Discretization of Euler's equations for incompressible fluids through semi-discrete optimal transport.

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Joint works with Jean-Marie Mirebeau et Thomas Gallouët

Brenier60: Calculus of Variations & Optimal Transport / January 2017 / IHP

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(... and borrowing many ideas from Yann...)

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 \longrightarrow With $u_t := \dot{s_t} \circ s_t^{-1}$ (= velocity in Eulerian coordinates), one recovers **Euler's equations** for incompressible fluids:

$$\begin{cases} \partial_t u + (u \cdot \nabla)u = -\nabla p & \text{ in } X \\ \operatorname{div} u = 0 & \text{ in } X \\ u \cdot n = 0 & \text{ on } \partial X \end{cases}$$

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This talk: Using this formulation for numerical computations (following Brenier):
→ Minimizing geodesics (with Jean-Marie Mirebeau, 2015)
→ Cauchy problem (with Thomas Gallouet, 2016).

1. Discretization of the Cauchy problem

Joint work with Thomas Gallouët

$$\begin{cases} \ddot{s}(t) \perp \mathbf{T}_{s(t)} S\\ s(t) \in S\\ (s(0), \dot{s}(0)) = (s_0, v_0) \end{cases}$$

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Simple example: Take
$$S = \mathbb{R} \times \{0\} \subseteq \mathbb{R}^2$$
, $s_0 = (0, 0)$, $v_0 = (1, 0)$
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 $\rightarrow \mathcal{C}^1$ convergence towards the geodesic requires $\frac{h}{\varepsilon} \longrightarrow 0$.

Leb = restriction of Lebesgue measure to a compact domain X $S = \{s : X \to X \mid s_{\#} \text{Leb} = \text{Leb}\} \longrightarrow$ "measure-preserving maps" $M = L^2(X, \mathbb{R}^d)$

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(NB: in \mathbb{R}^d $(d \ge 2)$, each iterations costs $N^3 \dots \longrightarrow$ different approach needed)

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Polar Factorization Theorem (Brenier): For every map m in $\mathbb{M} = L^2(X, \mathbb{R}^d)$, $d_{\mathbb{S}}^2(m) = W_2^2(\text{Leb}, m_{\#}\text{Leb})$

[Brenier '92]

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

$$\Pi_{\mathbb{S}}(m) = \{ \bar{s} \in \mathbb{S} \mid \bar{T} \circ \bar{s} = m \}$$



Objective: Constructing a finite-dimensional subspace of \mathbb{M} and computing $\Pi_{\mathbb{S}}$ $\longrightarrow X$ is partitioned into $(V_k)_{1 \leq k \leq N}$ with $\operatorname{Leb}(V_k) = \frac{1}{N}$ and $\operatorname{diam}(V_k) \simeq N^{-\frac{1}{d}}$



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space-discretization:

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Theorem: Let (u, p) be a regular (e.g. $\mathcal{C}^{1,1}$) solution to Euler's equations. Then, $\forall t \in [0, T], \quad \|\dot{m}_t - u_t \circ m_t\|_{L^2(X, \mathbb{R}^d)}^2 \leq C\left(\frac{h_N^2}{\varepsilon^2} + \varepsilon^2 + h_N\right) \quad \text{w.} \quad h_N = N^{-1/d}$

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[Gallouët–M., 2016]

 $\longrightarrow \text{ Proof: Gronwall on modulated energy } E_u(t) = \frac{1}{2} \|\dot{m}_t - u_t \circ m_t\|^2 + \frac{1}{2\varepsilon^2} d_{\mathbb{S}}^2(m_t)$ (Very similar to [Brenier, CMP 2000])

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

8
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: $p(\mathbf{x}) = \frac{1}{4}(\sin^2(\pi x_1) + \sin^2(\pi x_2))$



Objectives: \longrightarrow "Large-scale" computations, with more complex behaviour. \longrightarrow Preservation of the Hamiltonian by the discrete scheme.

