Optimal transport and its (semi-)discretization

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Outline

Lagrangian Formulation of (Some) PDEs

- We follow the evolution of a population of particles living in $\mathbb{R}^d$, described by its initial distribution $\rho_0 \in \mathcal{P}(\Omega)$ and by its **displacement**

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- Example of energies:

$$\mathcal{E}_{\mathrm{ent}}(\rho) = \begin{cases} \int \rho \log \rho & \text{if } \rho \in \mathcal{P}_2^{\mathrm{ac}}(\Omega), \\ +\infty & \text{otherwise.} \end{cases} \qquad \mathcal{E}_{\mathrm{inc}}(\rho) = \begin{cases} 0 & \text{if } \rho = \mathrm{Leb}_\Omega, \\ +\infty & \text{otherwise.} \end{cases}$$

$$\mathcal{E}_{\mathrm{cong}}(\rho) = \begin{cases} 0 & \text{if } \rho \leq \mathrm{Leb}_\Omega, \\ +\infty & \text{otherwise.} \end{cases} \qquad \mathcal{E}_{\mathrm{pot}}(\rho) = \int V \, d\rho.$$

Lagrangian-Eulerian dictionary

	$\dot{X} \in -\partial E(X)$	$\ddot{X} \in -\partial E(X)$
$\mathcal{E}_{\mathrm{inc}}$		incompressible Euler equation
$\mathcal{E}_{\mathrm{cong}} + \mathcal{E}_{\mathrm{pot}}$	crowd motion	pressureless Euler equation
$\mathcal{E}_{\mathrm{ent}} + \mathcal{E}_{\mathrm{pot}}$	linear Fokker-Planck equation	isentropic Euler equation

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- *Many* mathematicians have studied connections between OT and evolution PDEs.
- The energy E is typically non-convex, with values in $\mathbb{R} \cup \{+\infty\}$: in this introduction we will remain at a very formal level.

Fokker-Planck Case

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

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

From Lagrangian dynamic to the JKO scheme

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

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- We recover the JKO scheme: $\rho_\tau^{k+1} \in \arg\min_\rho \frac{1}{2\tau} \mathrm{W}_2^2(\rho_\tau^k, \rho) + \mathcal{E}(X).$

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Wasserstein distance between $\mu, \nu \in \mathcal{P}_p(\mathbb{R}^d)$:

$$\mathrm{W}_p(\mu, \nu) = \left(\min_{\gamma \in \Gamma(\mu,\nu)} \int \|x - y\|^p \, \mathrm{d}\gamma(x, y) \right)^{1/p},$$

where $\Gamma(\mu, \nu)$ is the set of *couplings* between μ, ν.

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- Optimal transport and Wasserstein distances W_p have found applications in geometry, functional inequalities, probabilities, PDEs, statistical learning.

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- T_μ is the *inverse cumulative distribution function*, also called *quantile function*.

$\mu = \frac{1}{N}\sum_{1 \le i \le N} \delta_{x_i}$ with $x_1 \le \ldots \le x_N \Longrightarrow T_\mu = x_i$ on $\left[\frac{i-1}{N}, \frac{i}{N}\right]$

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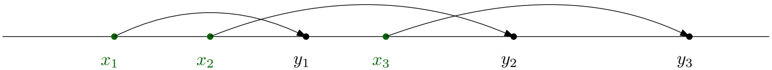

1D Wasserstein space and quantiles

- Given $\mu \in \mathcal{P}(\mathbb{R})$, there exists a unique nondecreasing $T_\mu \in \mathrm{L}^1([0,1])$ satisfying $T_{\mu\#}\lambda = \mu$, with $\lambda =$ Lebesgue measure on $[0,1]$.
- T_μ is the *inverse cumulative distribution function*, also called *quantile function*.

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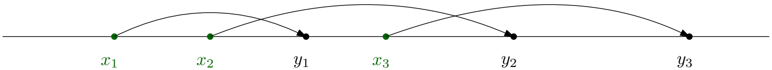

- The above formula remains true for any probability measures $\mu, \nu \in \mathcal{P}(\mathbb{R})$, i.e.

Theorem: $\mu \mapsto T_\mu$ is an isometry: $\mathrm{W}_p^p(\mu,\nu) = \|T_\mu - T_\nu\|_{\mathrm{L}^2(\lambda)}$.

