Computational optimal transport: recent speed-ups and applications

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Machine Learning in Infinite Dimensions, Bath

Who am I?

Background in **mathematics** and **data sciences**:

- **2012–2016** ENS Paris, mathematics.
- **2014–2015** M2 mathematics, vision, learning at ENS Cachan.
- **2016–2019** PhD thesis in **medical imaging** with Alain Trouvé at ENS Cachan.
- **2019–2021** **Geometric deep learning** with Michael Bronstein at Imperial College.
- **2021+** **Medical data analysis** in the HeKA INRIA team (Paris).

HeKA : a translational research team for public health

Hôpitaux

Inria

Inserm

Universités

My main motivation

Develop **robust and efficient** software that **stimulates other researchers**:

1. Speed up **geometric machine learning** on GPUs:
   $\Longrightarrow$ **pyKeOps** library for distance and kernel matrices, 600k+ downloads.
2. Scale up **pharmacovigilance** to the full French population:
   $\Longrightarrow$ **survivalGPU**, a fast re-implementation of the R survival package.
3. Ease access to modern statistical **shape analysis**:
   $\Longrightarrow$ **GeomLoss**, truly scalable optimal transport in Python.
   $\Longrightarrow$ **scikit-shapes**, alpha release now available.

Today’s talk – assuming that you would enjoy some nice simulations

1. A quick heads up on **fast geometric methods**.
2. Efficient discrete optimal transport **solvers**.
3. New applications for systems of **incompressible particles**.

How to code a N-body simulation?

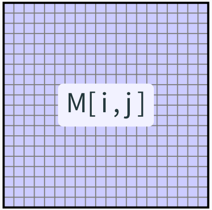
Scientific computing libraries represent most objects as tensors

Context. Constrained **memory accesses** on the GPU:

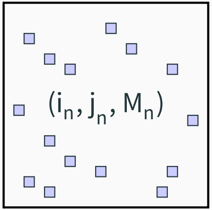
- **Long access times** to the registers penalize the use of large **dense** arrays.
- Hard-wired **contiguous** memory accesses penalize the use of **sparse** matrices.

Challenge. In order to reach optimal run times:

- **Restrict** ourselves to operations that are supported by the constructor: convolutions, FFT, etc.
- Develop new routines from scratch in C++/CUDA (FAISS, KPConv…): **several months of work**.



Dense array



Sparse matrix

The KeOps library: efficient support for symbolic matrices

Solution. KeOps – `www.kernel-operations.io`:

- For PyTorch, NumPy, Matlab and R, on **CPU and GPU**.
- **Automatic differentiation**.
- Just-in-time **compilation** of **optimized** C++ schemes, triggered for every new **reduction**: sum, min, etc.

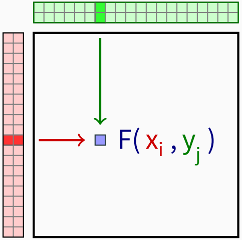
If the formula "F" is simple ($\leqslant$ 100 arithmetic operations):

"100k $\times$ 100k" computation $\rightarrow$ 10ms – 100ms,

"1M $\times$ 1M" computation $\rightarrow$ 1s – 10s.

Hardware ceiling of 10^{12} operations/s.

$\times$**10 to** $\times$**100 speed-up** vs standard GPU implementations for a wide range of problems.



Symbolic matrix

Formula + data

- Distances $d(x_i, y_j)$.
- Kernel $k(x_i, y_j)$.
- Numerous transforms.

A first example: efficient nearest neighbor search in dimension 50

Create large point clouds using **standard PyTorch syntax**:

```
import torch
N, M, D = 10**6, 10**6, 50
x = torch.rand(N, 1, D).cuda()  # (1M,  1, 50) array
y = torch.rand(1, M, D).cuda()  # ( 1, 1M, 50) array
```

Turn **dense** arrays into **symbolic** matrices:

```
from pykeops.torch import LazyTensor
x_i, y_j = LazyTensor(x), LazyTensor(y)
```

Create a large **symbolic matrix** of squared distances:

```
D_ij = ((x_i - y_j) ** 2).sum(dim=2)  # (1M, 1M) symbolic
```

Use an `.argmin()` **reduction** to perform a nearest neighbor query:

```
indices_i = D_ij.argmin(dim=1)  # -> standard torch tensor
```

The KeOps library combines performance with flexibility

Script of the previous slide = efficient nearest neighbor query,
on par with the bruteforce CUDA scheme of the **FAISS** library…
And can be used with **any metric**!

```
D_ij = ((x_i - x_j) ** 2).sum(dim=2)      # Euclidean
M_ij =  (x_i - x_j).abs().sum(dim=2)      # Manhattan
C_ij = 1 - (x_i | x_j)                    # Cosine
H_ij = D_ij / (x_i[...,0] * x_j[...,0])  # Hyperbolic
```

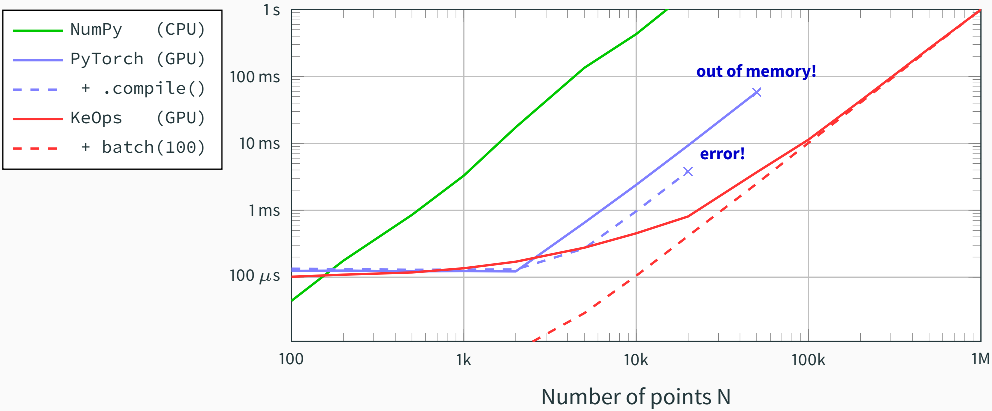
KeOps supports arbitrary **formulas** and **variables** with:

- **Reductions:** sum, log-sum-exp, K-min, matrix-vector product, etc.
- **Operations:** $+$, $\times$, sqrt, exp, neural networks, etc.
- **Advanced schemes:** batch processing, block sparsity, etc.
- **Automatic differentiation:** seamless integration with PyTorch.

KeOps lets users work with millions of points at a time

Benchmark of a Gaussian **convolution** $a_i \leftarrow \sum_{j=1}^{N} \exp(-\|x_i - y_j\|^2_{\mathbb{R}^3})\, b_j$

between **clouds of N 3D points** on a A100 GPU.



Yet another ML compiler?

Many impressive tools out there (Taichi, Numba, Triton, Halide...):

- Focus on **generality** (software + hardware).
- Increasingly easy to use via e.g. PyTorch 2.0.

KeOps fills a different niche (a bit like cuFFT, FFTW...):

- Focus on a **single major bottleneck**: geometric interactions.
- **Agnostic** with respect to Euclidean / non-Euclidean formulas.
- Fully compatible with PyTorch, NumPy, R.
- Can actually be **used by mathematicians**.

KeOps is a **bridge** between geometers (with a maths background)
and compiler experts (with a CS background).

Optimal transport?

Optimal transport (OT) generalizes sorting to spaces of dimension $D > 1$

If $A = (x_1, \dots, x_N)$ and $B = (y_1, \dots, y_N)$ are two clouds of N points in $\mathbb{R}^D$, we define:

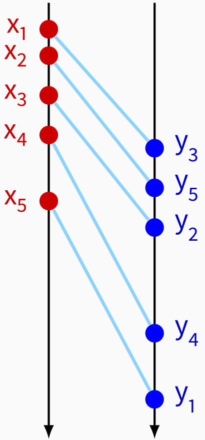
$$\text{OT}(A, B) = \min_{\sigma \in \mathcal{S}_N} \frac{1}{2N} \sum_{i=1}^{N} \| x_i - y_{\sigma(i)} \|^2$$

Generalizes **sorting** to metric spaces.

Linear problem on the permutation matrix P:

$$\text{OT}(A, B) = \min_{P \in \mathbb{R}^{N \times N}} \frac{1}{2N} \sum_{i,j=1}^{N} P_{i,j} \cdot \| x_i - y_j \|^2 ,$$

$$\text{s.t.} \quad P_{i,j} \geqslant 0 \qquad \underbrace{\textstyle\sum_j P_{i,j} = 1}_{\text{Each source point...}} \qquad \underbrace{\textstyle\sum_i P_{i,j} = 1}_{\text{is transported onto the target.}} .$$



assignment

$\sigma : [\![1, 5]\!] \to [\![1, 5]\!]$

Practical use

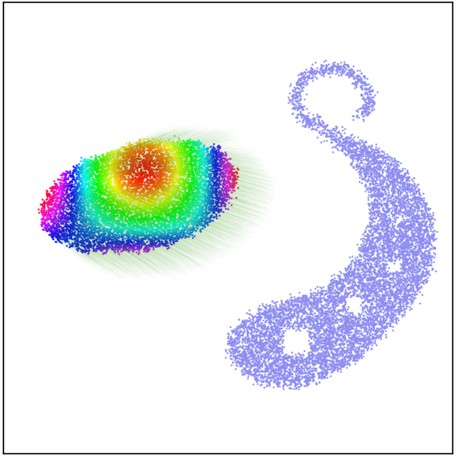
Alternatively, we understand OT as:

- Nearest neighbor **projection** + **incompressibility** constraint.
- Fundamental example of **linear optimization** over the transport plan $\mathrm{P}_{i,j}$.