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A. Discontinuous initial velocity



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- B. Rayleigh-Taylor instability (Inhomogeneous fluid)



10

 $X = [-1, 1] \times [-3, 3]$ 50k particles, 2000 timesteps, $t_{\text{max}} = 2$

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2. Semi-discrete optimal transport





► If the price of bread is uniform, people go the closest bakery:

$$Vor(y) = \{ x \in X; \forall z \in Y, \ c(x,y) \le c(x,z) \}$$



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Minimizes total distance walked ... but might exceed the capacity of bakery $y_0!$



▶ If prices are given by $\psi: Y \to \mathbb{R}$, people make a compromise:

$$\operatorname{Lag}_{\psi}(y) = \{ x \in X; \forall z \in Y, \ c(x, y) + \psi(y) \le c(x, z) + \psi(z) \}$$



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Lemma: The map T_{ψ} induced by this decomposition is a *c*-optimal transport between ρ and $\nu_{\psi} := T_{\psi \#} \nu = \sum_{y \in Y} \rho(\operatorname{Lag}_{y}(\psi)) \delta_{y}.$

Theorem: Finding an **optimal transport** between ρ and $\nu = \sum_{Y} \nu_y \delta_y$

 \iff finding **prices** ψ on Y such that $\nu_{\psi} = \nu$

[Gangbo McCann '96]

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 \iff finding **prices** ψ on Y such that $\nu_{\psi} = \nu$ [Gangbo McCann '96]

 \iff maximizing the **concave** function Φ [Aurenhammer, Hoffman, Aronov '98]

 $\Phi(\psi) := \sum_{y} \int_{\operatorname{Lag}_{y}(\psi)} [c(x, y) + \psi(y)] d\rho(x) - \sum_{y} \psi(y)\nu_{y}$

Byproduct of Kantorovich duality.

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In the simulations, we use a (damped) Newton's algorithm, solving a sequence of linearized **discrete** Monge-Ampère equations.

Simple damped Newton's algorithm, with global linear convergence, [Mirebeau 15] under (rather) general assumptions on ρ and c. [Kitagawa, M., Thibert 16]

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

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Near- $\mathcal{O}(N)$ vs $\mathcal{O}(N^3)$ complexity for fully discrete (combinatorial) OT.

3. Minimizing geodesics in $\operatorname{\mathbb{S}Diff}$

Joint work with Jean-Marie Mirebeau

Let S be a submanifold in \mathbb{R}^d , whose minimizing geodesics need to be approximated.

 $\blacktriangleright \text{ Minimizing geodesics: } \min_{s:[0,1] \to \mathbb{R}^d} \frac{1}{2} \int_0^1 \|\dot{s}_t\|^2 \, \mathrm{d} t \quad \text{where } \begin{cases} \forall t \in [0,1], \ s_t \in S \\ s_0 = s_*, s_1 = s^* \end{cases}$

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- **Relaxation:** Given a penalization parameter $\alpha > 0$, consider

$$\min_{m:[0,1]\to\mathbb{R}^d} \frac{1}{2} \int_0^1 \|\dot{m}_t\|^2 \,\mathrm{d}\,t + \alpha \left(\int_{[0,1]} \mathrm{d}_S^2(m_t) \,\mathrm{d}\,t + \|m_0 - s_*\|^2 + \|m_1 - s^*\|^2 \right)$$

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• **Time-discretization:** Given a number of timesteps $T \in \mathbb{N}$, consider

$$\min_{m_1,\dots,m_T \in \mathbb{R}^d} \frac{T}{2} \sum_{i=0}^{T-1} \|m_{i+1} - m_i\|^2 + \lambda \left(\sum_{i=1}^{T-1} \mathrm{d}_S^2(m_i) + \|m_0 - s_*\|^2 + \|m_T - s^*\|^2 \right)$$

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Imagine now that only a finite sample $S_K \subseteq S$ is known, with $Card(S_K) = K$. \longrightarrow How should $\lambda = \lambda(T, K)$ be chosen ?

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 \rightarrow combinatorial optimization pb (when $\lambda = +\infty$)

 λ too large \longrightarrow low-order approximation

Leb = restriction of Lebesgue measure to a compact domain X

 $\mathbb{SDiff} = \{s : X \to X \text{ diffeomorphism } | s_{\#} \text{Leb} = \text{Leb}\} \subseteq \mathbb{M} = L^2(X, \mathbb{R}^d)$

The endpoints s_* and s^* of the geodesic are two (fixed) elements in SDiff.

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C. relaxation involving measures over the set Γ of C^0 paths in X. [Brenier '89] [Schinerelman '94]
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Numerics: mostly in 1D using permutations

[Brenier '87, Brenier-Roesch '98]



