, $t_{\max} = 8$

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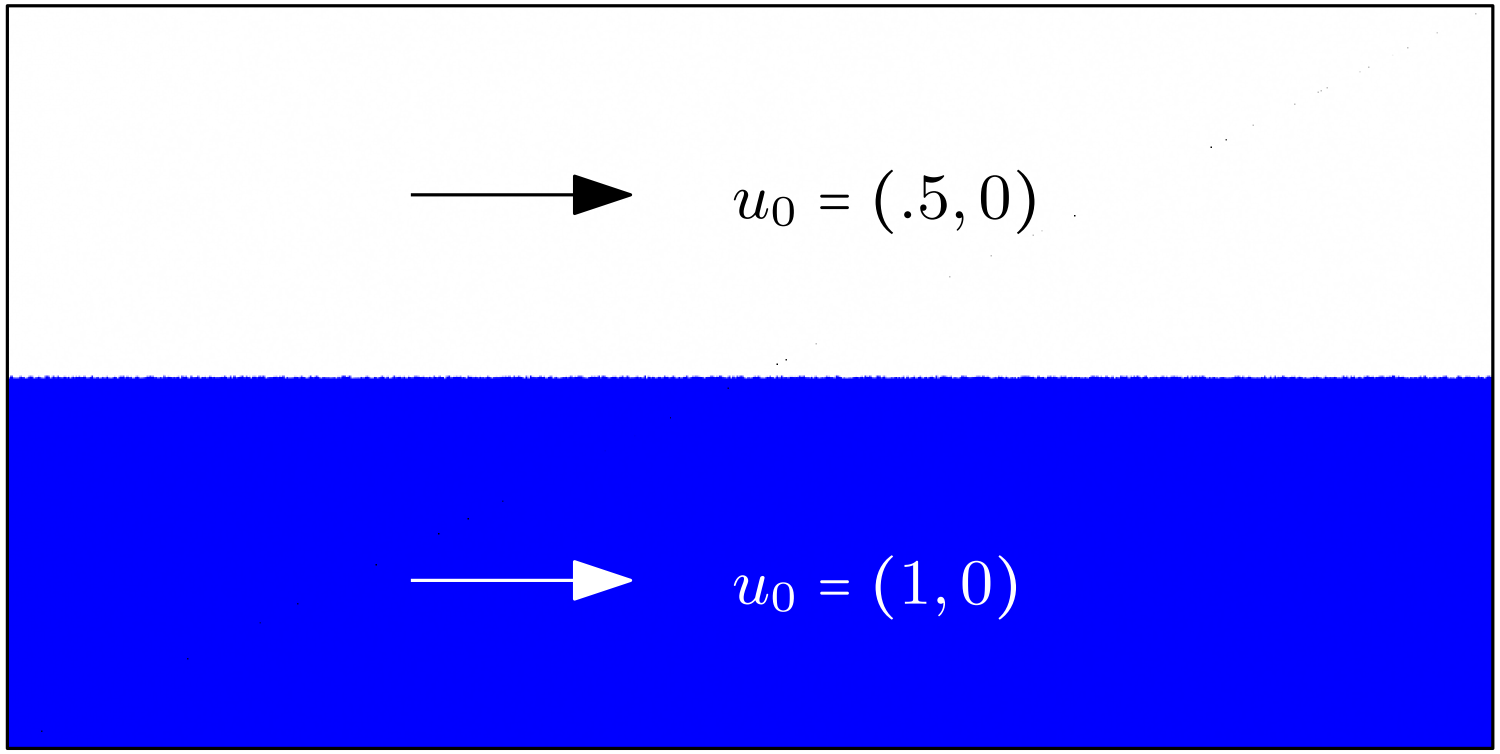

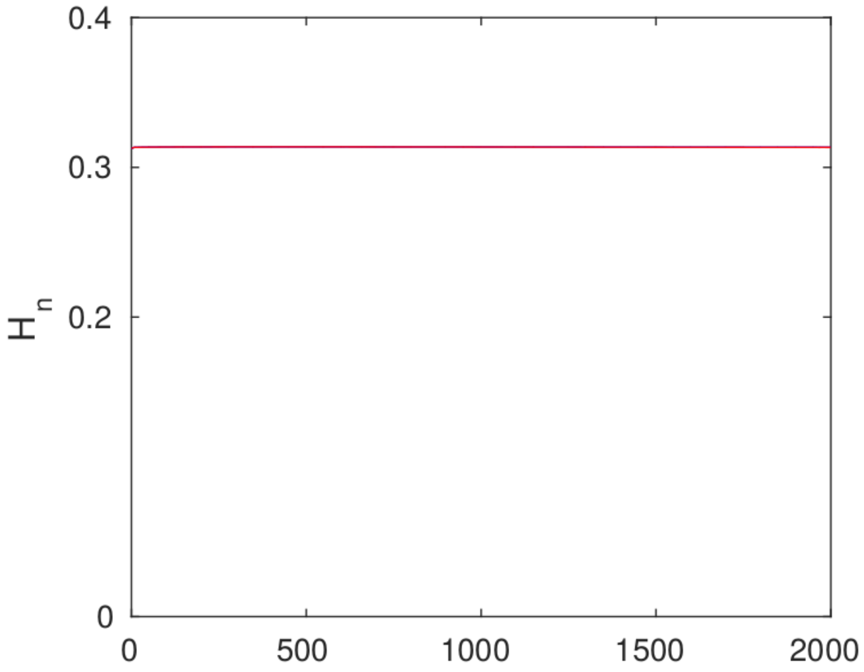

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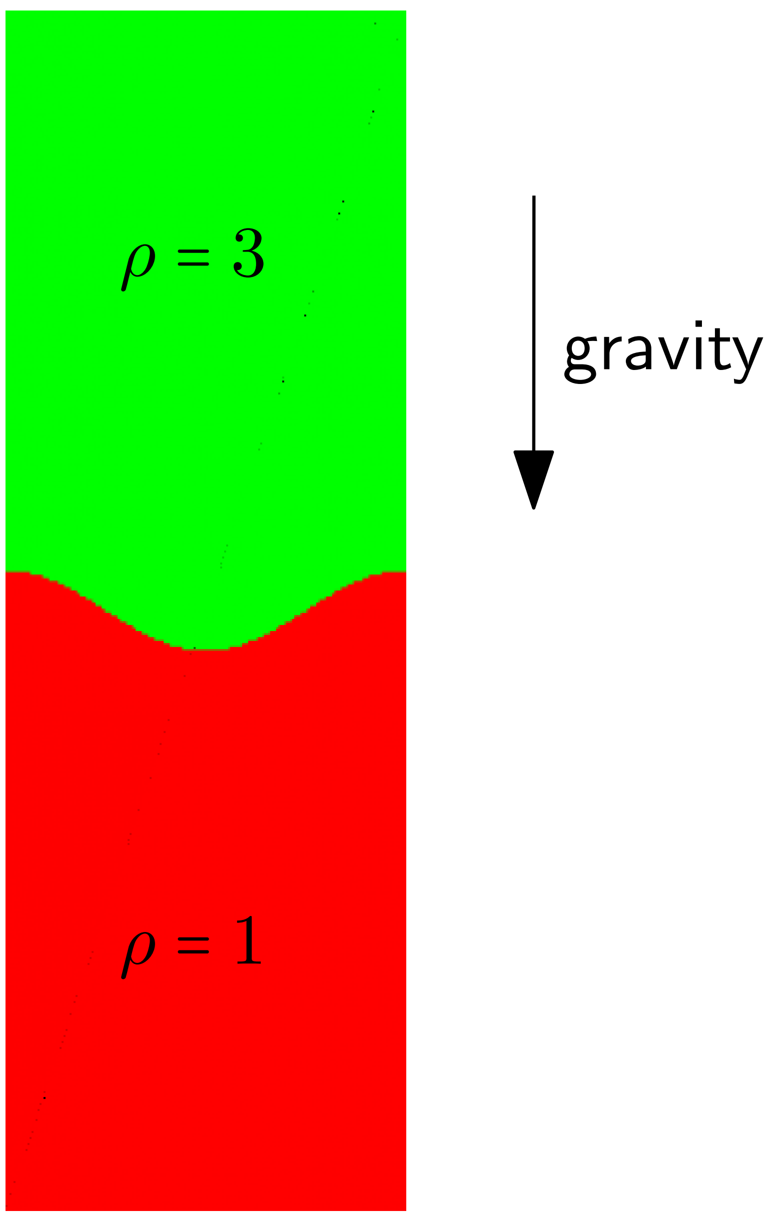