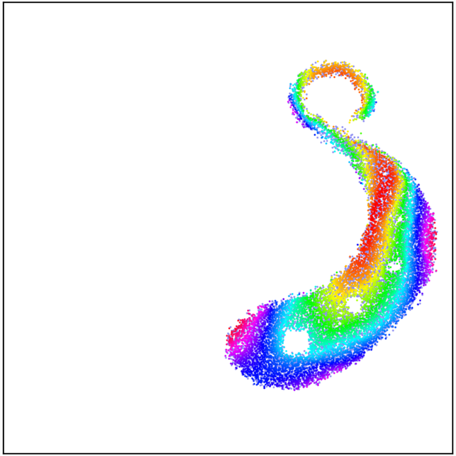
This theory induces two main quantities:

- The transport plan $\mathrm{P}_{i,j} \simeq$ the optimal mapping $x_i \mapsto y_{\sigma(i)}$.
- The "Wasserstein" distance $\sqrt{\mathrm{OT}(\mathrm{A}, \mathrm{B})}$.

The optimal transport plan

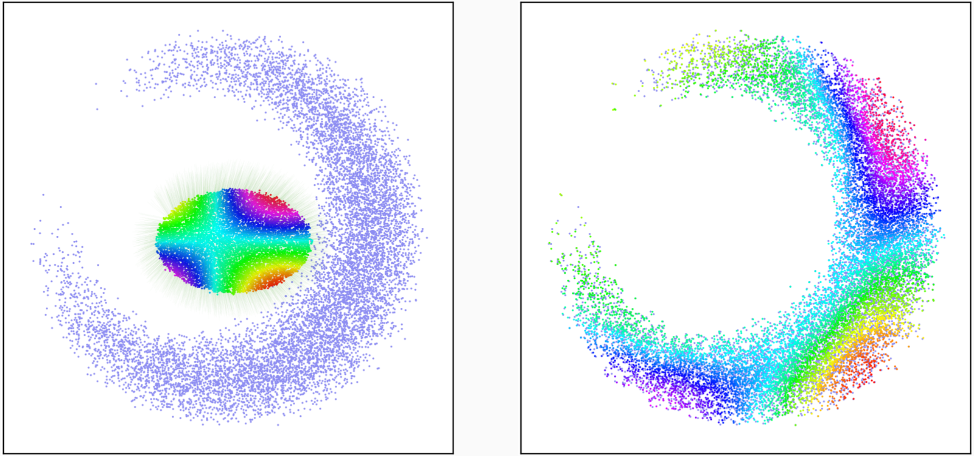


Before



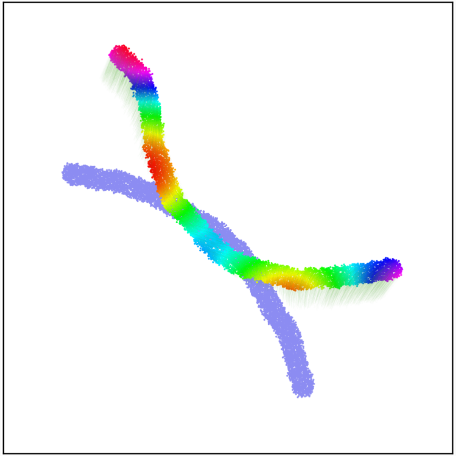
After

The optimal transport plan



Before After

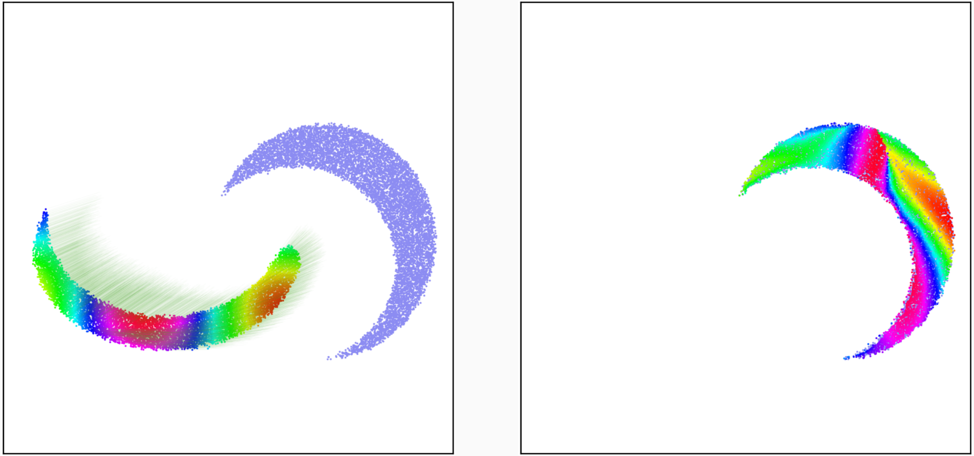
The optimal transport plan



Before

After

The optimal transport plan

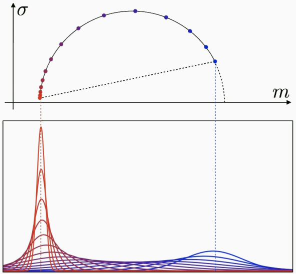


Before | After

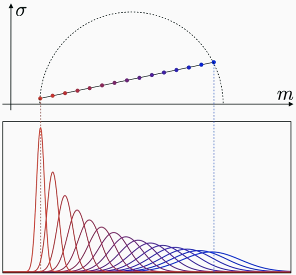
OT induces a geometry-aware distance between probability distributions [PC18]

Gauss map $\quad \mathcal{N} : (m, \sigma) \in \mathbb{R} \times \mathbb{R}_{\geqslant 0} \quad \mapsto \quad \mathcal{N}(m, \sigma) \in \mathbb{P}(\mathbb{R}).$

If the space of **probability distributions** $\mathbb{P}(\mathbb{R})$ is endowed with a given metric, what is the “pull-back” geometry on the space of **parameters** (m, σ)?



Fisher-Rao ($\simeq$ relative entropy) on $\mathcal{N}(m, \sigma)$
$\rightarrow$ Hyperbolic **Poincaré** metric on (m, σ).



OT on $\mathcal{N}(m, \sigma)$
$\rightarrow$ Flat **Euclidean** metric on (m, σ).

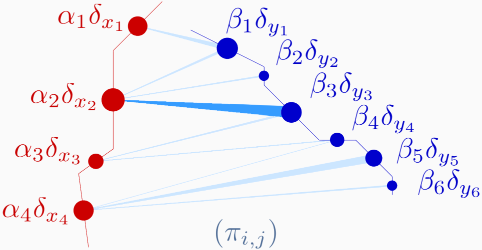
How to solve the OT problem?

Duality: central planning with NM variables $\simeq$ outsourcing with N + M variables

$$\mathrm{OT}(A, B) = \min_{\pi} \langle \pi , C \rangle, \text{ with } C(x_i, y_j) = \frac{1}{p}\|x_i - y_j\|^p \longrightarrow \text{Assignment}$$

$$\text{s.t. } \pi \geqslant 0, \quad \pi \mathbf{1} = A, \quad \pi^\top \mathbf{1} = B$$

$\sum_{i,j} \pi_{i,j} \, C(x_i, y_j)$

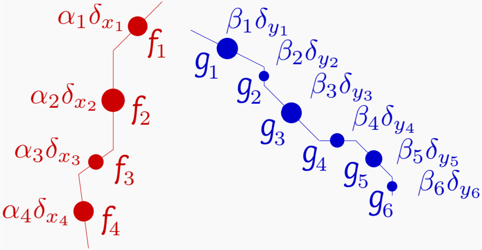


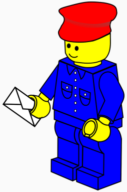
Duality: central planning with NM variables $\simeq$ outsourcing with N + M variables

$$\mathrm{OT}(\mathrm{A},\mathrm{B}) \;=\; \min_{\pi}\, \langle\, \pi\,,\, \mathrm{C}\,\rangle, \;\; \text{with } \mathrm{C}(x_i, y_j) \;=\; \tfrac{1}{p}\|x_i - y_j\|^p \qquad \longrightarrow \;\; \text{Assignment}$$

$$\text{s.t. } \pi \geqslant 0, \qquad \pi\,\mathbf{1} = \mathrm{A}, \qquad \pi^{\top}\mathbf{1} = \mathrm{B}$$

$\sum_{i,j} \pi_{i,j}\, \mathrm{C}(x_i, y_j)$





$\sum_i \alpha_i f_i + \sum_j \beta_j g_j$

$\longrightarrow$ FedEx

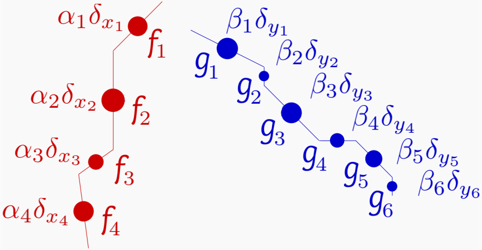
$$\max_{f\,,\,g} \quad \langle\, \mathrm{A}\,,\, f\,\rangle \,+\, \langle\, \mathrm{B}\,,\, g\,\rangle$$

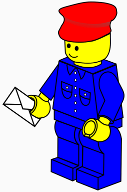
$$\text{s.t.} \quad f(x_i) \,+\, g(y_j) \,\leqslant\, \mathrm{C}(x_i, y_j),$$

Duality: central planning with NM variables $\simeq$ outsourcing with N + M variables

$$\mathrm{OT}(\mathsf{A},\mathsf{B}) = \min_{\pi} \langle \pi , \mathsf{C} \rangle, \text{ with } \mathsf{C}(x_i, y_j) = \tfrac{1}{p}\|x_i - y_j\|^p \quad \longrightarrow \quad \text{Assignment}$$

$$\text{s.t. } \pi \geqslant 0, \quad \pi \mathbf{1} = \mathsf{A}, \quad \pi^\top \mathbf{1} = \mathsf{B}$$





$\sum_{i,j} \pi_{i,j} \mathsf{C}(x_i, y_j)$

$\sum_i \alpha_i f_i + \sum_j \beta_j g_j$

$$= \max_{f,g} \quad \langle \mathsf{A} , f \rangle + \langle \mathsf{B} , g \rangle \quad \longrightarrow \quad \text{FedEx}$$

$$\text{s.t.} \quad f(x_i) + g(y_j) \leqslant \mathsf{C}(x_i, y_j),$$

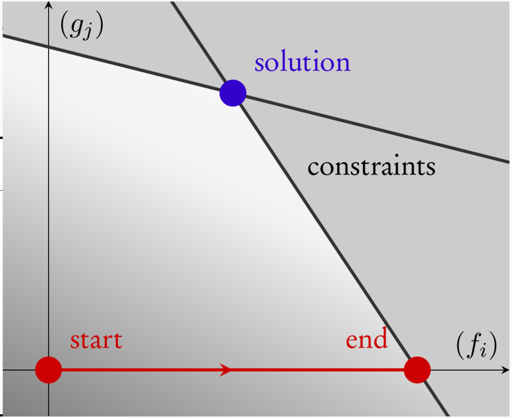
Being too greedy... doesn't work!