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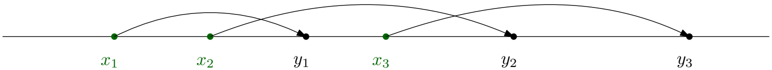

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- When μ is a density and $\nu = \sum_{i=1}^N \alpha_i\delta_{y_i}$, the optimal transport plan induces a partition (a mesh?) of $\mathrm{spt}(\mu)$ into intervals $(V_i)_{1\le i\le N}$ with $\mu(V_i) = \alpha_i$.

Wasserstein geodesics

Proposition: Let $\mu_0, \mu_1 \in \mathcal{P}_2(\mathbb{R}^d)$, and let $\gamma \in \Gamma_{\mathrm{opt}}(\mu_0, \mu_1)$. Then, the *curve*

$$\mu_t = \Pi_{t\#}\gamma, \text{ with } \Pi_t(x, y) = (1-t)x + ty$$

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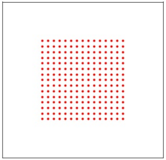

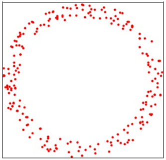

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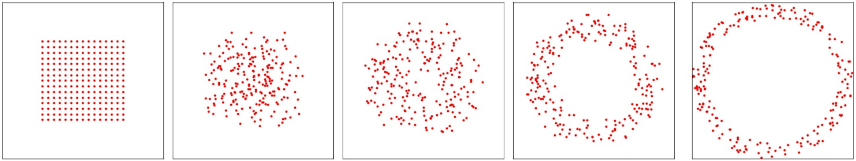

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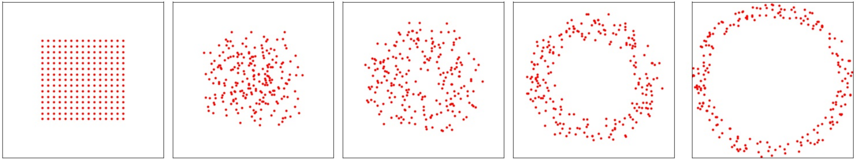

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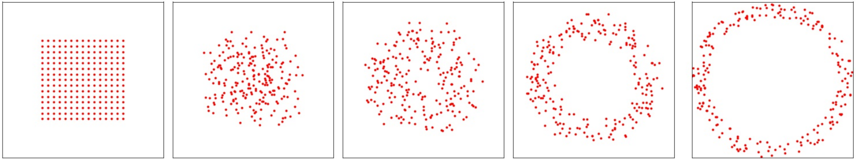
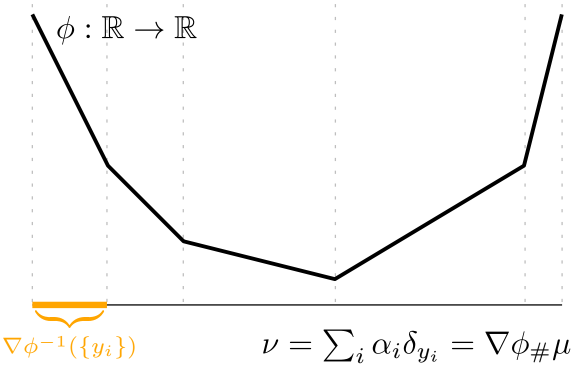


- All minimizing geodesics are of this form.
- There may exist **uncountably many geodesics**, e.g. if $\mathrm{spt}(\mu_0) \subseteq \mathbb{R} \times \{0\}$ and $\mathrm{spt}(\mu_0) \subseteq \{0\} \times \mathbb{R}$ on $\mathbb{R}^2$, any $\gamma \in \Gamma(\mu_0, \mu_1)$ is optimal!