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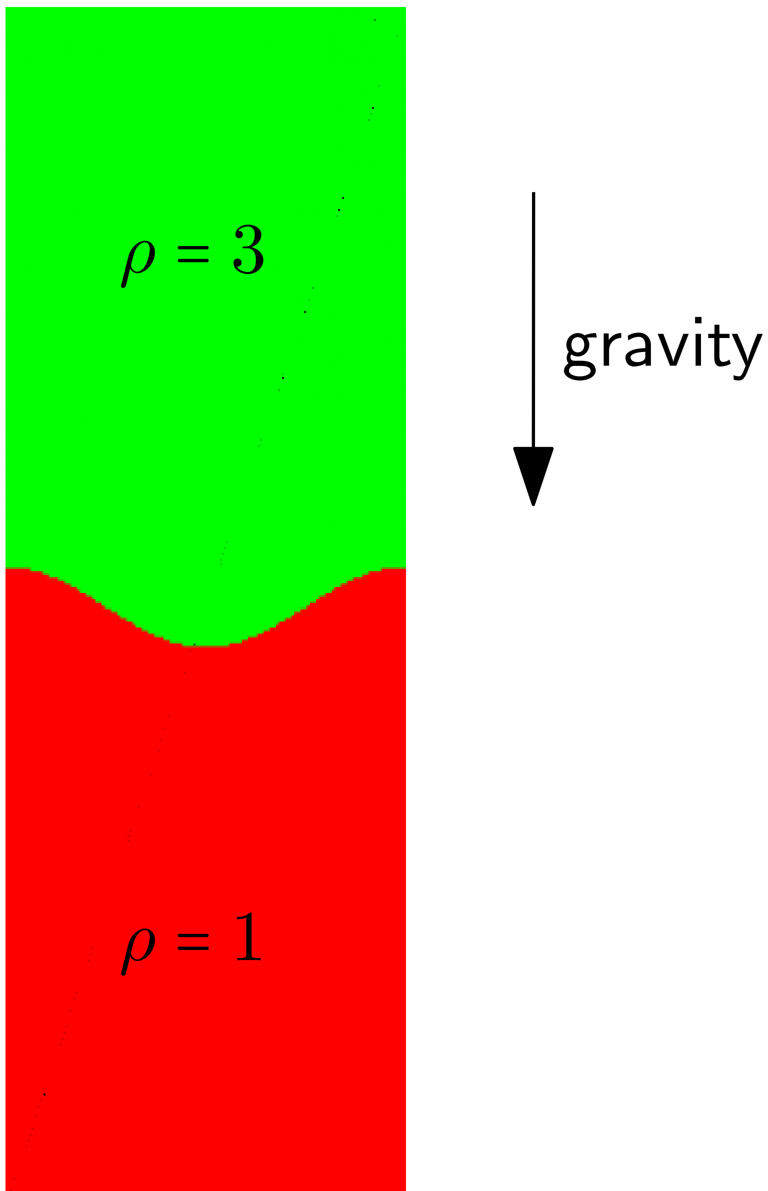

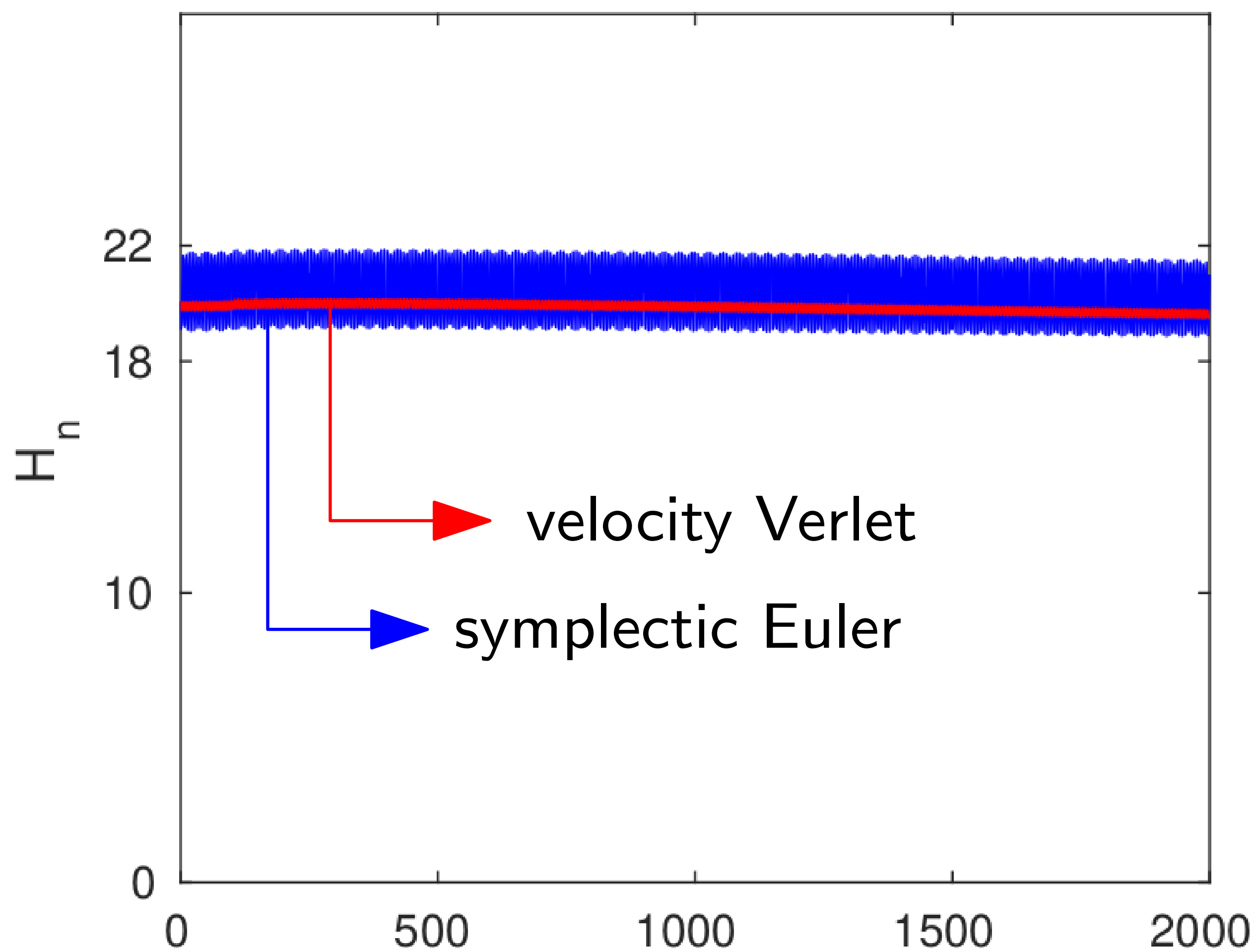

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3. General picture

Lagrangian formulation of (some) PDEs

- We track the evolution of a **population of particles** ($=$ probability distribution) $\rho_0 \in \mathcal{P}_2(\mathbb{R}^d)$, whose **displacement field** $s : [0, T] \to \mathrm{L}^2(\rho_0, \mathbb{R}^d)$ satisfies

$$\dot{s} \in -\partial E(s) \quad \textit{(gradient flow)}$$

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- **Main assumption:** The energy/entropy E only depends on the distribution of particles, i.e. $E(s) = \mathcal{E}(s_{\#}\rho_0)$, with $\mathcal{E} : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R} \cup \{+\infty\}$.

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$$\mathcal{E}_{\mathrm{ent}}(\rho) = \begin{cases} \int \rho \log \rho & \text{if } \rho \in \mathcal{P}_2^{\mathrm{ac}}(\Omega) \\ +\infty & \text{if not} \end{cases} \qquad \mathcal{E}_{\mathrm{inc}}(\rho) = \begin{cases} 0 & \text{if } \rho = \mathrm{Leb}_\Omega \\ +\infty & \text{if not} \end{cases}$$

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- **NB: E is typically non-convex, with values in $\mathbb{R} \cup \{+\infty\}$.**

Lagrangian-Eulerian dictionnary

	$\dot{s} \in -\partial E(s)$
$\mathcal{E}_{\text{inc}}$	
$\mathcal{E}_{\text{cong}} + \mathcal{E}_{\text{pot}}$	crowd motion
$\mathcal{E}_{\text{ent}} + \mathcal{E}_{\text{pot}}$	linear Fokker-Planck equation

Wasserstein gradient-flows:

[Otto '99],
[Jordan-Kinderlehrer-Otto '98],
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- **Moreau-Yosida regularization:** $E_\varepsilon(s) := \inf_{s'} \frac{1}{2\varepsilon}\|s - s'\|^2 + E(s')$

$\longrightarrow$
$$\dot{s}_\varepsilon = -\nabla E_\varepsilon(s_\varepsilon)$$
or $\ddot{s}_\varepsilon = -\nabla E_\varepsilon(s_\varepsilon)$

4. Gradient flows and Moreau-Yosida regularization

Gradient flow case

We consider $\mathcal{E}(\rho) = \int f(\rho) + \rho V$ and $E(s) = \mathcal{E}(s_{\#}\rho_0)$ with $s \in \mathrm{L}^2(\rho_0, \mathbb{R}^d)$

- If $\dot{s}_t = v_t \circ s_t$ and $\rho_t := s_{t\#}\rho_0$, then: 1) $\dot{\rho}_t + \mathrm{div}(\rho_t v_t) = 0$,

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Proof of 2): $\frac{d}{dt}\mathcal{E}(\rho_t) = \frac{d}{dt}\int f(\rho_t) + \rho_t V = \int (f'(\rho_t) + V)\dot{\rho}_t$

$= -\int (f'(\rho_t) + V)\mathrm{div}(\rho_t v_t)$ [by 1)]

$= \int \langle \nabla f'(\rho_t) + \nabla V | v_t \rangle \,\mathrm{d}\,\rho_t$ [by Stokes]

$= \int \langle (\nabla f'(\rho_t) + \nabla V) \circ s_t | \dot{s}_t \rangle \,\mathrm{d}\,\rho_0$ [$y = s_t(x)$]