$$\mathrm{OT}(\alpha,\beta) = \max_{\substack{(f_i)\in\mathbb{R}^{\mathrm{N}} \\ (g_j)\in\mathbb{R}^{\mathrm{M}}}} \sum_{i=1}^{\mathrm{N}} \alpha_i f_i + \sum_{j=1}^{\mathrm{M}} \beta_j g_j$$

$$\text{s.t. } \forall\, i, j,\ f_i + g_j \leqslant \mathbf{C}(x_i, y_j)$$

Algorithm 3.1: Naive greedy algorithm

1: $f_i,\ g_j \leftarrow \mathbf{0}_{\mathbb{R}^{\mathrm{N}}},\ \mathbf{0}_{\mathbb{R}^{\mathrm{M}}}$
2: **repeat**
3: $\quad f_i \leftarrow \min_{j=1}^{\mathrm{M}} \left[\, \mathbf{C}(x_i, y_j) - g_j \,\right]$
4: $\quad g_j \leftarrow \min_{i=1}^{\mathrm{N}} \left[\, \mathbf{C}(x_i, y_j) - f_i \,\right]$
5: **until** convergence.
6: **return** $f_i,\ g_j$



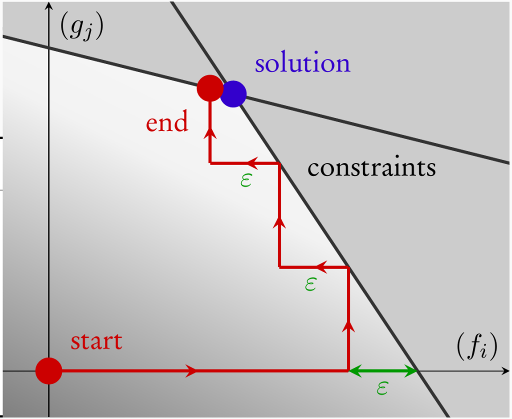
The auction algorithm: take it easy with a slackness $\varepsilon > 0$

$$\mathrm{OT}(\alpha,\beta) = \max_{\substack{(f_i)\in\mathbb{R}^{\mathrm{N}}\\(g_j)\in\mathbb{R}^{\mathrm{M}}}} \sum_{i=1}^{\mathrm{N}} \alpha_i f_i + \sum_{j=1}^{\mathrm{M}} \beta_j g_j$$

$$\text{s.t. } \forall\, i,j,\ f_i + g_j \leqslant \mathbf{C}(x_i,y_j)$$

Algorithm 3.2: Pseudo-auction algorithm

1: $f_i,\ g_j \leftarrow \mathbf{0}_{\mathbb{R}^{\mathrm{N}}},\ \mathbf{0}_{\mathbb{R}^{\mathrm{M}}}$
2: **repeat**
3: $\quad f_i \leftarrow \min_{j=1}^{\mathrm{M}} \left[\,\mathbf{C}(x_i,y_j) - g_j\,\right] - \varepsilon$
4: $\quad g_j \leftarrow \min_{i=1}^{\mathrm{N}} \left[\,\mathbf{C}(x_i,y_j) - f_i\,\right]$
5: **until** $\forall\, i,\ \exists\, j,\ f_i + g_j \geqslant \mathbf{C}(x_i,y_j) - \varepsilon\,.$
6: **return** $f_i,\ g_j$

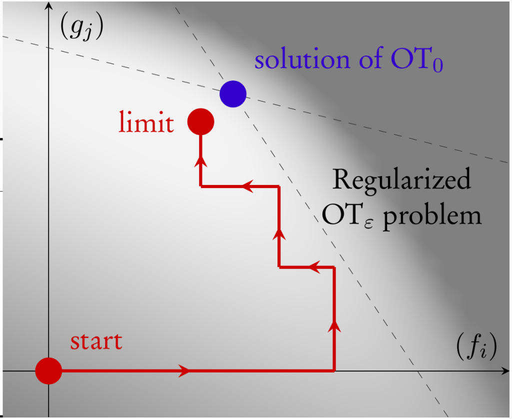


The Sinkhorn algorithm: use a softmin, get a well-defined optimum

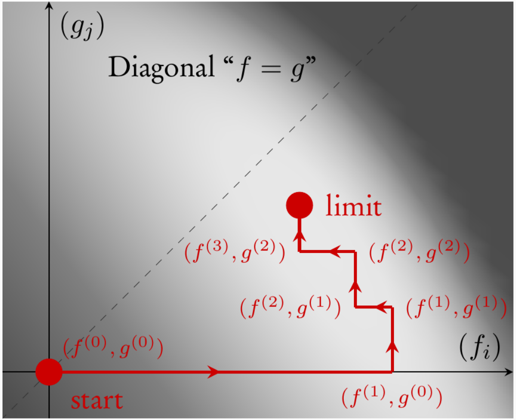
$$\mathrm{OT}(\alpha,\beta) = \max_{\substack{(f_i)\in\mathbb{R}^{\mathrm{N}} \\ (g_j)\in\mathbb{R}^{\mathrm{M}}}} \sum_{i=1}^{\mathrm{N}} \alpha_i f_i + \sum_{j=1}^{\mathrm{M}} \beta_j g_j - \varepsilon \log \langle \alpha_i \otimes \beta_j, \exp \tfrac{1}{\varepsilon}[f_i \oplus g_j - \mathbf{C}_{ij}] \rangle$$

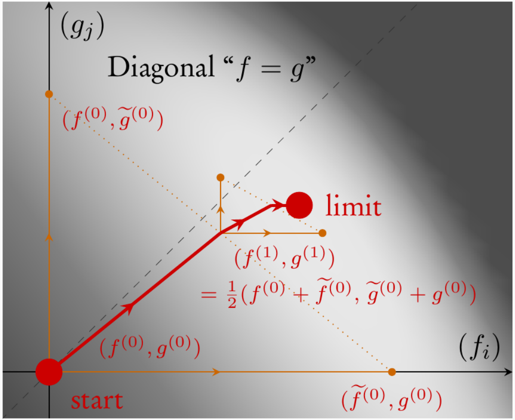
Algorithm 3.3: Sinkhorn or "soft-auction" algorithm

1: $f_i,\ g_j \leftarrow \mathbf{0}_{\mathbb{R}^{\mathrm{N}}},\ \mathbf{0}_{\mathbb{R}^{\mathrm{M}}}$
2: **repeat**
3: $\quad f_i \leftarrow -\varepsilon \log \sum_{j=1}^{\mathrm{M}} \beta_j \exp \tfrac{1}{\varepsilon}[\,g_j - \mathbf{C}(x_i, y_j)\,]$
4: $\quad g_j \leftarrow -\varepsilon \log \sum_{i=1}^{\mathrm{N}} \alpha_i \exp \tfrac{1}{\varepsilon}[\,f_i - \mathbf{C}(x_i, y_j)\,]$
5: **until** convergence up to a set tolerance.
6: **return** $f_i,\ g_j$



The symmetric Sinkhorn algorithm: stay close to the diagonal if A $\simeq$ B





Remark 1: a streamlined algorithm

One key operation – the soft, **weighted distance transform**:

$$\forall i \in [1, \mathsf{N}], \;\; f(x_i) \leftarrow \min_{y \sim \beta} \big[\mathsf{C}(x_i, y) - g(y)\big] = -\varepsilon \log \sum_{j=1}^{\mathsf{M}} \beta_j \exp \tfrac{1}{\varepsilon}\big[g_j - \mathsf{C}(x_i, y_j)\big] \,.$$

Similar to the chamfer distance transform, convolution with a Gaussian kernel…

Fast implementations with **pyKeOps**:

- If $\mathsf{C}(x_i, y_j)$ is a closed formula: **bruteforce** scales to N, M $\simeq$ 100k in 10ms on a GPU.
- If A and B have a low-dimensional support:
  use a clustering and **truncation** strategy to get a x10 speed-up.
- If A and B are supported on a 2D or 3D grid and $\mathsf{C}(x_i, y_j) = \frac{1}{2}\|x_i - y_j\|^2$:
  use a **separable** distance transform to get a second x10 speed-up.
  (N.B.: FFTs run into numerical accuracy issues.)

Remark 2: annealing works!

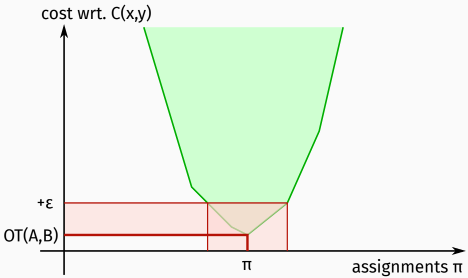
The **Auction/Sinkhorn** algorithms:

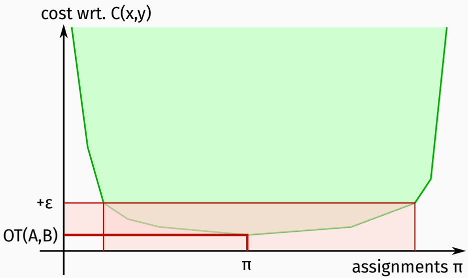
- Improve the dual cost by at least ε at each (early) step.
- Reach an ε-optimal solution with $(\max \text{C}) \,/\, \varepsilon$ steps.

Simple heuristic: run the optimization with **decreasing values** of ε.

ε-scaling
= **simulated annealing**
= **multiscale** strategy
= **divide and conquer**

Remark 3: the curse of dimensionality





In **low dimension**:

- $\|x - y\|$ takes large and small values.
- The OT objective is **peaky** wrt. π.
- ε-optimal solutions are **useful**.
- OT(discrete samples) $\simeq$ OT(underlying distributions)

In **high dimension**:

- $\|x - y\|$ gets closer to a constant.
- The OT objective is **flat** wrt. π.
- ε-optimal solutions are **random**.
- OT(discrete samples) $\neq$ OT(underlying distributions)

To recap 80+ years of work...