► Time-discretization of geodesic with endpoints $s_*, s^* \in \mathbb{S}$ $\mathcal{E}_{N,T,\lambda} : (\mathbb{M}_N)^T \to \mathbb{R}$,

$$\mathcal{E}_{N,T,\lambda}(m) := \frac{T}{2} \sum_{i=0}^{T-1} \|m_{i+1} - m_i\|_2^2 + \lambda \left(\|m_0 - s_*\|_2^2 + \|m_T - s^*\|_2^2 + \sum_{i=1}^{T-1} \mathrm{d}_{\mathbb{S}}^2(m_i) \right)$$

action

boundary conditions

incompressibility



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Then, with
$$\mu_m = \frac{1}{N} \sum_{k=1}^N \delta_{\gamma_k} \in \operatorname{Prob}(\Gamma)$$
,

$$\begin{aligned} \mathcal{E}_{N,T,\lambda}(m) &= \mathcal{E}(\mu_m) \\ &+ \lambda \sum_{i=1}^T W_2^2(e_{t_i \#} \mu_m, \text{Leb}) \\ &+ \text{boundary cond.} \end{aligned}$$



► Time-discretization of geodesic with endpoints $s_*, s^* \in \mathbb{S}$ $\mathcal{E}_{N,T,\lambda} : (\mathbb{M}_N)^T \to \mathbb{R}$,

$$\mathcal{E}_{N,T,\lambda}(m) := \frac{T}{2} \sum_{i=0}^{T-1} \|m_{i+1} - m_i\|_2^2 + \lambda \left(\|m_0 - s_*\|_2^2 + \|m_T - s^*\|_2^2 + \sum_{i=1}^{T-1} \mathrm{d}_{\mathbb{S}}^2(m_i) \right)$$

• Given $m = (m_1, \ldots, m_T) \in \mathbb{M}_N^T$, let $\gamma_k \in \mathcal{C}^0([0, 1], \mathbb{R}^d)$ be PL with $\gamma_k(t_i) = m_i(V_k)$



Then, with
$$\mu_m = \frac{1}{N} \sum_{k=1}^N \delta_{\gamma_k} \in \operatorname{Prob}(\Gamma)$$
,

$$\mathcal{E}_{N,T,\lambda}(\boldsymbol{m}) = \mathcal{E}(\boldsymbol{\mu}_{\boldsymbol{m}}) + \lambda \sum_{i=1}^{T} W_2^2(e_{t_i \#} \boldsymbol{\mu}_{\boldsymbol{m}}, \text{Leb})$$

+ boundary cond.

 \rightarrow \simeq Common discretization for both relaxations! \rightarrow Choice of penalization parameter?

Regular generalized geodesic: a probability measure $\mu \in \operatorname{Prob}(\Gamma)$ s.t. (Regularity) $\exists p$ with Lipschitz gradient s.t. $\forall \gamma \in \operatorname{spt}(\mu), \quad \ddot{\gamma} = -\nabla p \circ \gamma,$ (Incompressibility) $e_{t\#}\mu = \operatorname{Leb}$ for all t(Boundary conditions) $(e_0, e_1)_{\#}\operatorname{Leb} = (s_*, s^*)_{\#}\operatorname{Leb}$

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Theorem: Let μ be a regular generalized geodesic in SDiff between s_* and s^* ,

 $m_N \in \arg \min \mathcal{E}_{N,T_N,\lambda_N}$ with $\lambda_N = N^{2d}$ and $T_N \lambda_N \to 0$,

Then, up to subsequences, $\mu_{m_N} \in \operatorname{Prob}(\Gamma)$ converges weakly to a minimizing generalized geodesic between s_* and s^* .

[Mirebeau-M., 2015]

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 $\begin{array}{ll} \text{Main step: } \limsup_N \mathcal{E}_{N,T_N,\lambda_N}(m_N) \leq \mathcal{E}(\mu^{\text{opt}}). \end{array} \\ \text{more precisely, we need} \quad \min_{m \in \mathbb{M}_N^T} \mathcal{E}_{N,T,\lambda}(m) \leq \mathcal{E}(\mu^{\text{opt}}) + \mathcal{O}(Th_N^2\lambda) \end{array} \end{array}$

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It turns out that one can take D := dim(spt(μ^{opt}))
→ For a classical solution s : [0,1] → S, dim(spt(μ^{opt})) = d. (λ_N = N^d)
→ For a regular generalized solution, dim(spt(μ^{opt})) ≤ 2d. (λ_N = N^{2d})

Energy estimate for classical solutions

Proposition: Assume that the minimizing geodesic s between s_* and s^* is classical and that $s \in L^{\infty}([0,1], H^1(X))$. Then, with $h_N = N^{-1/d}$,

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Then, $\mathcal{E}_{N,T,\lambda}(m)$ is upper bounded using the Poincaré-Wirtinger inequality.