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(Lagrangian)

[Evans-Gangbo-Savin '08]

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Examples: $f(r) = r \log r \longrightarrow \dot{\rho}_t = \Delta \rho_t + \mathrm{div}(\rho_t \nabla V)$

$f(r) = \frac{1}{m} r^m \longrightarrow \dot{\rho}_t = \Delta \rho_t^m + \mathrm{div}(\rho_t \nabla V)$

Gradient flow case

We consider $\mathcal{E}(\rho) = \int f(\rho) + \rho V$ and $E(s) = \mathcal{E}(s_{\#}\rho_0)$ with $s \in \mathrm{L}^2(\rho_0, \mathbb{R}^d)$

- If $\dot{s}_t = v_t \circ s_t$ and $\rho_t := s_{t\#}\rho_0$, then: 1) $\dot{\rho}_t + \mathrm{div}(\rho_t v_t) = 0$,

  2) $\frac{d}{dt}\mathcal{E}(\rho_t) = \langle \nabla(f'(\rho_t) + \nabla V) \circ s_t | \dot{s}_t \rangle_{\mathrm{L}^2(\rho_0)}$

$$\boxed{\nabla E(s) = (\nabla f'(\rho) + \nabla V) \circ s, \text{ with } \rho = s_{\#}\rho_0}$$

- Formally $\dot{s}_t = -\nabla E(s_t)$ leads to the equations

$$\boxed{\begin{cases} \dot{s}_t = v_t \circ s_t \\ \rho_t = s_{t\#}\rho_0 \\ v_t = -(\nabla f'(\rho_t) + \nabla V) \end{cases}}$$

(Lagrangian)
[Evans-Gangbo-Savin '08]

$$\boxed{\dot{\rho}_t + \mathrm{div}[\rho_t(\nabla f'(\rho_t) + \nabla V)] = 0}$$

(Eulerian)
[Otto '99]

Examples: $f(r) = r \log r \longrightarrow \dot{\rho}_t = \Delta\rho_t + \mathrm{div}(\rho_t \nabla V)$

$f(r) = \frac{1}{m} r^m \longrightarrow \dot{\rho}_t = \Delta\rho_t^m + \mathrm{div}(\rho_t \nabla V)$

- **Regular** lagrangian trajectory associated to heat flow ($\neq$ Brownian motion!)

(Numerical) approximation of gradient flows

- **Minimizing-movement (JKO) scheme**: for $\tau > 0$ define a time-discretization by

$$\boxed{s_\tau^{n+1} \in \arg\min_s \frac{1}{2\tau} \|s_\tau^n - s\|^2 + E(s)}$$

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  Main difficulty: $\mathcal{E}(\frac{1}{N}\sum_i \delta_{y_i}) = +\infty$. Possible solutions:

  - spreading the mass $\frac{1}{N}\delta_{y_i}$ uniformly over a Voronoi/Laguerre cell or a ball:

    [Blanchet-Calvez-Carrillo '08] [Benamou-Carlier-M.-Oudet '14]
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  - replacing $\mathcal{E}(\mu)$ by $\mathcal{E}(\mu * \eta_\varepsilon)$: [Carrillo-Craig-Patacchini '18]

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- **Moreau-Yosida regularization:** $E_\varepsilon(s) := \inf_{s'} \frac{1}{2\varepsilon}\|s - s'\|^2 + E(s')$

  $$\boxed{\dot{s} \in -\partial E(s) \longrightarrow \dot{s}_\varepsilon = -\nabla E_\varepsilon(s_\varepsilon)}$$

Moreau-Yosida regularization in Wasserstein space

- **Wasserstein distance** between two probability measures $\rho, \mu \in \mathcal{P}_2(\mathbb{R}^d)$,

$$\mathrm{W}_2^2(\rho,\mu) = \min_T \int \|x - T(x)\|^2 \,\mathrm{d}\,\rho(x) \text{ under the constraint } T_\# \rho = \mu$$

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Space-discretization: assume that μ = uniform over a finite set = $\frac{1}{N}\sum_{1\leq i\leq N} \delta_{y_i}$

5. Lagrangian discretization of crowd motion

Crowd motion model

$\Omega \subset \mathbb{R}^d, |\Omega| > 1, \rho_0 \in \mathcal{P}^{\mathrm{ac}}(\Omega)$ [Maury, Roudneff-Chupin, Santambrogio '09]

- The crowd is subjet to two forces: $\mathrm{E}_{\mathrm{pot}}(s) = \int V(s(x))\,\mathrm{d}\,\rho_0(x)$

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- Eulerian formulation of the model:

$$\boxed{\begin{cases} \partial_t \rho - \mathrm{div}(\rho\nabla V + \rho\nabla p) = 0 \\ \rho(0) = \rho_0 \\ \rho \le \mathrm{Leb}_\Omega \\ p \ge 0,\ p(1-\rho) = 0 \end{cases}}$$

Computing $\mathcal{E}_{\mathrm{cong},\varepsilon}$ (congestion)

- Let $\Omega \subseteq \mathbb{R}^d$, with $|\Omega| > 1$ and let $K = \{\sigma \in \mathcal{P}(\Omega) \mid \sigma \leq \mathrm{Leb}_\Omega\}$.
- To measure whether $\mu = \frac{1}{N}\sum_i \delta_{y_i}$ is close to being "non-congested", we use

$$\boxed{\mathcal{D}^{\mathrm{cong}}(y_1, \cdots, y_N) := \frac{N}{2} \min_{\sigma \in K} \mathrm{W}_2^2(\sigma, \tfrac{1}{N}\textstyle\sum_i \delta_{y_i})} \quad (*)$$

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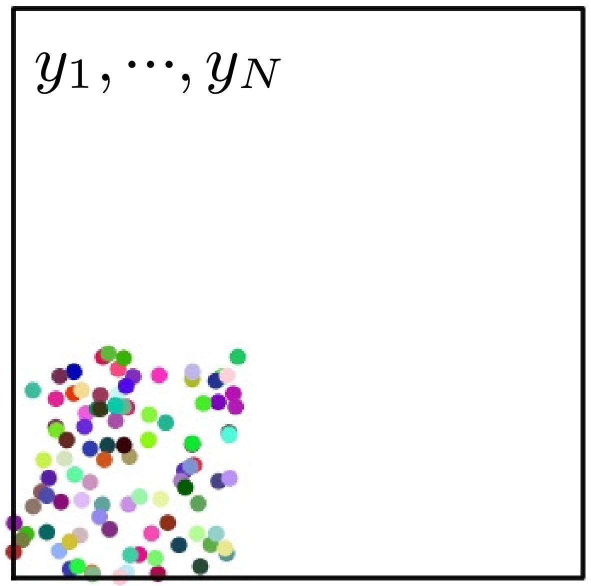

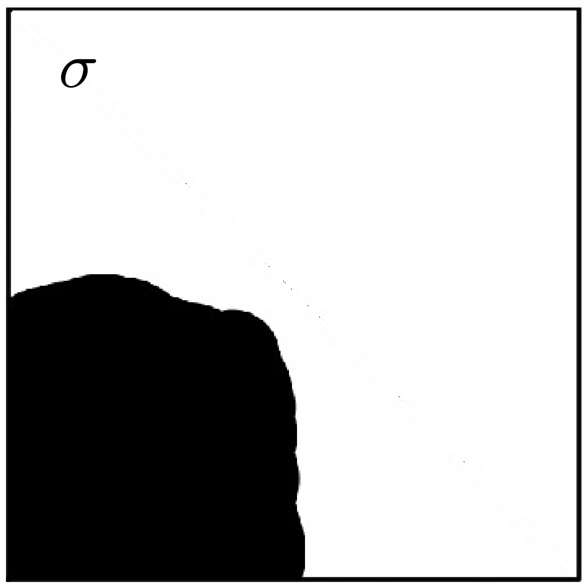

Prop: 1) $\exists ! \sigma$ minimizer of $(*)$

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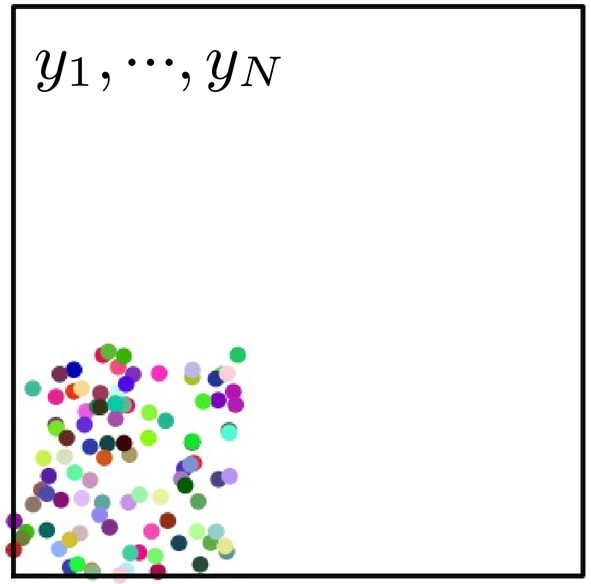