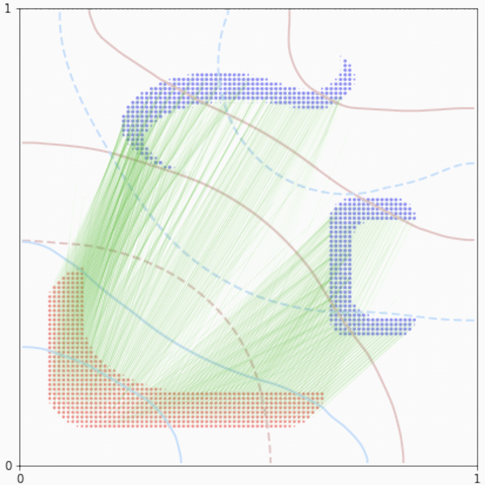
Key dates for discrete optimal transport with N points:

- [Kan42]: **Dual** problem of Kantorovitch.
- [Kuh55]: **Hungarian** methods in $O(\mathrm{N}^3)$.
- [Ber79]: **Auction** algorithm in $O(\mathrm{N}^2)$.
- [KY94]: **SoftAssign** = Sinkhorn + simulated annealing, in $O(\mathrm{N}^2)$.
- [GRL$^+$98, CR00]: **Robust Point Matching** = Sinkhorn as a loss.
- [Cut13]: Start of the **GPU era.**
- [Mér11, Lév15, Sch19]: **multi-scale** solvers in $O(\mathrm{N} \log \mathrm{N})$.

- **Solution,** today: **Multiscale Sinkhorn algorithm, on the GPU**.

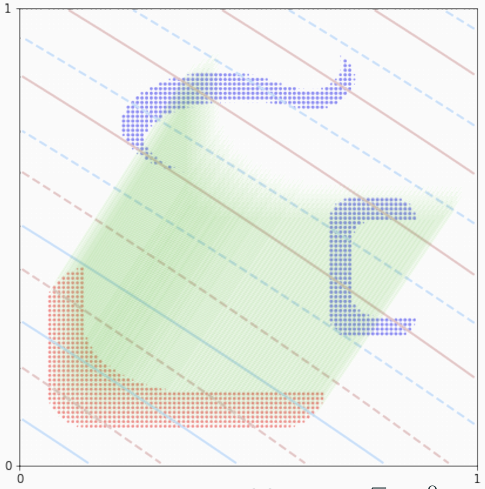
$\Longrightarrow$ Generalized **QuickSort** algorithm.

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}\mathrm{OT}(\alpha,\beta)$



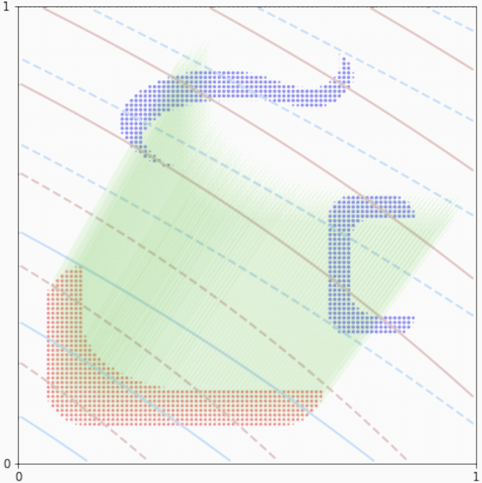
OT plan in 2D.

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}\mathrm{OT}(\alpha, \beta)$



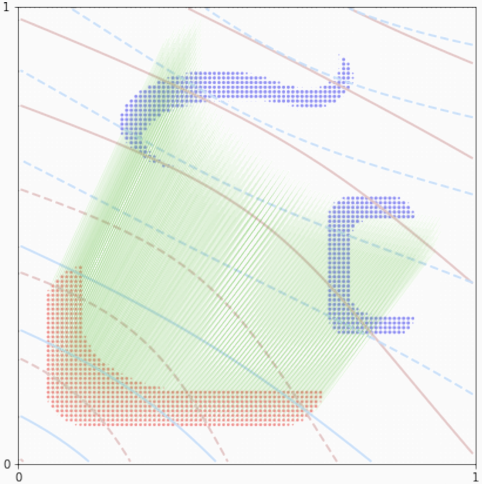
Iteration 0, blur $\sigma = \sqrt{\varepsilon} = 2^0$

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}\mathrm{OT}(\alpha, \beta)$



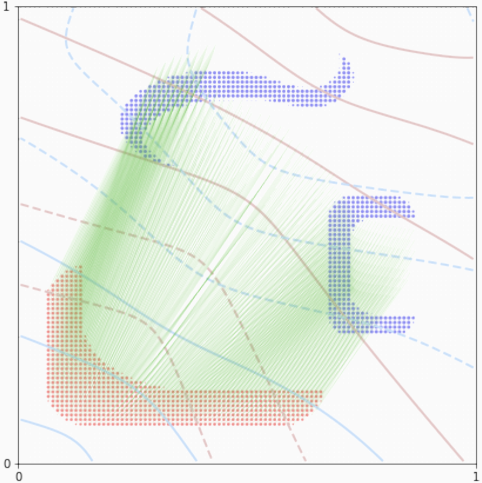
Iteration 1, blur $\sigma = \sqrt{\varepsilon} = 2^{-1}$

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}\mathbf{OT}(\alpha, \beta)$



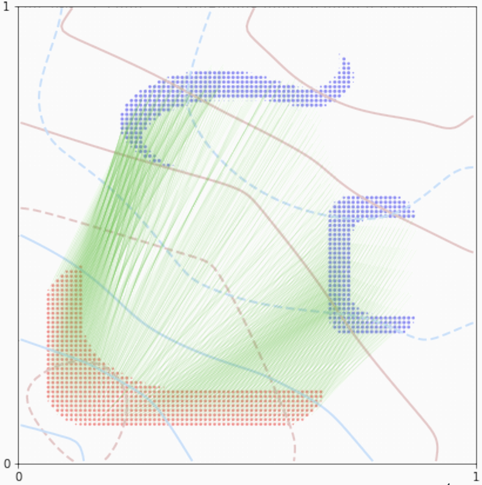
Iteration 2, blur $\sigma = \sqrt{\varepsilon} = 2^{-2}$

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}\mathrm{OT}(\alpha, \beta)$



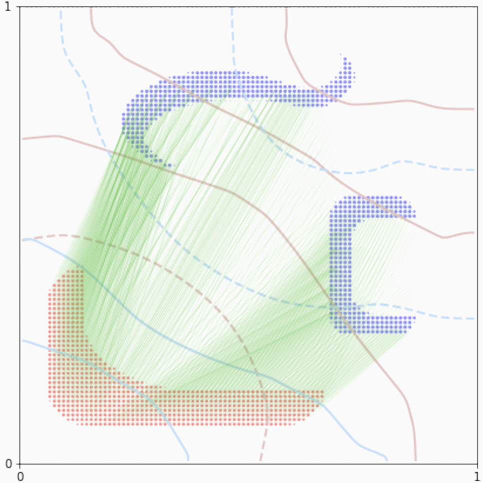
Iteration 3, blur $\sigma = \sqrt{\varepsilon} = 2^{-3}$

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}\mathrm{OT}(\alpha, \beta)$



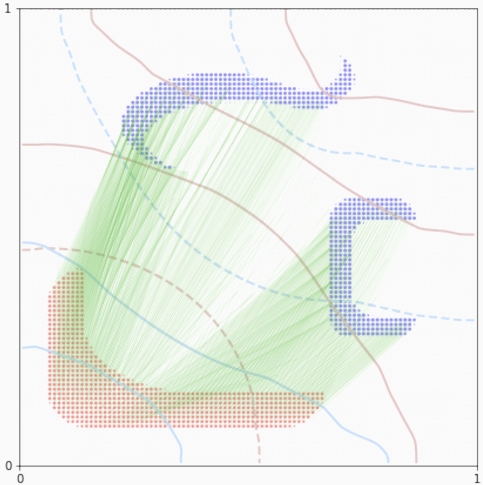
Iteration 4, blur $\sigma = \sqrt{\varepsilon} = 2^{-4}$

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}$ OT(α, β)



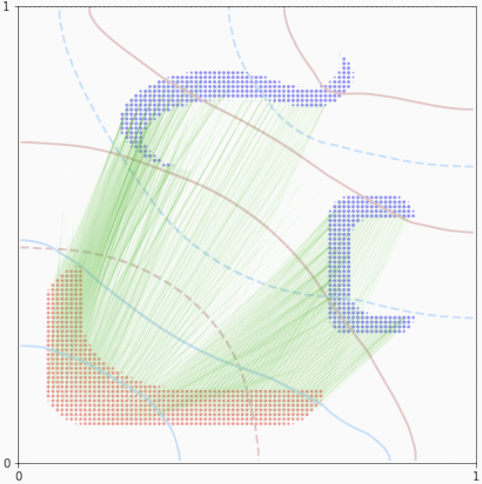
Iteration 5, blur $\sigma = \sqrt{\varepsilon} = 2^{-5}$

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}\mathbf{OT}(\alpha, \beta)$



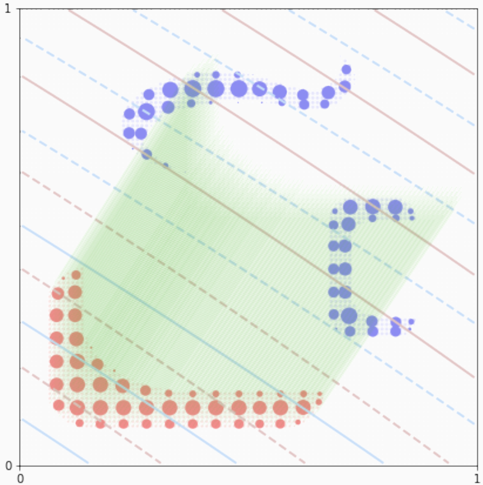
Iteration 6, blur $\sigma = \sqrt{\varepsilon} = 2^{-6}$