Characterization of quadratic optimal transport

Theorem (Brenier) Let $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ with $\mu \ll \mathrm{Leb}$. Then

(i) there exists a unique map $T = \nabla\phi$, with ϕ convex, transporting μ to ν,



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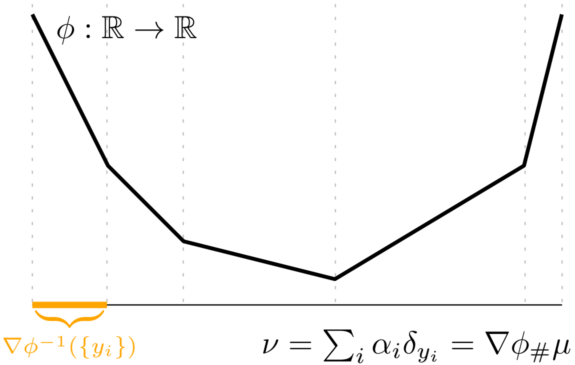

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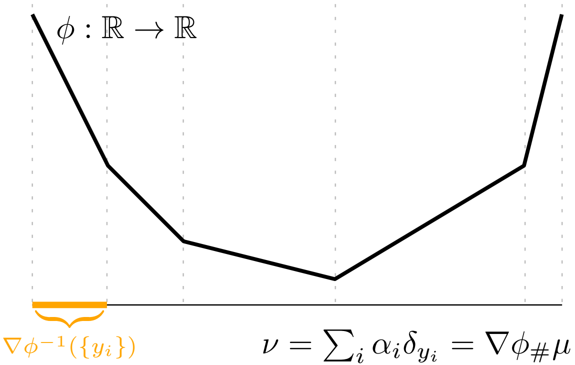

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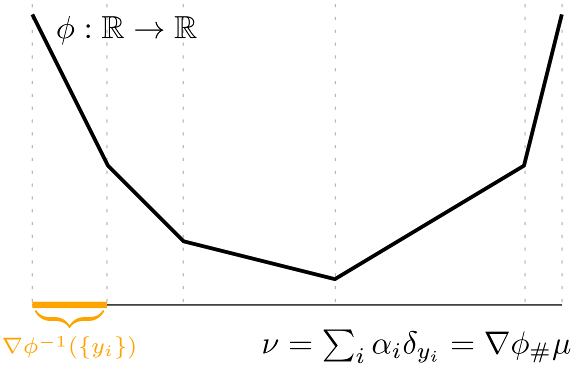

Proof relies on the dual problem to optimal transport, due to Kantorovich.

Kantorovich duality, quadratic case

- Quadratic optimal transport is equivalent to the maximal correlation problem:

$$\min_{\gamma\in\Gamma(\mu,\nu)} \int \|x-y\|^2 \,\mathrm{d}\gamma(x,y) = M_2(\mu) + M_2(\nu) - 2 \max_{\gamma\in\Gamma(\mu,\nu)} \int \langle x|y\rangle \,\mathrm{d}\gamma(x,y).$$

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Def: We will call **Kantorovich functional** $\mathcal{K}_\mu(\psi) = \int \psi^* \mathrm{d}\mu$, where ψ^* denotes the convex conjugate of ψ, i.e. $\psi^*(x) = \max_{y\in Y} \langle x|y\rangle - \psi(y)$

- Maximum correlation problem $\longleftrightarrow$ unconstrained convex minimization problem:

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- The Monge-Ampère operator is linearized (in $\phi = \psi^*$!) into :

$$\det(D^2(\phi + v)) \simeq \det(D^2\phi)(1 + \mathrm{Tr}(D^2\phi^{-1}D^2 v))$$

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- Setting $\phi = \psi^*$ and $\tilde{v} = v(\nabla\phi)$, we get

$$\left\langle D^2\mathcal{K}_\mu(\psi) v | v\right\rangle = \int \left\langle \mathrm{D}^2\phi^{-1} \cdot \nabla\tilde{v} | \nabla\tilde{v}\right\rangle \mathrm{d}\mu$$

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$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{K}_\mu(\psi_t) = -\int v(\nabla\psi_t^*)\mathrm{d}\mu.$$

Taking the time-derivative of $\nabla\psi_t^* \circ \nabla\psi_t = \mathrm{id}$, we see that

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\mathcal{K}_\mu(\psi_t) = \int \left\langle \nabla v(\nabla\psi_t^*) | D^2\psi_t^* \cdot \nabla v(\nabla\psi_t^*)\right\rangle \mathrm{d}\mu.$$

i.e. $\left\langle D^2\mathcal{K}_\mu(\psi)v | v\right\rangle = \int \left\langle \nabla v(\nabla\psi^*) | D^2\psi^* \cdot \nabla v(\nabla\psi^*)\right\rangle \mathrm{d}\mu$