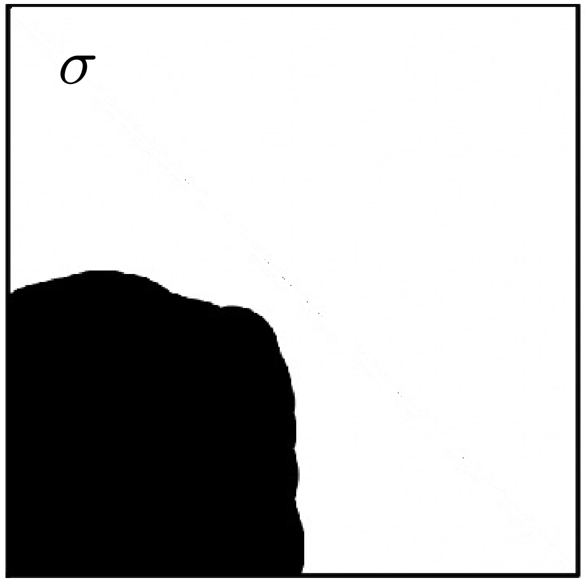

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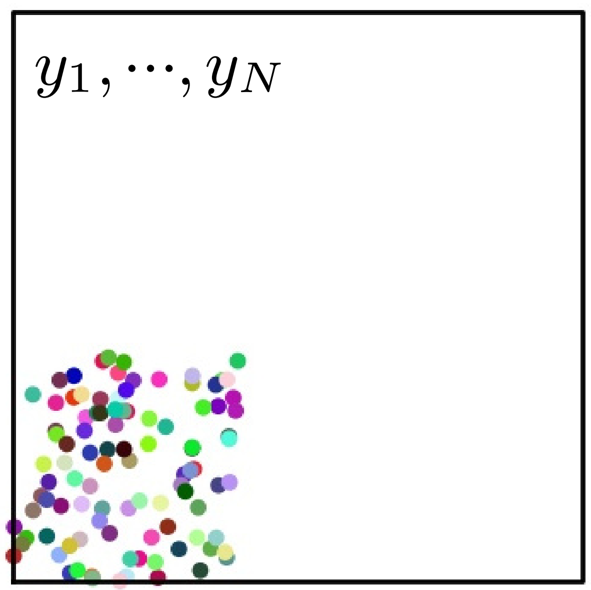

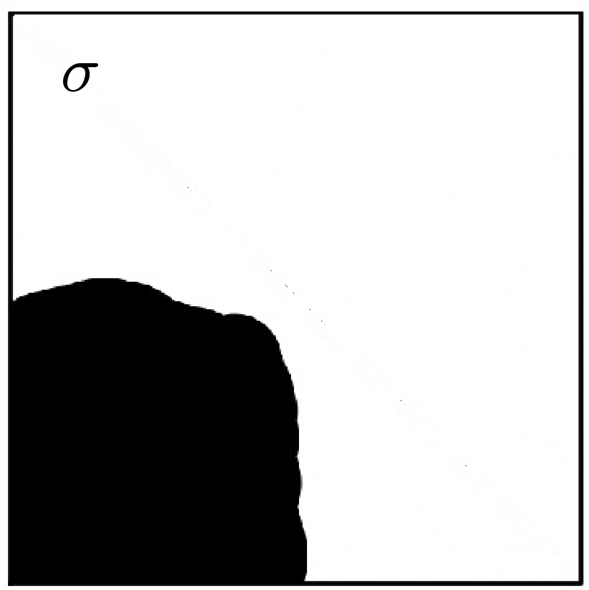

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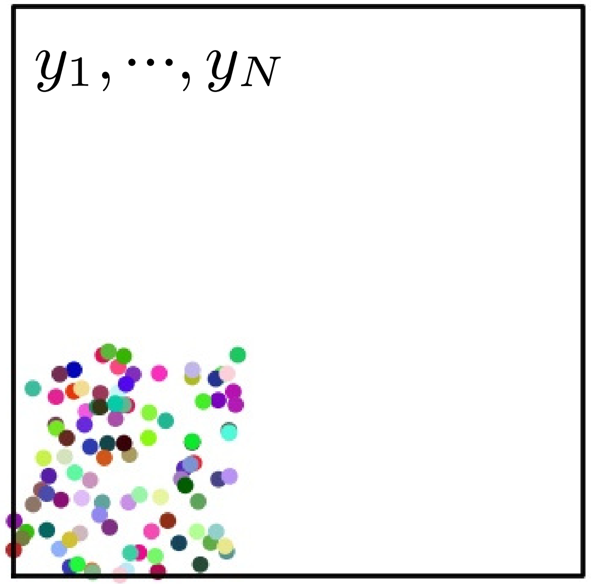

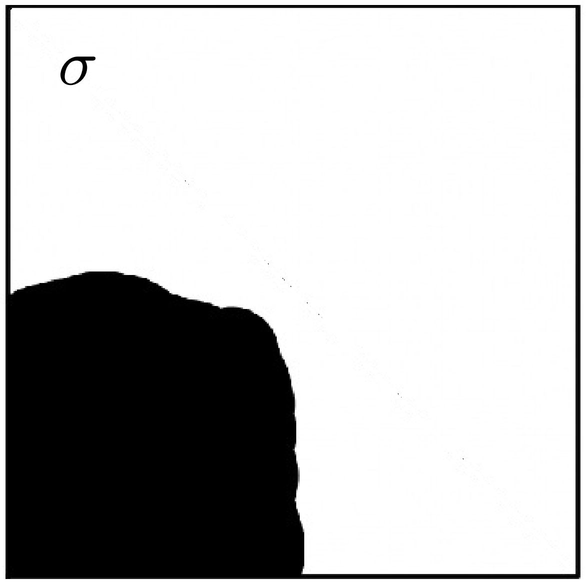

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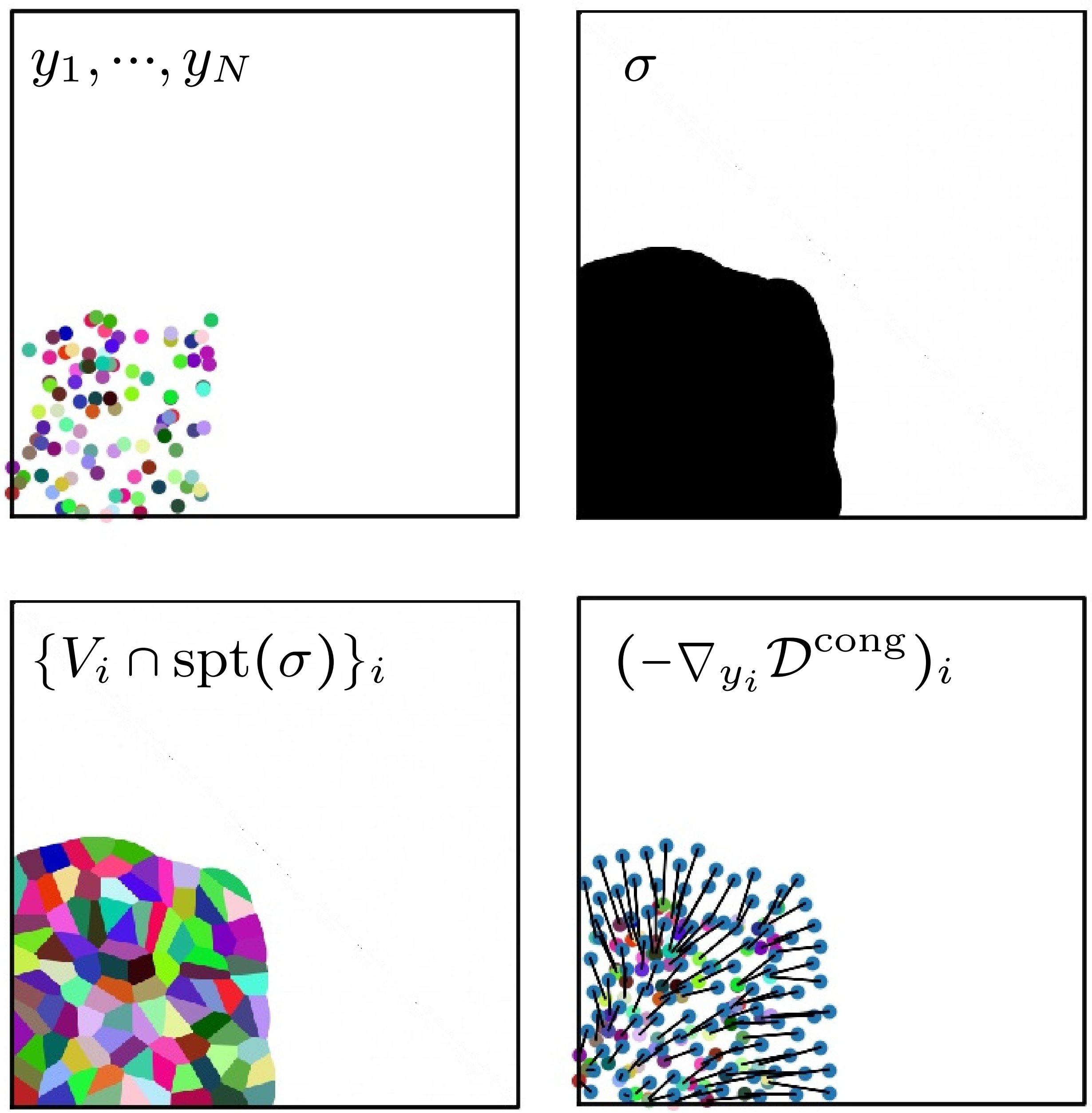

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- $\boxed{\text{Kantorovich potential} \simeq -\text{ pressure}}$
- $\mathcal{D}^{\mathrm{cong}}, \nabla\mathcal{D}^{\mathrm{cong}}$ and σ are also computed in *near-linear* time in 2D/3D.