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}\textbf{OT}(\alpha, \beta)$



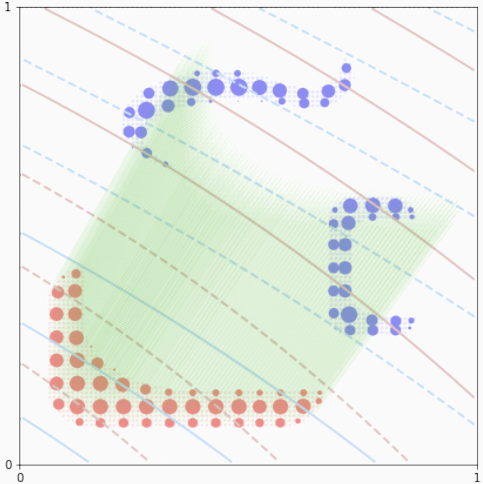
Iteration 7, blur $\sigma = \sqrt{\varepsilon} = .01$

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}\mathrm{OT}(\alpha, \beta)$



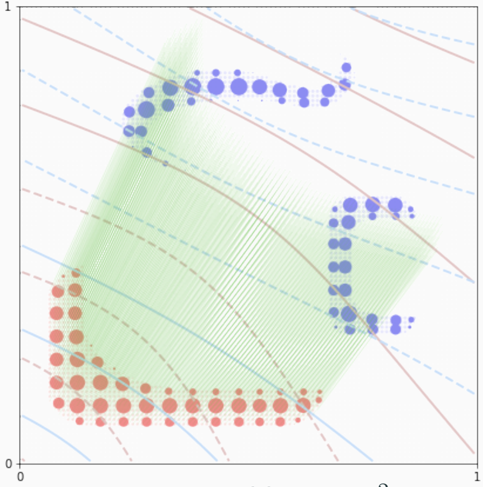
Iteration 0, blur $\sigma = 2^0$

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}\text{OT}(\alpha, \beta)$



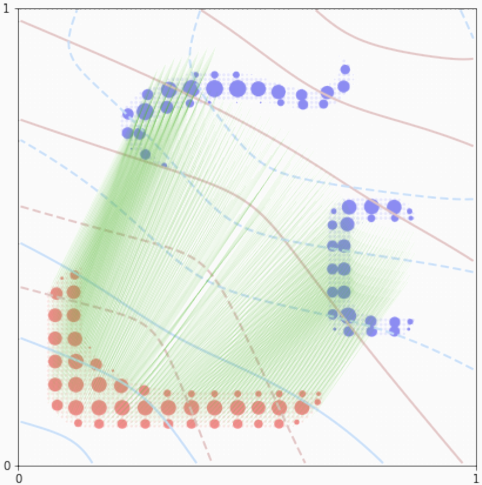
Iteration 1, blur $\sigma = 2^{-1}$

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}\mathrm{OT}(\alpha,\beta)$



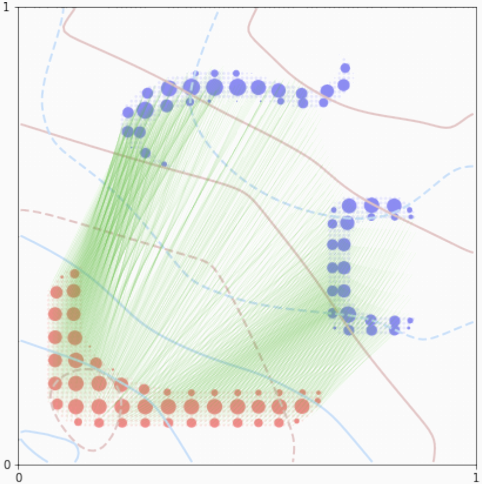
Iteration 2, blur $\sigma = 2^{-2}$

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}\text{OT}(\alpha, \beta)$



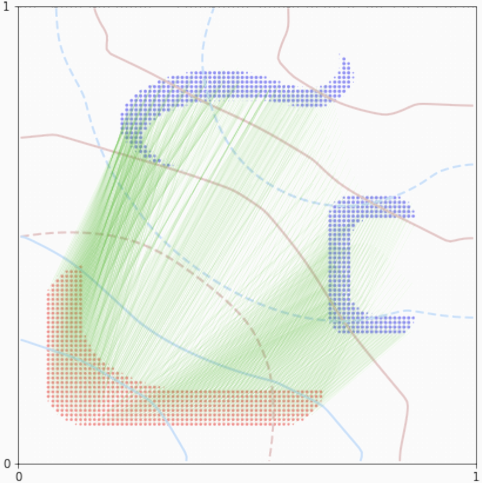
Iteration 3, blur $\sigma = 2^{-3}$

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}\mathrm{OT}(\alpha, \beta)$



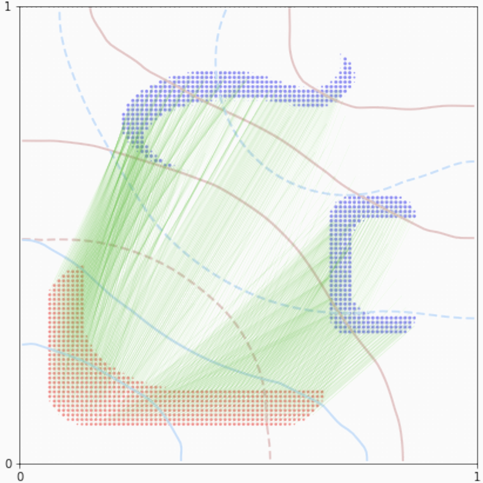
Iteration 4, blur $\sigma = 2^{-4}$

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}\text{OT}(\alpha, \beta)$



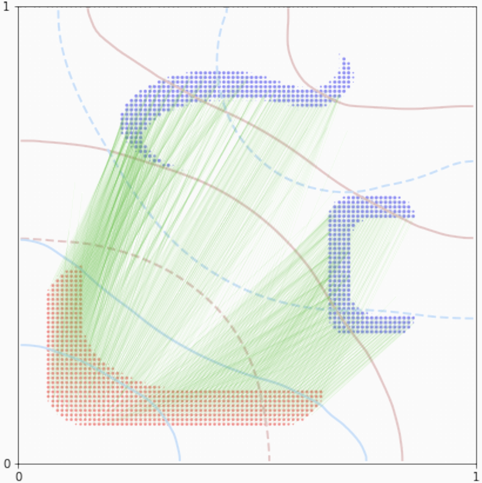
Iteration 5, blur $\sigma = 2^{-5}$

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}\mathrm{OT}(\alpha, \beta)$



Iteration 6, blur $\sigma = 2^{-6}$

Visualizing F, G and the Brenier map $\nabla F(x_i) = -\frac{1}{\alpha_i}\partial_{x_i}\mathrm{OT}(\alpha, \beta)$



Iteration 7, blur $\sigma = .01$

Scaling up optimal transport to anatomical data

Progresses of the last decade add up to a $\times$**100** - $\times$**1000** acceleration:

$$\text{Sinkhorn GPU} \xrightarrow{\times 10} \text{+ KeOps} \xrightarrow{\times 10} \text{+ Annealing} \xrightarrow{\times 10} \text{+ Multi-scale}$$

With a precision of 1%, on a modern gaming GPU:

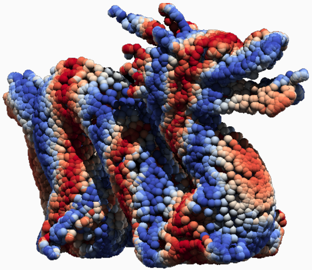
`pip install geomloss`

+

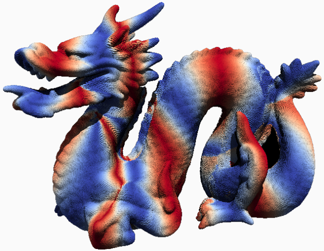
modern GPU

(1 000 €)

$\Longrightarrow$

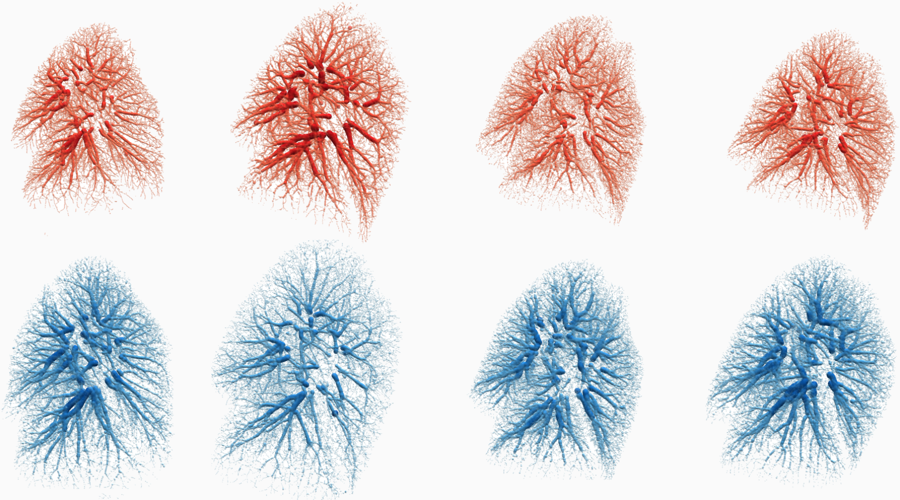


10k points in 30-50ms



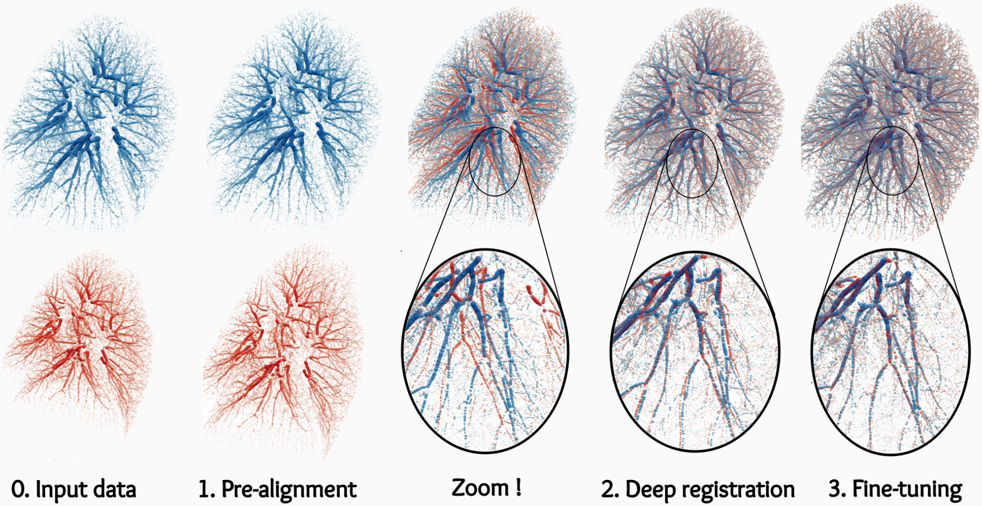
100k points in 100-200ms

A typical example in anatomy: lung registration “Exhale – Inhale”