- Setting $\phi = \psi^*$ and $\tilde{v} = v(\nabla\phi)$, we get

$$\left\langle D^2\mathcal{K}_\mu(\psi)v | v\right\rangle = \int \left\langle \mathrm{D}^2\phi^{-1} \cdot \nabla\tilde{v} | \nabla\tilde{v}\right\rangle \mathrm{d}\mu$$

- For $\mu \equiv 1$, a Newton method for minimizing $\mathcal{K}(\cdot) + \langle\nu|\cdot\rangle$ at ψ will involve the linear operator $\tilde{v} \mapsto \mathrm{div}((\mathrm{D}^2\psi^*)^{-1}\nabla\tilde{v})$

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Kantorovich functional and computational geometry

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$$V_i(\Psi) = \{x \in \mathbb{R}^d \mid \forall j, \langle x | y_i \rangle - \psi_i \ge \langle x | y_j \rangle - \psi_j\}.$$
- In general, y_i does **NOT** belong to its Laguerre cell $V_i(\Psi)$.

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Moreover, Ψ is $\mathcal{C}^1$ and $\partial_{y_i} \mathcal{K}_\mu(\Psi) = -\mu(V_i(\Psi))$. [Aurenhammer, Hoffman, Aronov]

$\nabla \mathrm{K}(\Psi)$ is consistent with continuous case: $\nabla \mathcal{K}(\psi) = -\nabla \psi^*_\# \mu = \sum_i \mu(V_i(\Psi)) \delta_{y_i}$.

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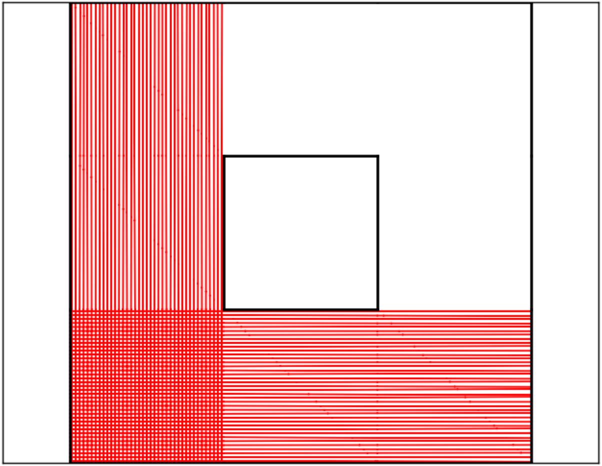
- Computing $\mathrm{D}G(\Psi)$ is as costly as computing $G \rightsquigarrow$ Newton's method

$$\boxed{\Psi^{k+1} = \Psi^k - \mathrm{D}G(\Psi^k)^{-1}(G(\Psi^k) - \nu).}$$

Difficulty: $\mathrm{D}G(\Psi^k)$ is in general not invertible $\rightsquigarrow$ damping.

Numerical example: Newton iterations



Source: Piecewise linear density on $X = [0,3]^2$ / **Target:** Uniform grid in $[0,1]^2$.

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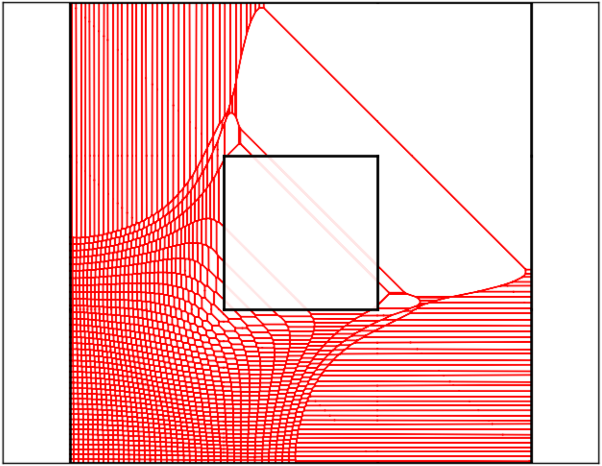

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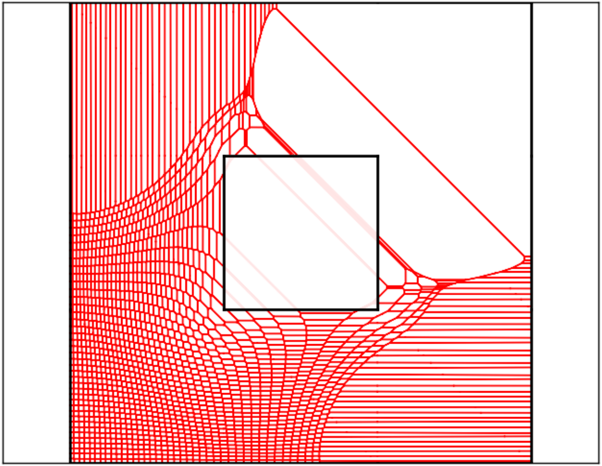