Discretization of the crowd motion model

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[with $s|_{\omega_i} = y_i$] $\Longleftrightarrow$

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We let $\mu_N(t) = \frac{1}{N} \sum_i \delta_{y_i(t)} \in \mathcal{P}(\Omega)$ the corresponding distribution of particles.

Convergence theorem

Consider

$$\boxed{\begin{cases} \dot{y}_i = -\nabla V(y_i) - \frac{1}{\varepsilon_N}\nabla_{y_i}\mathcal{D}^{\mathrm{cong}}(y_1(t),\cdots,y_N(t)) \\ y_i(0) = \fint_{\omega_i} x\,\mathrm{d}\,\rho_0 \end{cases}}$$

Denote $\mu_N = \frac{1}{N}\sum_i \delta_{y_i} \in \mathcal{P}(\Omega)$ and $\sigma_N = \arg\min \frac{1}{2\varepsilon}\,\mathrm{W}_2^2(\mu_N,\cdot) + \mathcal{E}_{\mathrm{cong}}(\cdot)$.

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Theorem: For every N, choose $\varepsilon_N \to 0$ and assume that $V \in \mathcal{C}^1, V \geq 0$ and

$$\frac{1}{\varepsilon_N} \mathrm{W}_2^2(\rho_0, \mu_N(0)) \leq C \qquad \text{and} \qquad \frac{1}{\varepsilon_N^2} \int_0^T \mathrm{W}_2^2(\mu_N, \sigma_N)\,\mathrm{d}\,t \leq C$$

Then $\mu_N \rightharpoonup \rho \in \mathcal{C}^0([0,T], \mathcal{P}(\Omega))$, where ρ satisfies in the sense of distribution,

$$\begin{cases} \partial_t \rho + \mathrm{div}(\rho v) = 0 \\ v = -\nabla V - \nabla p, \\ \rho \leq 1 \\ p \geq 0,\ \ p(1-\rho) = 0, \end{cases} \qquad \text{for some } p \in \mathrm{L}^2([0,T], \mathrm{H}^1(\Omega))$$

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- The assumption (*) is always true in 1D, and can be checked numerically in 2D.

Proof techniques

- **Existence of a limit.** Let $\sigma_N = \Pi_K(\mu_N)$ and $\mathcal{E}_N(t) = \int V \,\mathrm{d}\mu_N + \frac{1}{2\varepsilon_N} \mathrm{W}_2^2(\mu_N, \sigma_N)$.

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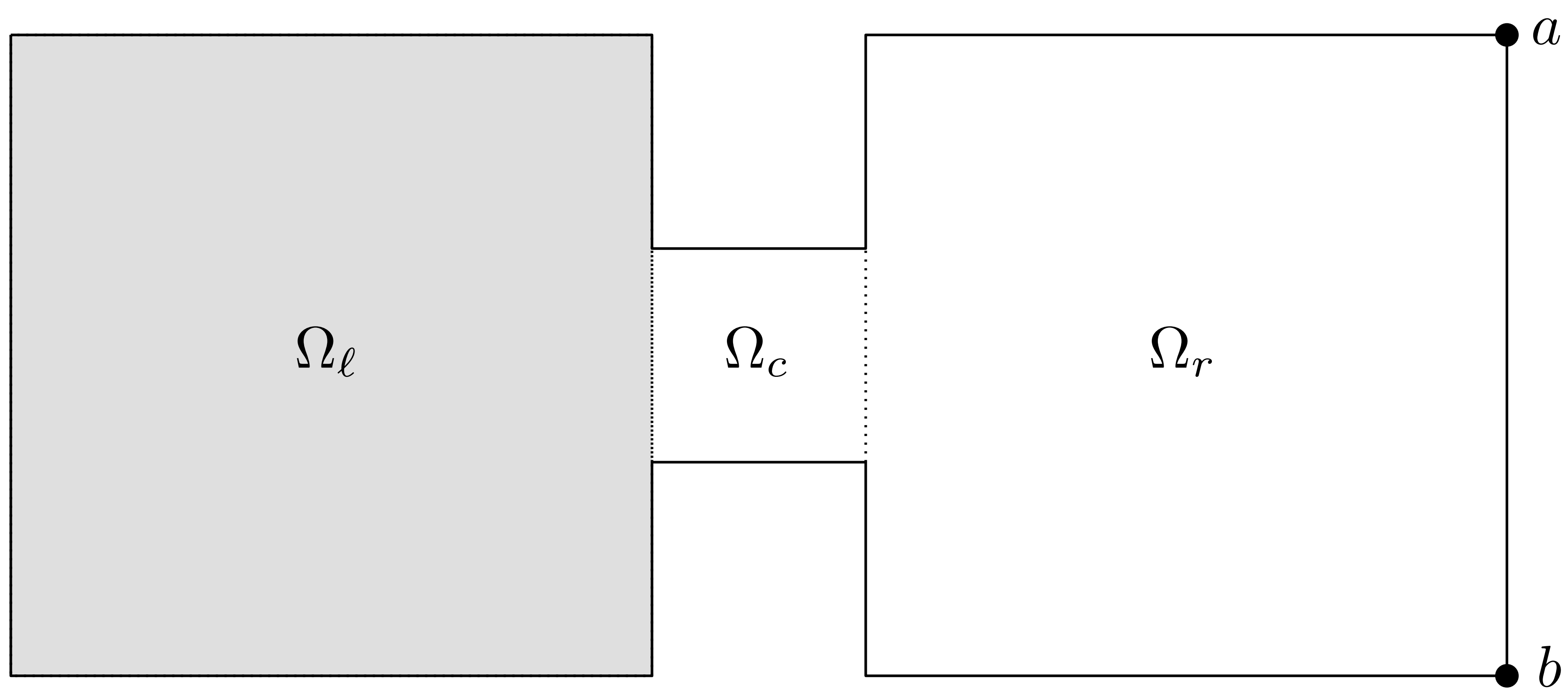
Numerical example



initial density: $\rho_0 \simeq 0.78 \cdot \mathrm{Leb}_{\Omega_\ell}$

potential: V = geodesic distance to $\{a,b\}$, i.e. V satisfies the Eikonal equation

$$\begin{cases} \|\nabla V\| = 1 \text{ in } \Omega_\ell \cup \Omega_c \cup \Omega_r \\ V(a) = V(b) = 0 \end{cases}$$

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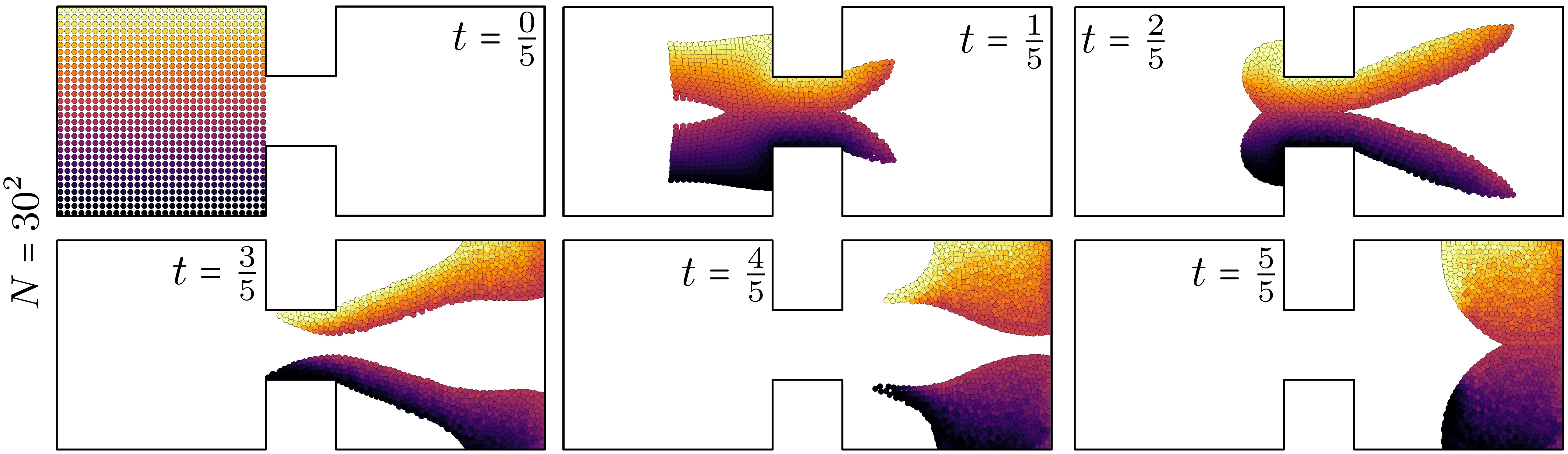