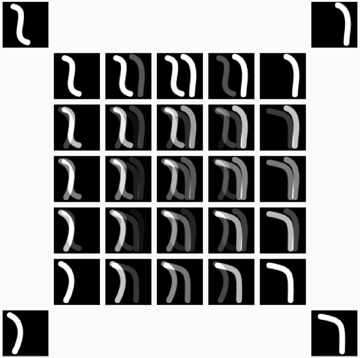
Complex deformations, high **resolution** (50k–300k points), high **accuracy** (< 1mm).

Three-steps registration



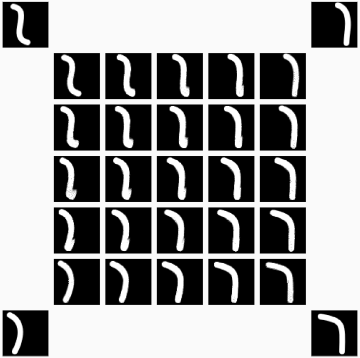
Wasserstein barycenters [AC11]

$$\text{Barycenter } \textcolor{red}{A}^* = \arg\min_{\textcolor{red}{A}} \sum_{i=1}^{4} \lambda_i \, \text{Loss}(\textcolor{red}{A}, \textcolor{blue}{B}_i)\,.$$



Euclidean barycenters.

$$\text{Loss}(\textcolor{red}{A}, \textcolor{blue}{B}) = \|\textcolor{red}{A} - \textcolor{blue}{B}\|_{L^2}^2$$



Wasserstein barycenters.

$$\text{Loss}(\textcolor{red}{A}, \textcolor{blue}{B}) = \text{OT}(\textcolor{red}{A}, \textcolor{blue}{B})$$

Wasserstein barycenters

From a computational perspective:

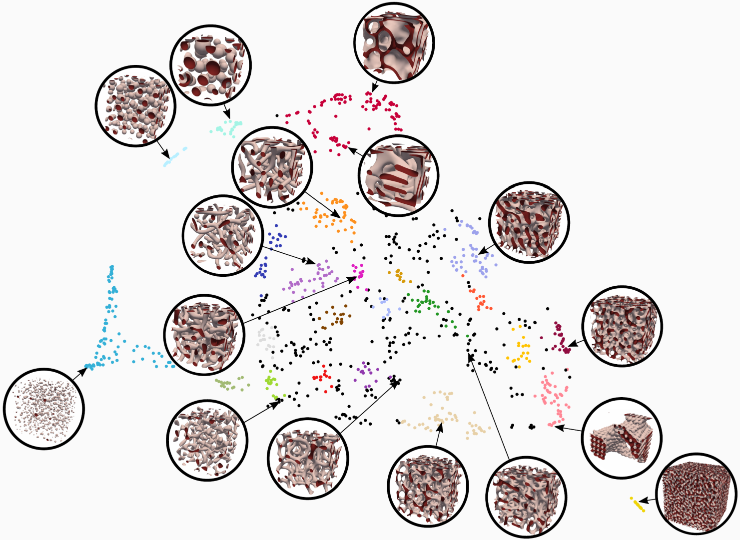
- The problem is **convex** (easy) wrt. the weights.
- The support of the barycenter lies in the **convex hull** of the input distributions.

The **curse of dimensionality** hits hard:

- In high dimension, identifying the support can become **NP-hard**.
- In dimensions 2 and 3, we can just use a grid and recover **super fast** algorithms. Computing OT distances and barycenters between **density maps** is a solved problem.

$\Longrightarrow$ We can now **easily** do manifold learning (= non-linear Model Order Reduction) in Wasserstein spaces of **2D and 3D** distributions.

An example: Anna Song's exploration of 3D shape textures [Son22]



Incompressible particles

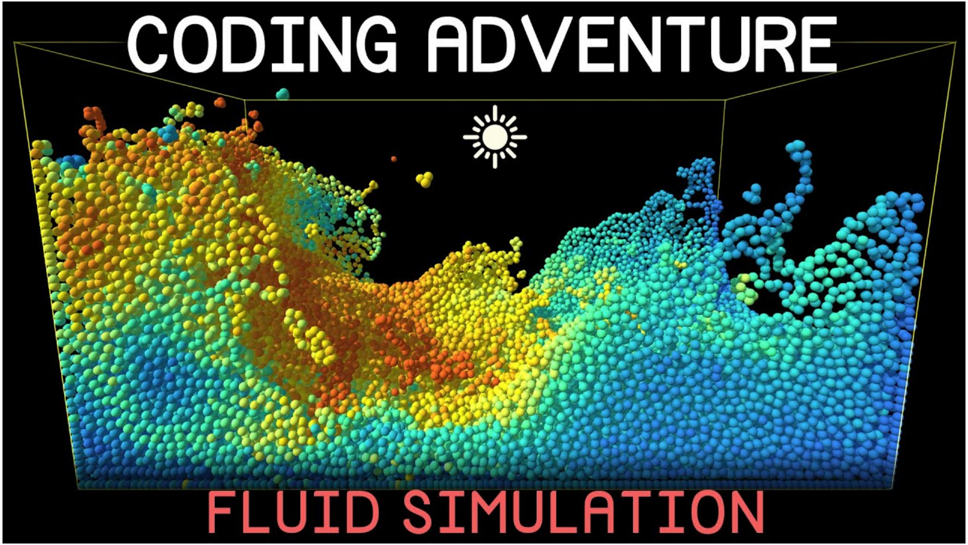
Two very talented postdocs

Maciej Buze
Heriot-Watt University

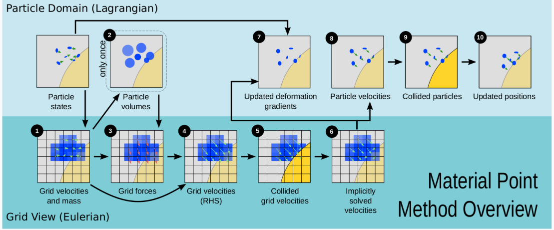
Antoine Diez
Kyoto University

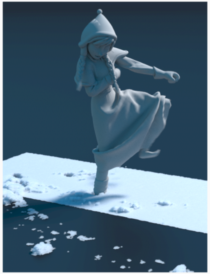
Original motivation: the N-body problem [Pri11]

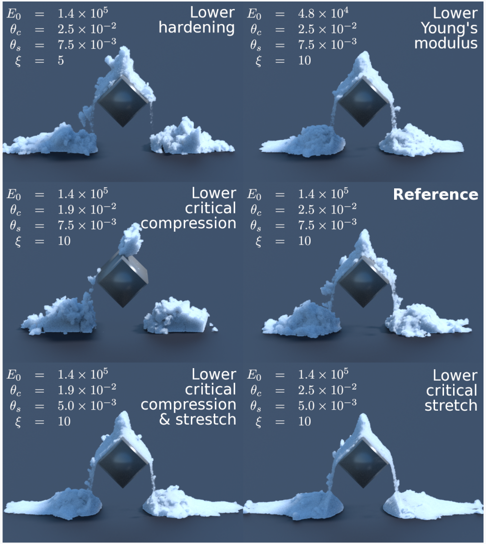
Coding a simple fluid simulation is now a matter of hours [Lag23]



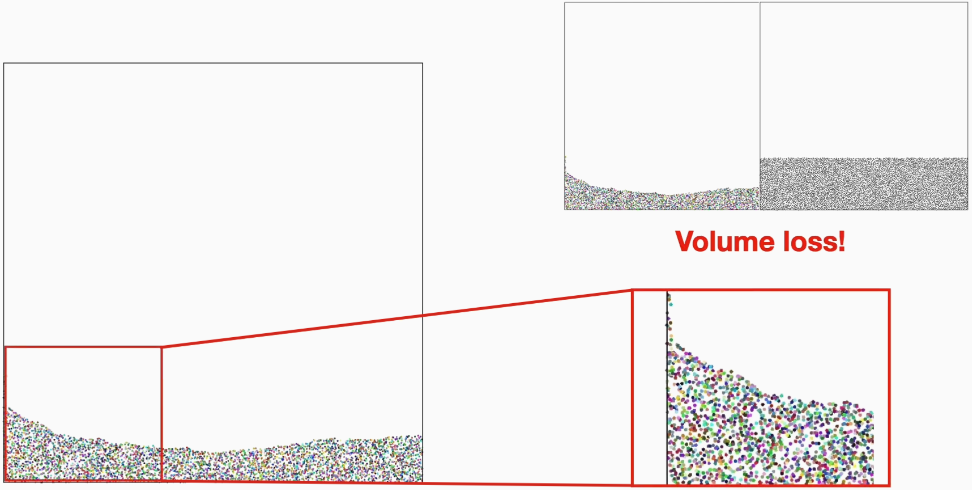
The material point method: Disney's Frozen [SSC+13]