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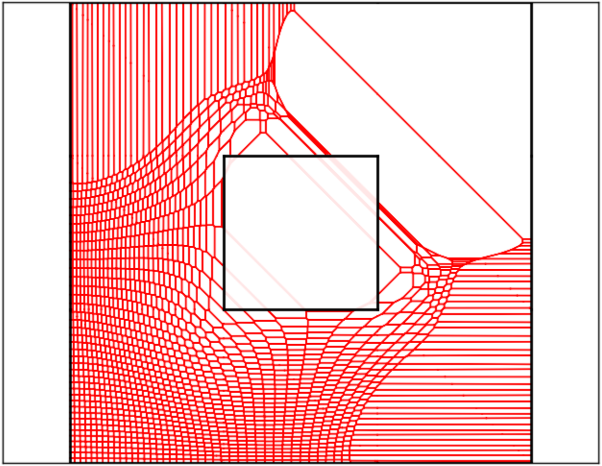

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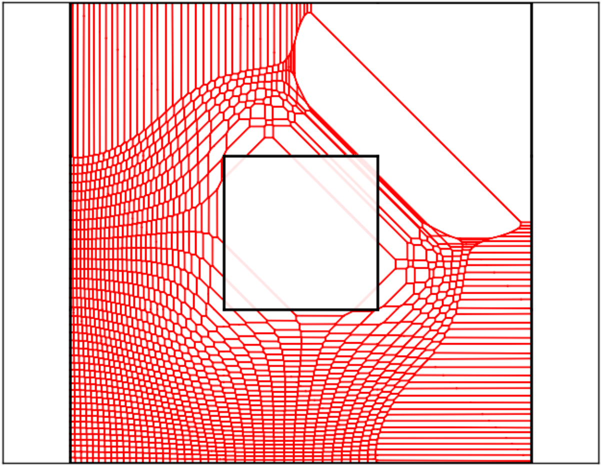

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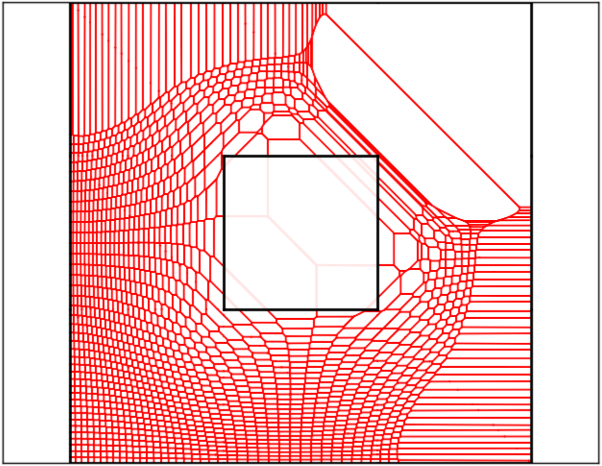

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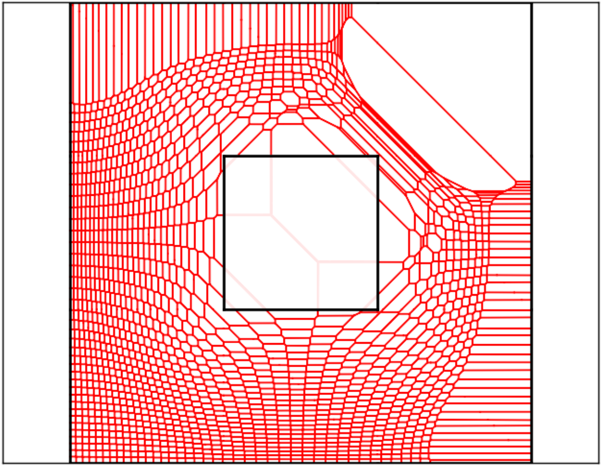