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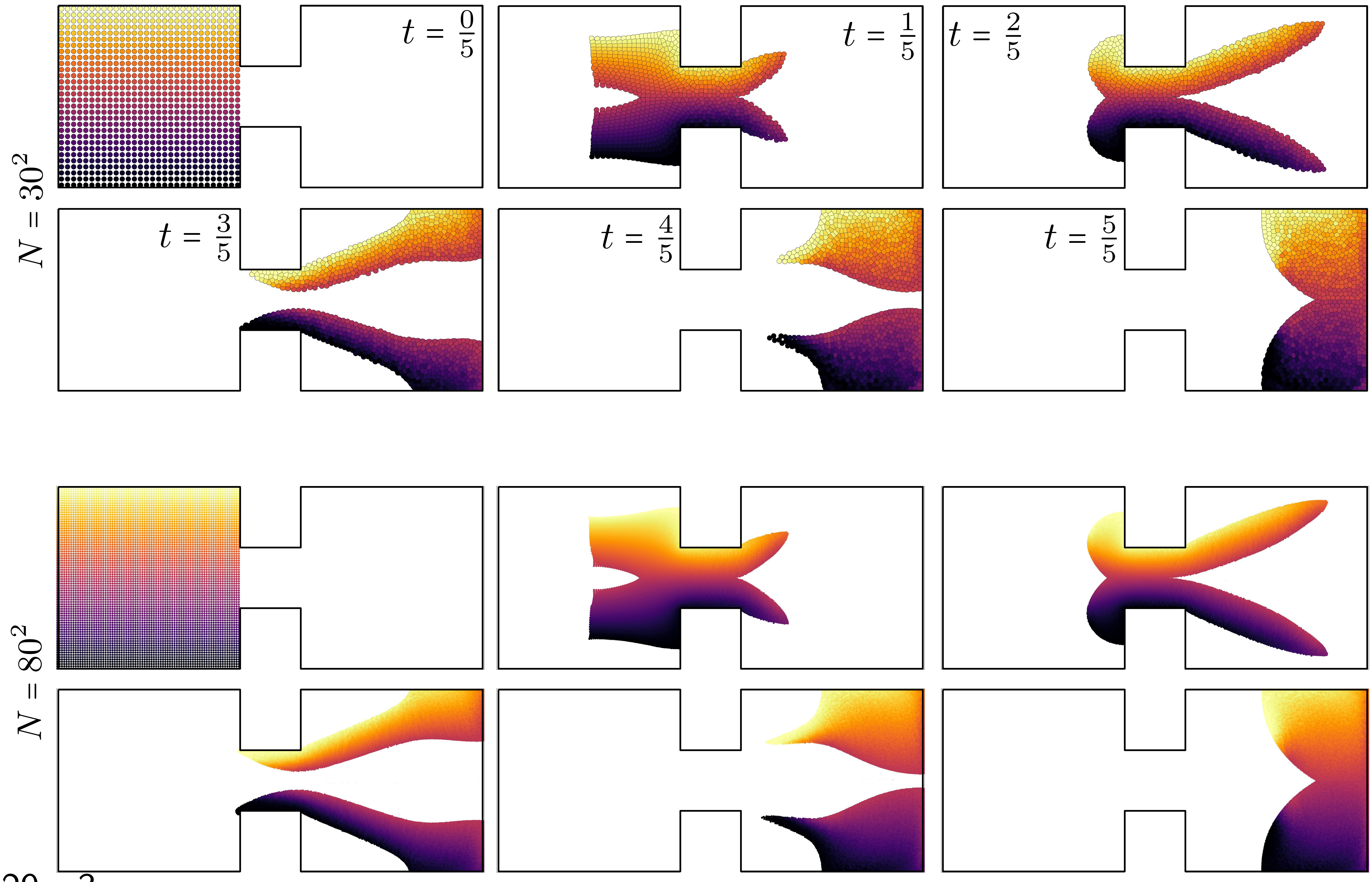

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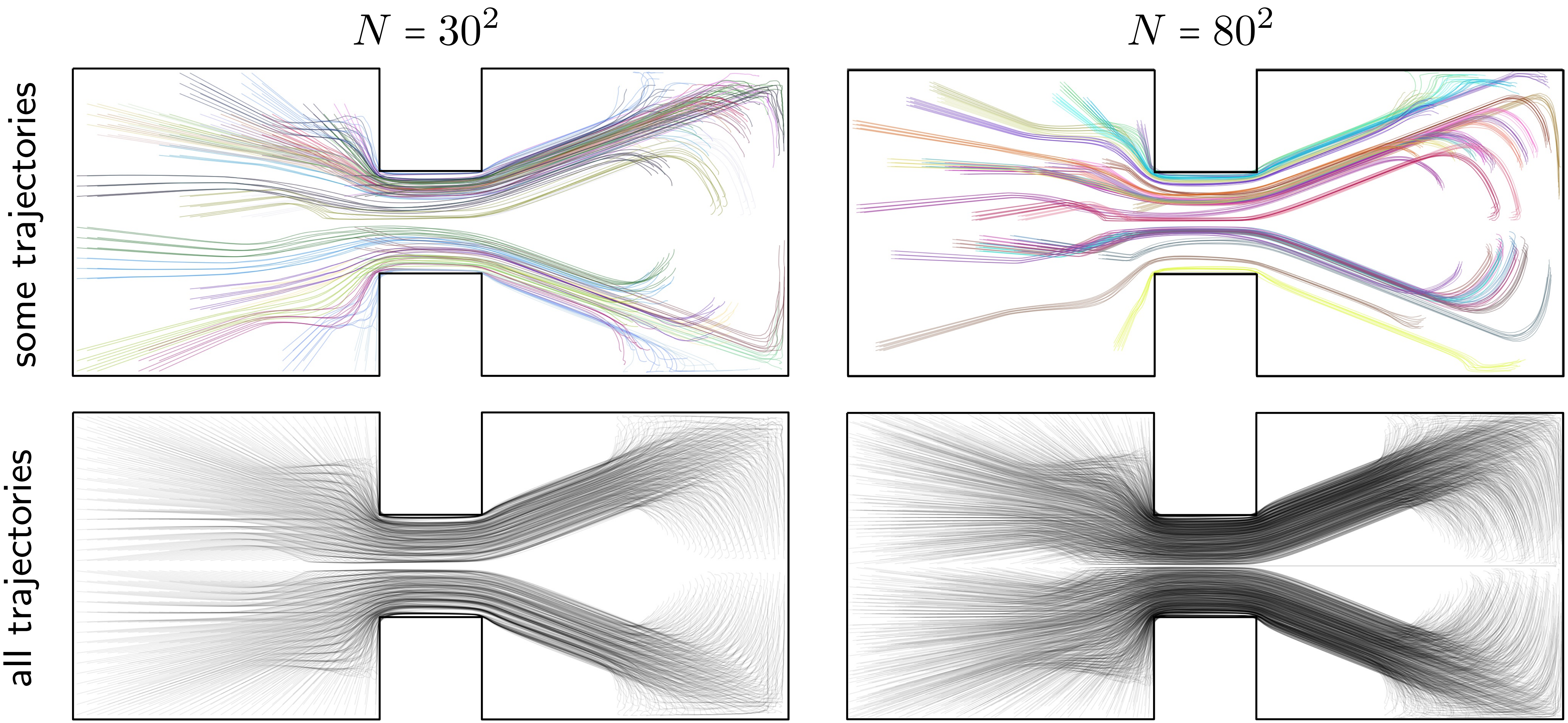

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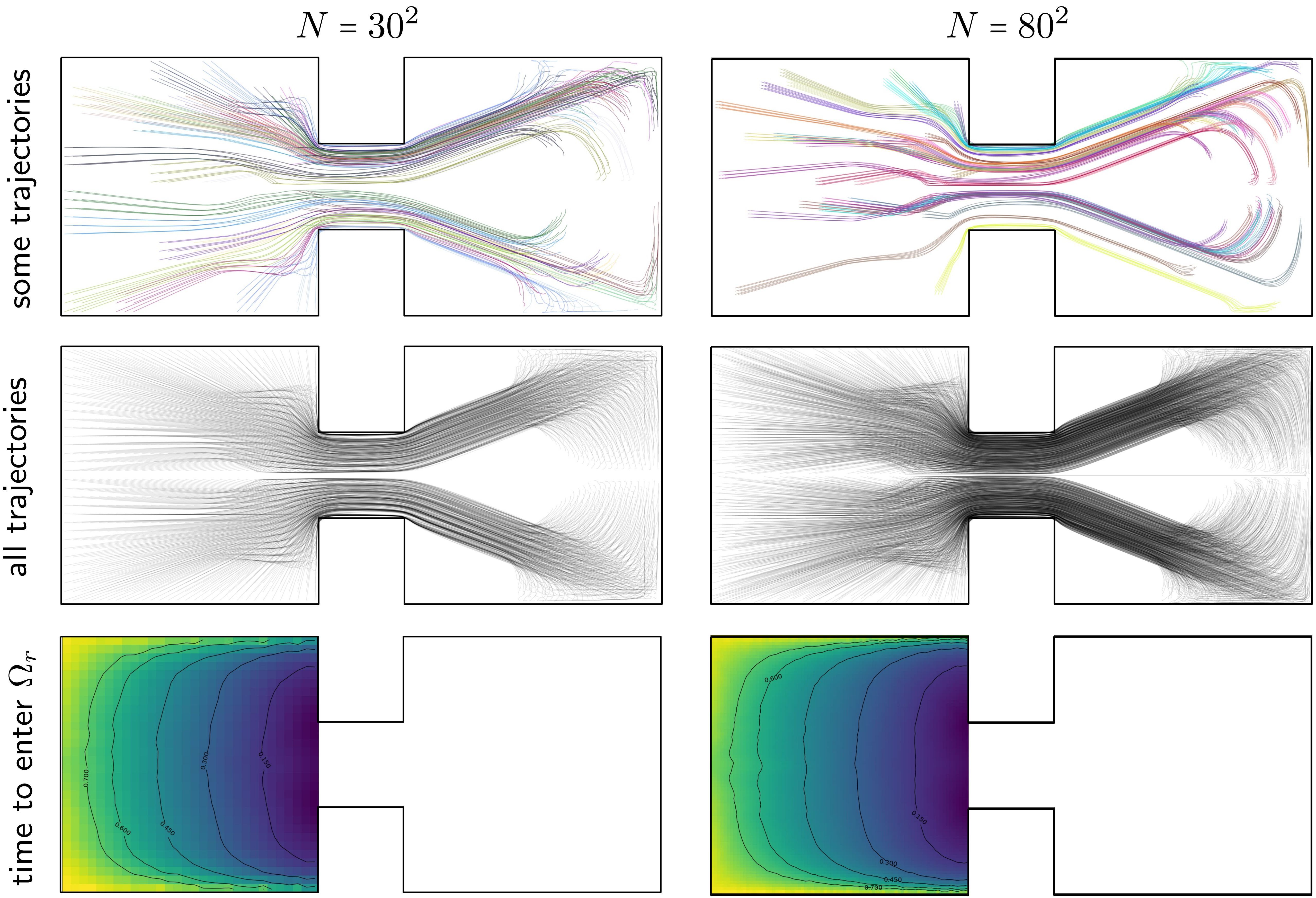