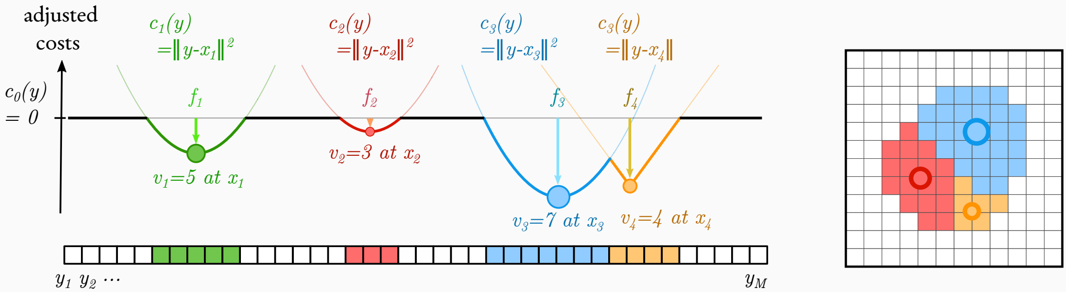


How can we enforce a volume preservation constraint? [QLDGJ22]



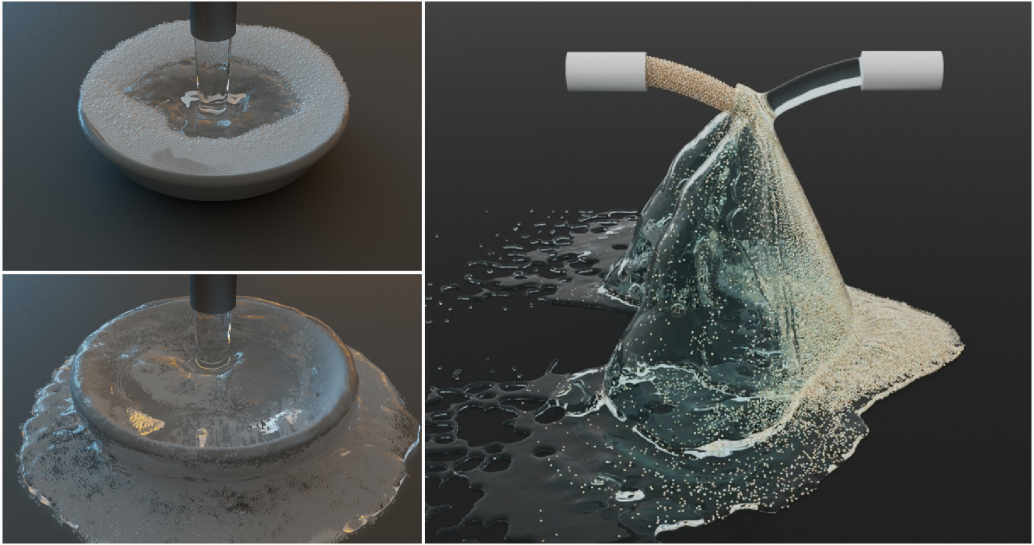
2D FLIP Simulation

Use power diagrams i.e. semi-discrete optimal transport

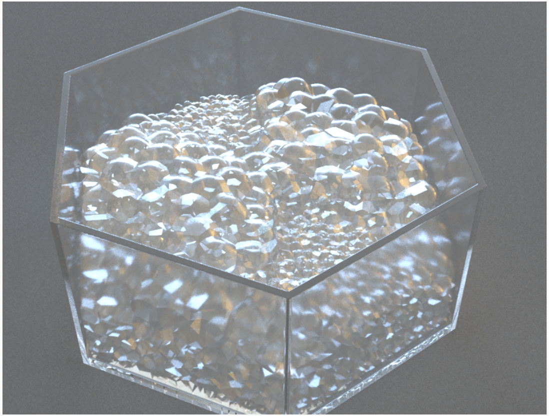


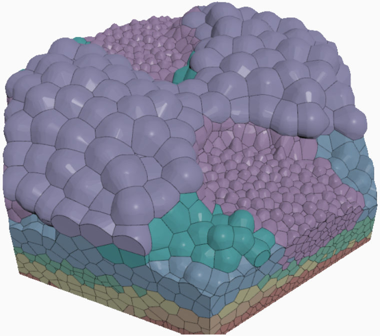
- The f_i's maximize the dual objective $\sum_{i=1}^N v_i f_i + \int_{y \in \Omega} \min_{i=0}^N [\, c_i(y) - f_i \,] \,\mathrm{d}y$.
- **Optimality** conditions $\iff$ $\mathrm{Vol}(\mathrm{Cell}_i) = v_i$.
- To **compute the cells**, the objective and its gradient:
  - If $c_i(y) = \|y - x_i\|^2$ for all cells, use a clever **grid-free** algorithm.
  - Otherwise, just use **KeOps**.

Power plastics [QLY+23]



Power plastics [QLY+23] – without the eye candy





Main numerical ingredients

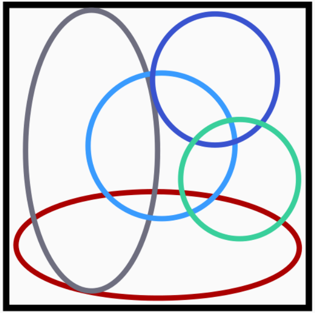
These simulations alternate between:

1. **Moving the particles** according to your favorite N-body model.
2. Computing Laguerre **cells** with the **correct volumes**:
    - (Multiscale) Sinkhorn for tolerance $> 5\%$.
    - (Quasi-)Newton for tolerance $< 1\%$.
3. **Correcting** the particle positions to enforce the volume-preservation constraint:
    - Jump to the centroid of the cell.
    - Or add a spring for smoother trajectories.

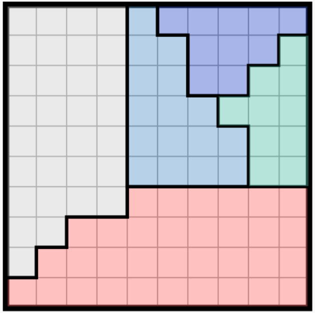
See e.g. Thomas Gallouët for a rigorous analysis with Mérigot, Lévy, etc.

But today: new applications with **custom cost functions** (thanks KeOps).

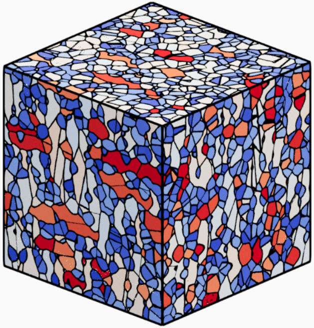
Anisotropic power diagrams let us model polycrystalline metals [BFR+24]



Ellipsoids.

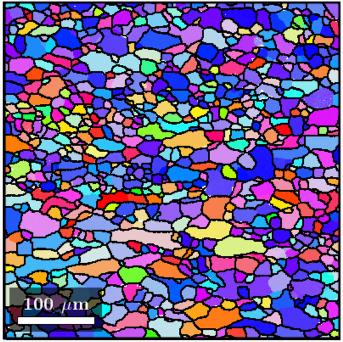


Pixel cells.

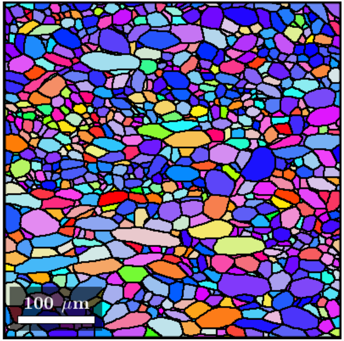


5,000 crystals in 3D.

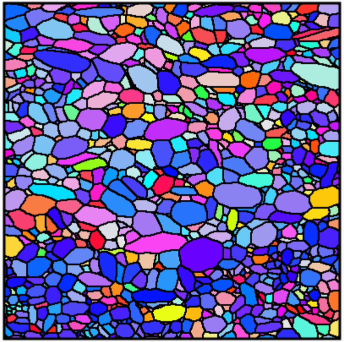
Fit to real EBSD scan of low-carbon steel [BFR+24]



Data from Tata steel.



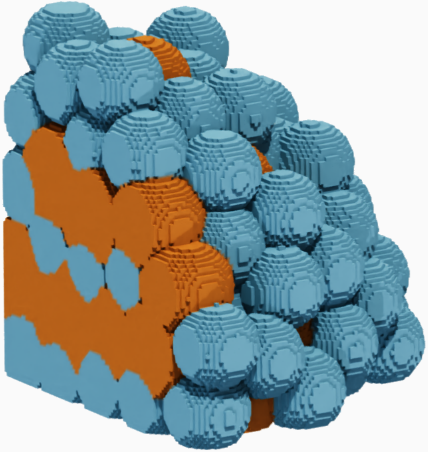
Our APD model.



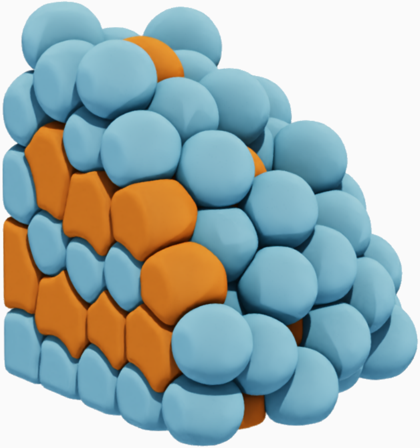
New synthetic image.

We can generate new, realistic 3D images with **prescribed properties** in seconds.

Change the cost function to simulate hard (blue) and soft (orange) cells [DF24]

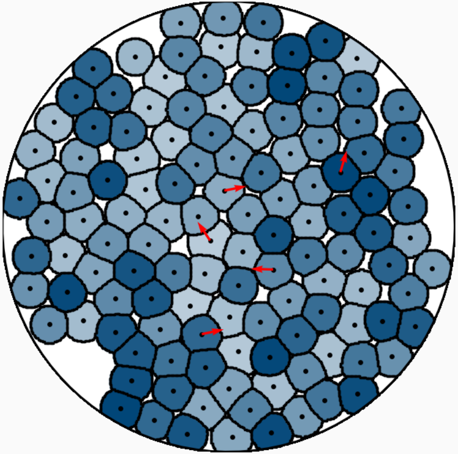


The **raw** 100x100x100 pixel grid…

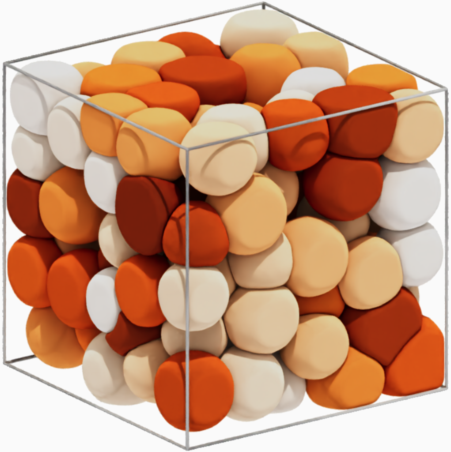


with some Hollywood **makeup**.