Prop: Assume that the generalized minimizing geodesic in Π is associated to a pressure $p: [0,1] \times \Omega \to \mathbb{R}$ with Lipschitz gradient. Then, with $h_N = N^{-1/2d}$,

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$$X = B(0,1) \subseteq \mathbb{R}^2 \qquad (s_*,s^*) = (\mathrm{id},-\mathrm{id})$$

Classical solutions: clockwise/counterclockwise rotations μ_{\pm}



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Examples of generalized solutions:

linear combination $\mu_{\frac{1}{2}}$ of μ_{\pm} constructed from rotations NB: dim $(spt(\mu_{\frac{1}{2}})) = 2$



Brenier's generalized solution: $\mu \in \operatorname{Prob}(\Gamma)$:

$$\operatorname{spt}(\mu) = \{t \mapsto x \cos(\pi t) + v \sin(\pi t) \in \Gamma; \\ (x, v) \in X \times \mathbb{R}^2, \|v\|^2 = 1 - \|x\|^2\}$$

 \longrightarrow non-deterministic solution, $\dim(\operatorname{spt}(\mu)) = 3$





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Computed trajectories for $N = 10^5$, T = 17



Numerical result: Beltrami Flow in Square

Stationary flow on $[0,1]^2$:speed: $u(\mathbf{x}) = (\cos(\pi x_1)\sin(\pi x_2), \sin(\pi x_1)\cos(\pi x_2))$ [Brenier-Roesch]pressure: $p(\mathbf{x}) = \frac{1}{4}(\sin^2(\pi x_1) + \sin^2(\pi x_2))$



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Exact Lagrangian solution: $s_0^e = \text{id}$ $\dot{s}_t^e = u \circ s_t$

NB: s^e is minimizing on [0, 1]

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Reconstruction problem:

 $\min \mathcal{E}_{N,T,\lambda}$ $s_* = s_0^e$, $s^* = s_{t_{\max}}^e$
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Parameters:

 $t_{\max} \in \{0.9, 1.1, 1.3, 1.5\}$

Numerical result: Beltrami Flow in Square



NB: qualitatively similar results by Luca Nenna and J.D. Benamou

Numerical result: Comparison of Trajectories



Square, $t_{\rm max} = 1.5$

Comparison of Minkowski dimensions

Minkowski dimension Let $S \subseteq \Gamma$ be a compact subset of a metric space.

 $\overline{\dim}(S) = \limsup_{N \to \infty} \log(N) / \log(1/\delta_N)$

where $\delta_N = \text{minimum radius required to cover } S$ with N balls.

Estimation of dim(spt(μ)) via log(N)/log($1/\delta_N$)



Perspectives

- A) More realistic numerical schemes for the Cauchy problem (e.g. without ε)?
- B) Changing the polar factorization theorem \rightarrow other fluid models, e.g. fluid-structure interactions / Camassa-Holm equation [Gallouet-Vialard 16], pressureless Euler equation with congestion [Maury-Preux '15]

C) Viscosity?

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[Arnold 1966]



$$\rightarrow T_{id} SDiff = divergence-free vector fields$$

$$= \{ \nabla p \mid p : X \to \mathbb{R} \}^{\perp}$$

 \longrightarrow Formally, a path $s : [0, 1] \rightarrow \mathbb{SDiff}$ is a **geodesic** iff $\ddot{s}_t \perp T_{s_t} \mathbb{SDiff}$

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 $\iff \exists p: [0,1] \times X \to \mathbb{R}, \ddot{s}_t = -\nabla p_t \circ s_t$

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 $\begin{array}{l} \longrightarrow \text{ Formally, a path } s: [0,1] \rightarrow \mathbb{S}\text{Diff is a geodesic iff} \\ \ddot{s}_t \perp \mathrm{T}_{s_t} \mathbb{S}\text{Diff} & \Longleftrightarrow \ddot{s}_t \circ s_t^{-1} \perp \mathrm{T}_{\mathrm{id}} \mathbb{S}\text{Diff} \\ & \Longleftrightarrow \exists t : [0,1] \times X \rightarrow \mathbb{R}, \\ \ddot{s}_t = -\nabla p_t \circ s_t \end{array}$

 \longrightarrow With $u_t := \dot{s_t} \circ s_t^{-1}$ (= velocity in Eulerian coordinates), one recovers **Euler's equations** for incompressible fluids:

$$\begin{cases} \partial_t u + (u \cdot \nabla)u = -\nabla p & \text{ in } X \\ \operatorname{div} u = 0 & \text{ in } X \\ u \cdot n = 0 & \text{ on } \partial X \end{cases}$$

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Use this formulation for numerical computations (following Brenier): \longrightarrow Minimizing geodesics (with Jean-Marie Mirebeau, 2015) \longrightarrow Cauchy problem (with Thomas Gallouet, 2016).