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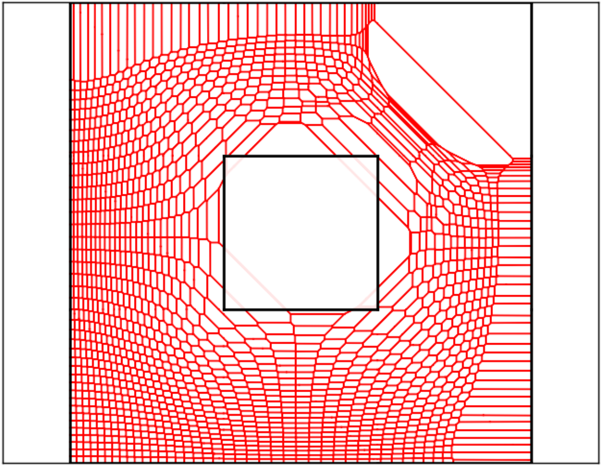

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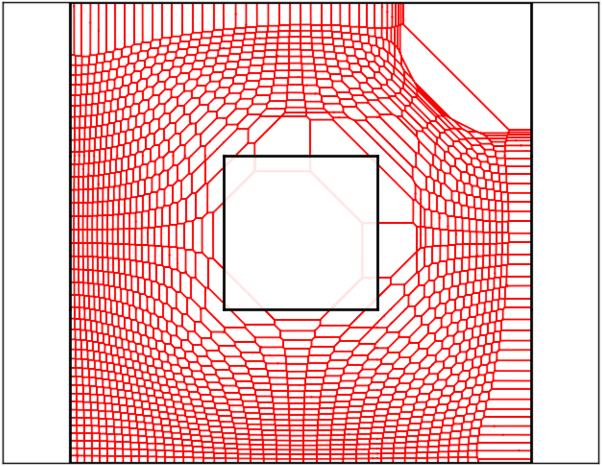

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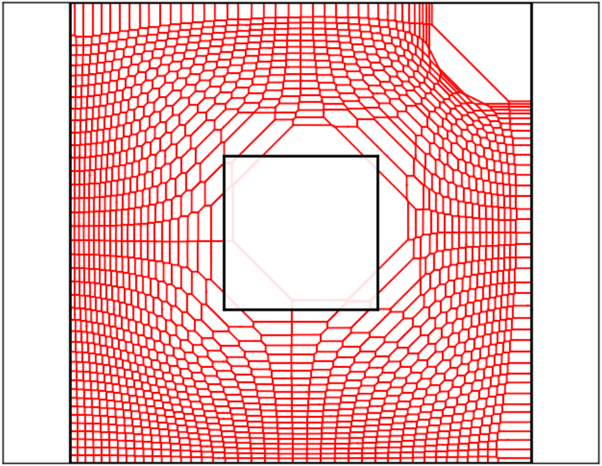

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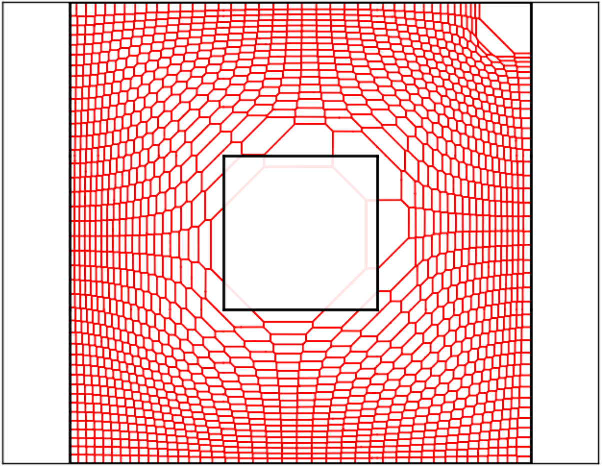

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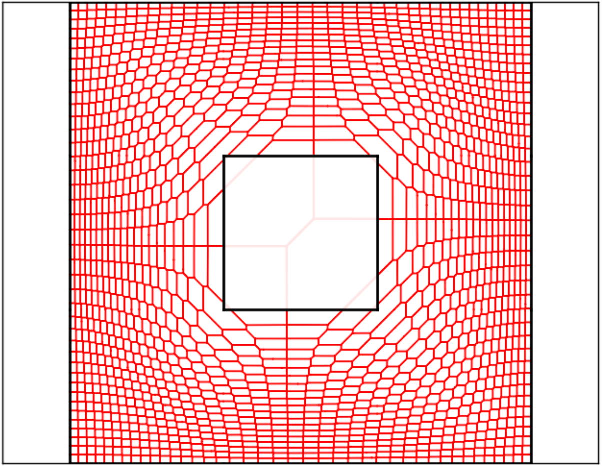

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Newton's method for semi-discrete OT is able to handle huge problems in 2D/3D, up to $N \sim 10^8$ in 3D. See e.g. Geogram (Bruno Lévy) or SDOT (Hugo Leclerc).