6. Linear diffusion

Computing $\mathcal{E}_{\mathrm{ent},\varepsilon}$ (entropy)

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[Klartag, M., Santambrogio '17]

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- **Applications to density estimation in statistics?**

Convergence theorem

Consider

$$\boxed{\begin{cases} \dot{y}_i = -\nabla V(y_i) - \frac{1}{\varepsilon_N} \nabla_{y_i} \mathcal{D}_\varepsilon^{\mathrm{ent}}(y_1(t), \cdots, y_N(t)) \\ y_i(0) = ⨍_{\omega_i} x \,\mathrm{d}\,\rho_0 \end{cases}}$$

Denote $\mu_N = \frac{1}{N}\sum_i \delta_{y_i} \in \mathcal{P}(\Omega)$ and $\sigma_N = \arg\min \frac{1}{2\varepsilon} \mathrm{W}_2^2(\mu_N, \cdot) + \mathcal{E}_{\mathrm{ent}}(\cdot)$.

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Theorem: For every N, choose $\varepsilon_N \to 0$ and assume that $V \in \mathcal{C}^1, V \geq 0$ and

$$\frac{1}{\varepsilon_N}\mathrm{W}_2^2(\rho_0,\mu_N(0)) \leq C \quad \text{and} \quad \lim_{N\to+\infty}\frac{1}{\varepsilon_N}\int_0^T \mathrm{W}_2^2(\mu_N,\sigma_N)\,\mathrm{d}\,t = 0$$

Then $\mu_N \rightharpoonup \rho \in \mathcal{C}^0([0,T],\mathcal{P}(\Omega))$, where ρ satisfies in the sense of distribution,

$$\begin{cases} \partial_t\rho + \mathrm{div}(\rho v) = 0 \\ v = -\nabla V - \nabla p, \\ p = \log\rho \end{cases}$$

[M., Stra, Santambrogio '18]

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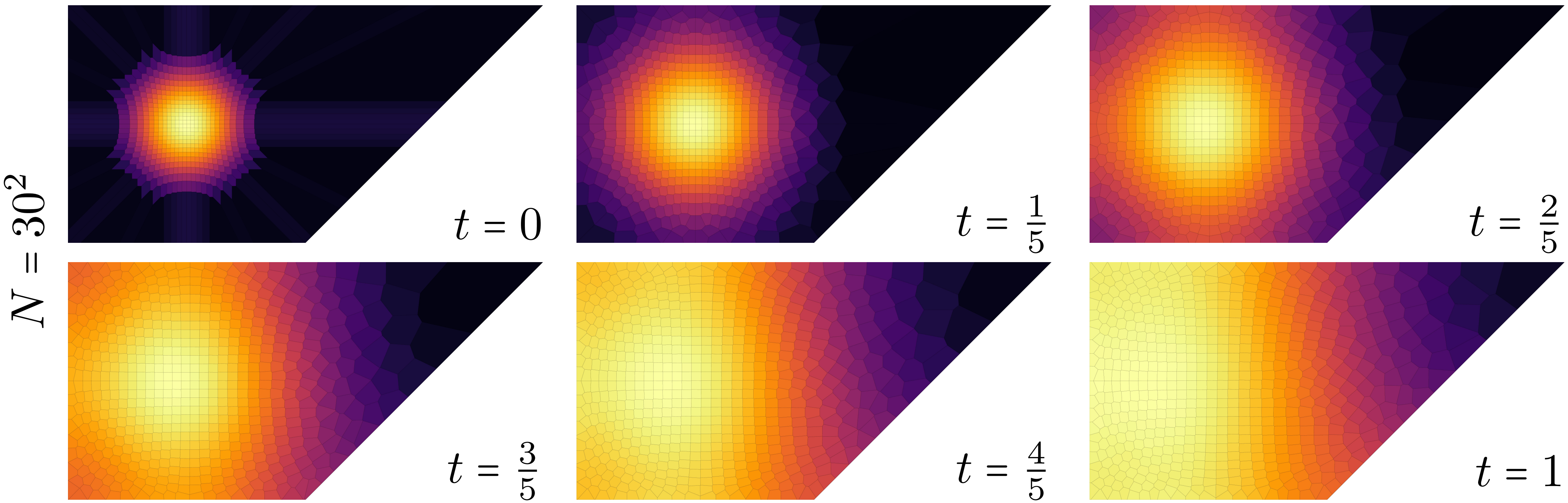
- The assumption (*) is always true in 1D, and can be checked numerically in 2D. (it is less strong than in the crowd motion case)