Run-and-tumble motion [DF24]

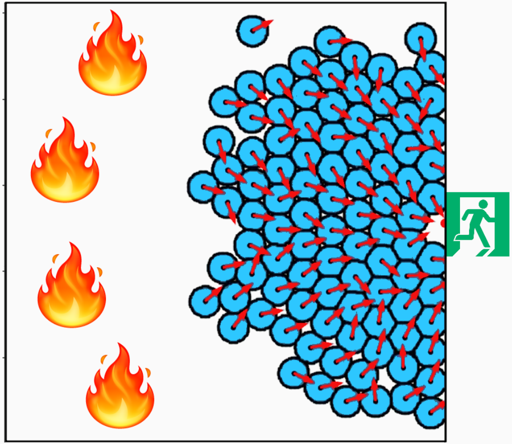


2D disk.

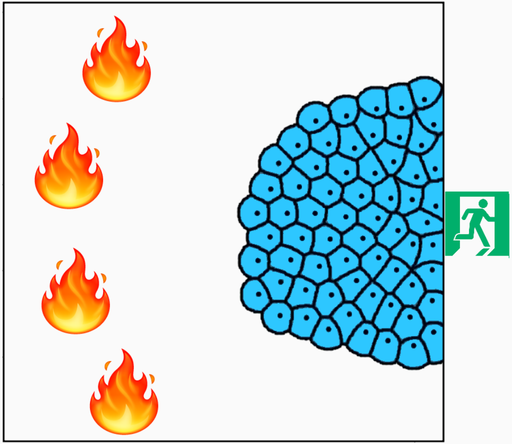


3D cube.

Fire alarm! [DF24]

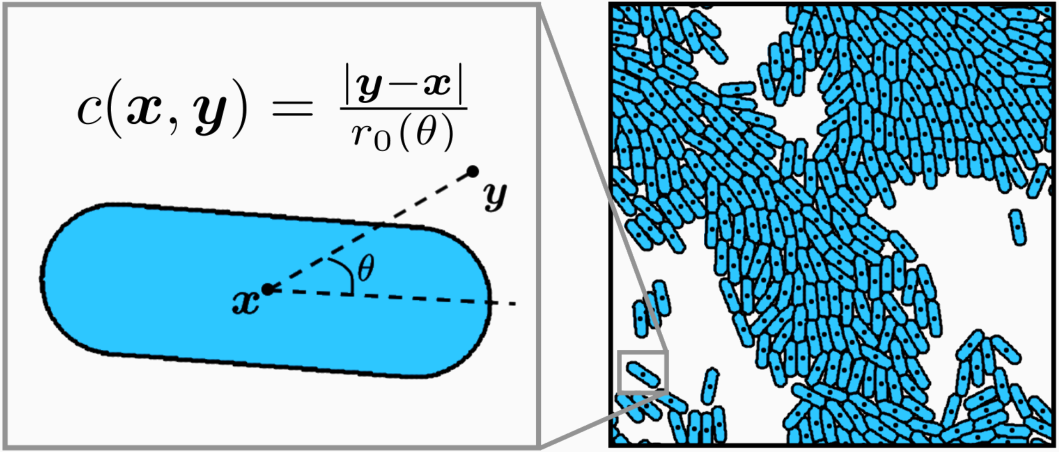


Hard particles **burn**.

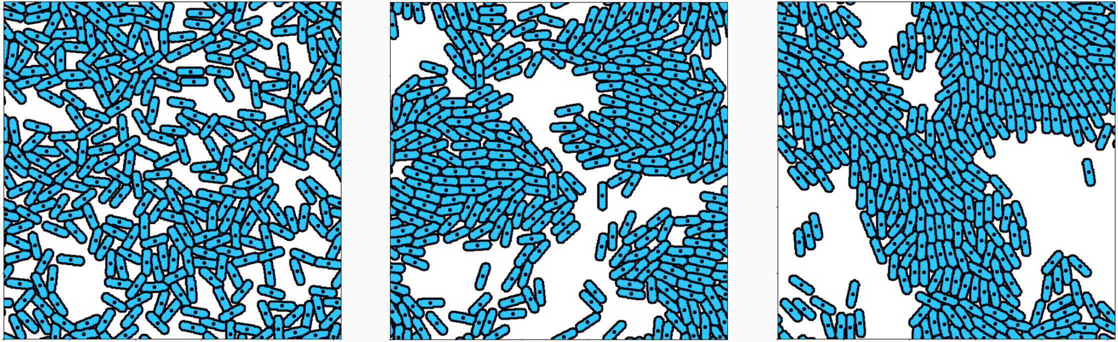


Soft particles **escape**.

Self-organizing swarms of blind, incompressible swimmers [DF24]



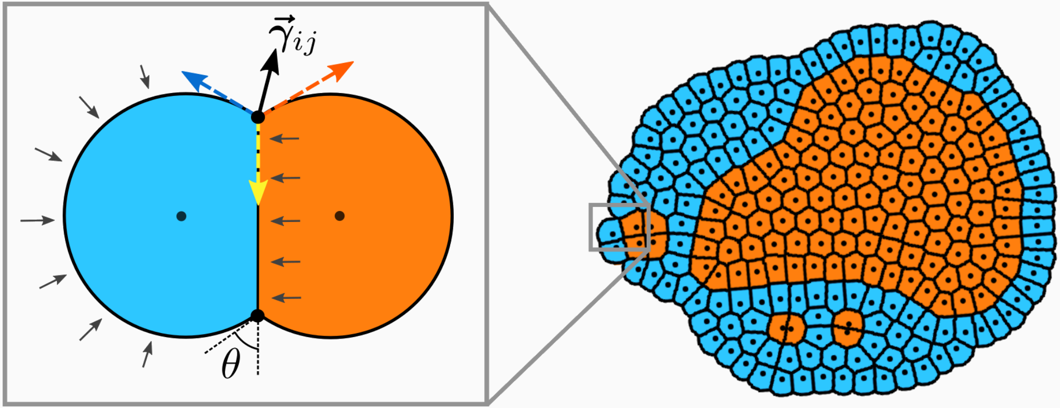
Self-organizing swarms of blind, incompressible swimmers [DF24]



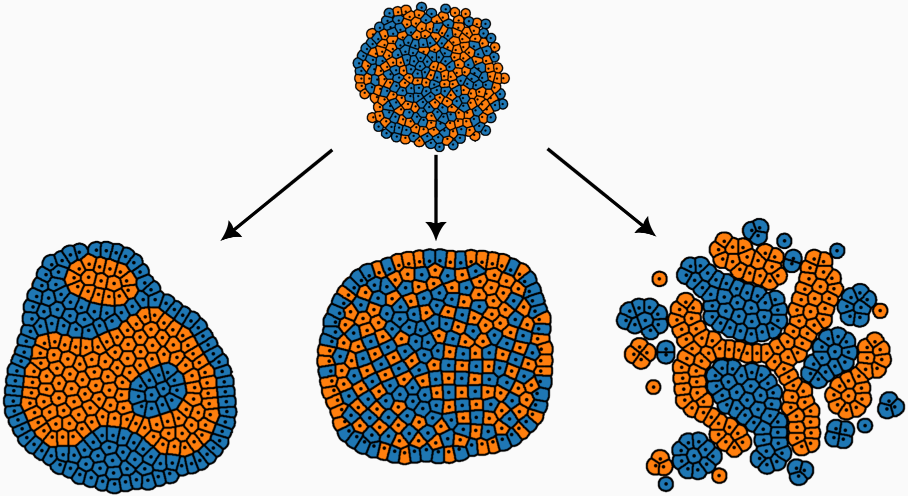
$t = 0$ $t = 4$ $t = 30$

Order emerges out of blind collisions and re-alignments.

Surface tension [DF24]



Surface tension [DF24] – playing with the energy parameters



Conclusion

Genuine team work


Benjamin Charlier


Joan Glaunès


Thibault Séjourné


F.-X. Vialard


Gabriel Peyré


Alain Trouvé


Marc Niethammer


Shen Zhengyang


Olga Mula


Hieu Do

Key points

- Optimal Transport = volume preservation = **generalized sorting** :

  $\longrightarrow$ Super-fast solvers on **simple domains**, especially 2D/3D spaces.

  $\longrightarrow$ **Fundamental tool** at the intersection of geometry and statistics.

- **"Video-game physics"** is great for modelling:

  $\longrightarrow$ **Expressive**, real-time simulations that you can implement without being a Finite Elements guru: XPBD, DiffPD, Taichi…

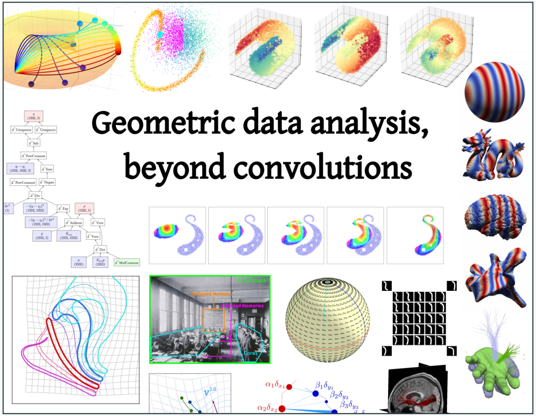
- GPUs are more **versatile** than you think.

  $\longrightarrow$ Ongoing work to provide **fast GPU backends** to researchers, going beyond what Google and Facebook are ready to pay for.

2026 target for scientific Python: **interactive, web-based** simulations à la ShaderToy.

Documentation and tutorials are available online

$\Longrightarrow$ www.kernel-operations.io $\Longleftarrow$



www.jeanfeydy.com/geometric_data_analysis.pdf

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