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Denote $G(\Psi) = -\nabla \mathcal{K}(\Psi) = (\mu(V_i(\Psi)))_{1 \leq i \leq N}$.

Prop.: Assume $\mu \in \mathcal{C}^0(X)$, X convex and $\Psi \in \mathbb{R}^N$ is such that $\forall i, G_i(\Psi) > 0$. Then,

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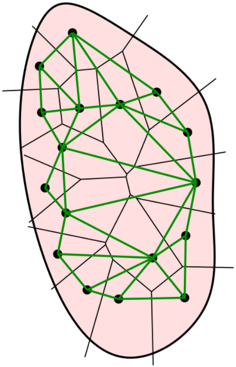

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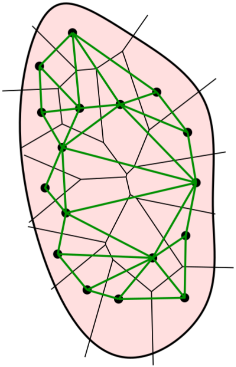

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(Estimation follows from [Eymard, Gallouët, Herbin '00])

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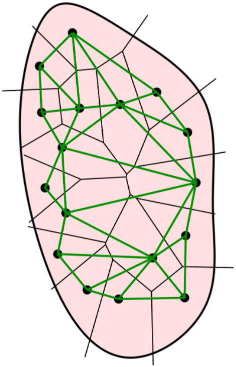

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- Finite-volume discretization of $\tilde{v} \mapsto \mathrm{div}((\mathrm{D}^2\psi^*)^{-1}\nabla\tilde{v})$?

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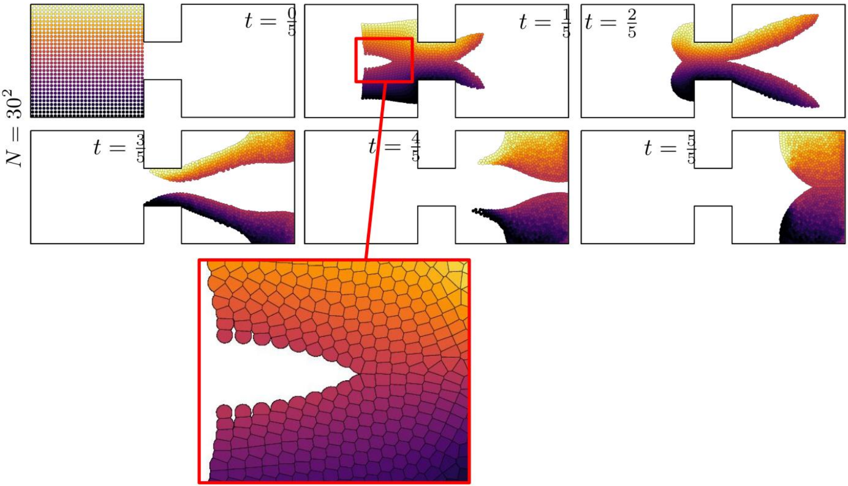
Crowd motion



- Macroscopic crowd motion model [Maury, Roudneff-Chupin, Santambrogio]
- Particle discretization relies on a Moreau-Yosida regularization of the Lagrangian energy $\mathcal{E}_{\mathrm{cong}}$ ($\rightsquigarrow$ partial optimal transport) [M., Santambrogio, Stra]
- By OT, a moving mesh is automatically associated to the moving particle cloud!

Summary/questions

- OT can be used to interpret/reformulate some PDEs from fluid mechanics.
- This leads to new Eulerian numerical schemes (which will be the main object of this workshop), but also to Lagrangian (particle) discretization of evolution PDE.

`https://github.com/sd-ot` `https://github.com/BrunoLevy/geogram`

- Can OT be useful to construct (moving) meshes for finite volumes ?