Numerical example



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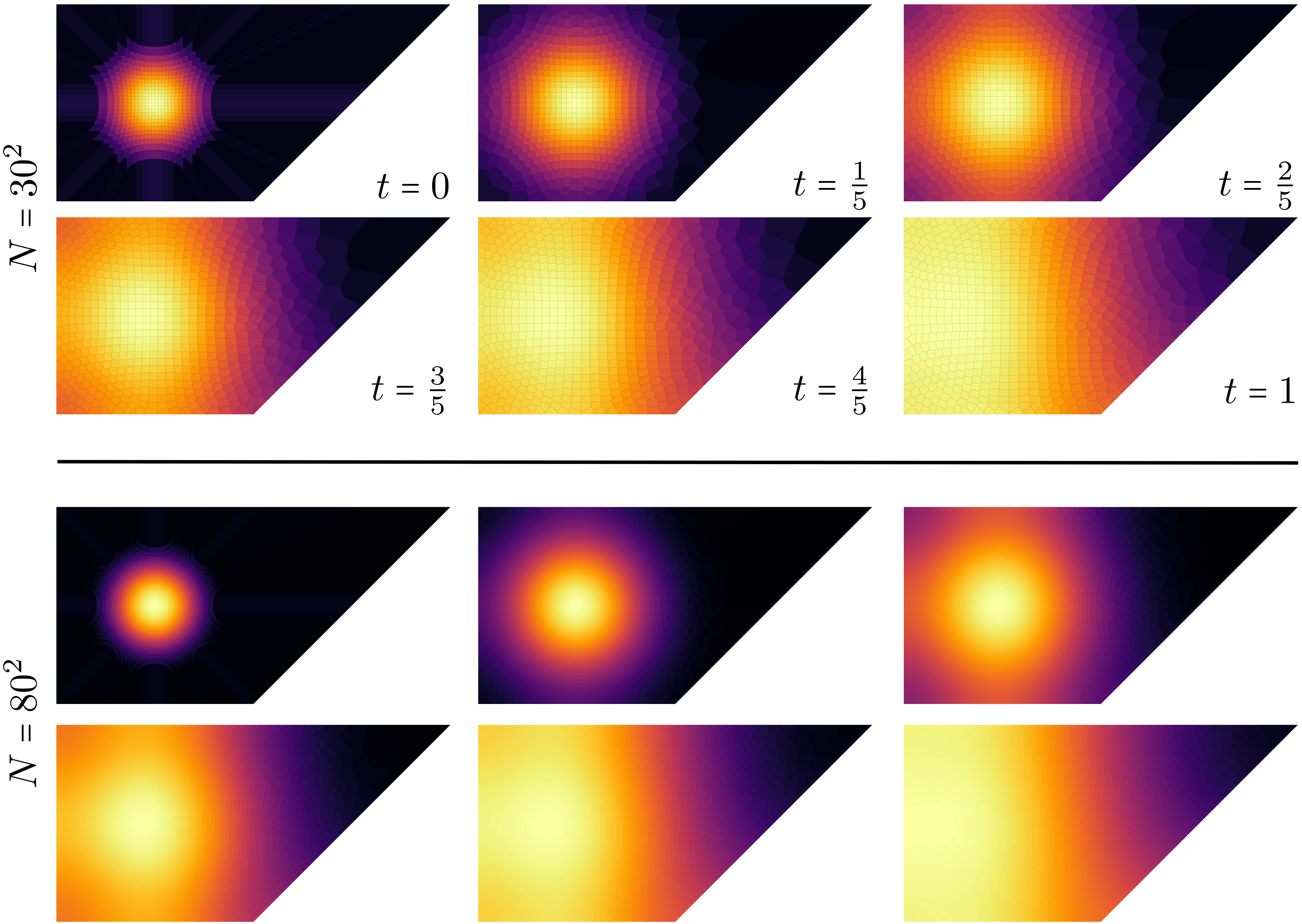
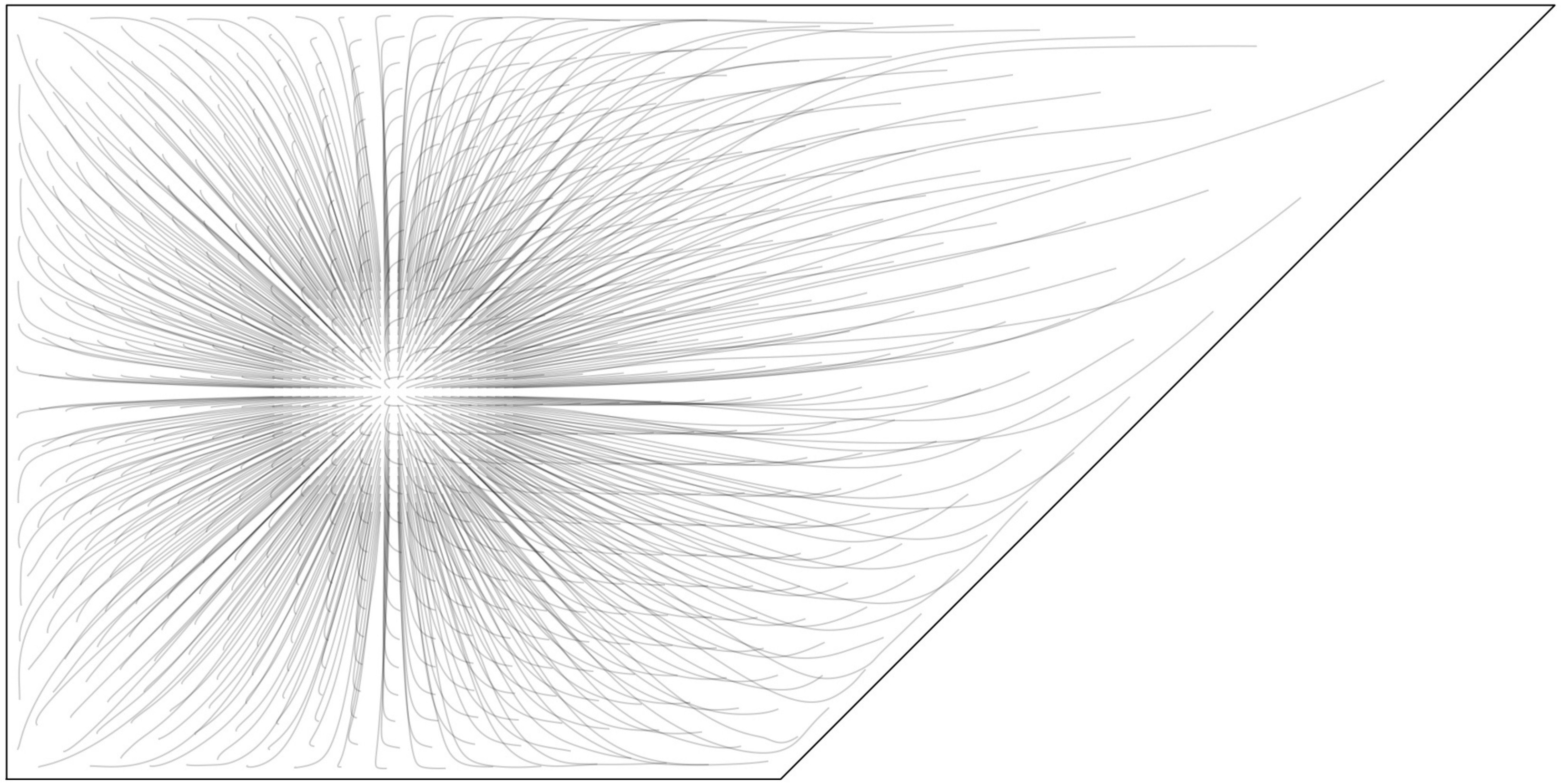
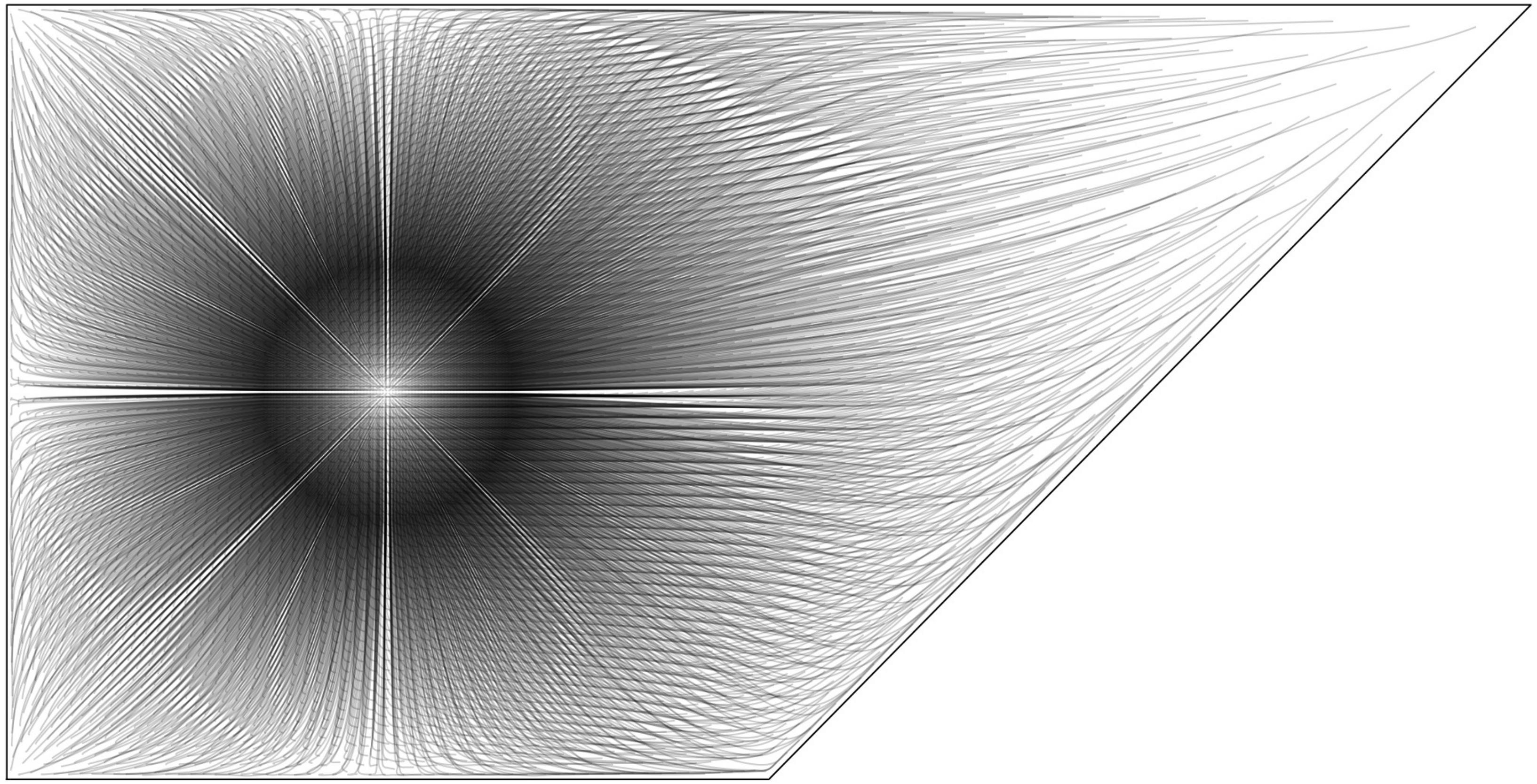


Numerical example

$N = 30^2$



$N = 80^2$



Summary

Optimal transport can be used to construct particle discretization of (some) evolution PDEs with congestion/incompressibility constraints or diffusion terms

$\boxed{\texttt{https://github.com/sd-ot}}$

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Some perspectives:

- more general models: non-linear diffusion, reaction terms (e.g. tumor growth), multiple population, surface tension, interaction forces (e.g. Keller-Segel) ?
- convergence towards Lagrangian solutions (à la [Evans-Gangbo-Savin '05]) ?
- using the ε-entropy (resp. ε-relative entropy) as regularization/data fidelity terms in statistics or inverse problems ?

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Thank you for your attention!