Fast geometric learning with symbolic matrices

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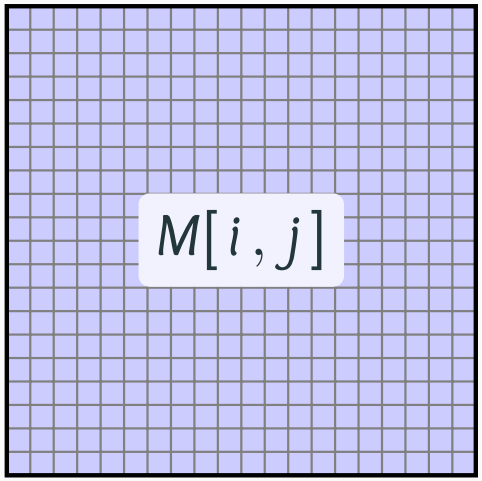
Joint work with B. Charlier, J. Glaunès (numerical foundations),
T. Séjourné, F.-X. Vialard, G. Peyré (optimal transport theory),
P. Roussillon, P. Gori, A. Trouvé (applications to computational anatomy),
F. Sverrisson, B. E. Correia, M. Bronstein (applications to protein sciences).

Symbolic matrices?

Machine learning libraries represent most objects as tensors



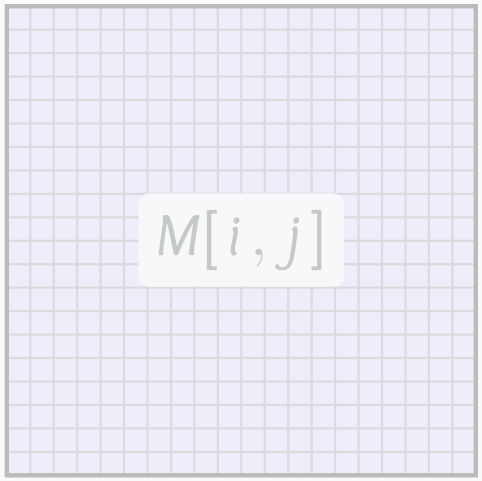
Dense matrix

Coefficients only

Dense matrices – large, contiguous **arrays** of numbers:

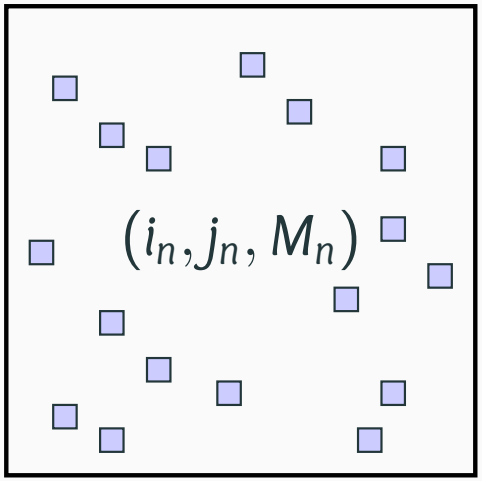
+ **Convenient** and well supported.
– Heavy load on the **memories** of our GPUs, with **time-consuming transfers** that take place between compute units.

Machine learning libraries represent most objects as tensors



Dense matrix

Coefficients only



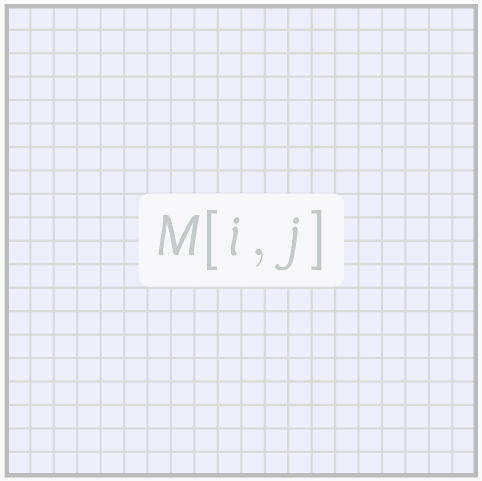
Sparse matrix

Coordinates + coeffs

Sparse matrices – tensors that have **few non-zero entries:**

+ Represent **large tensors** with a small memory footprint.
– Outside of **graph** processing, few objects are **sparse enough** to really benefit from this representation.

Machine learning libraries represent most objects as tensors



Dense matrix

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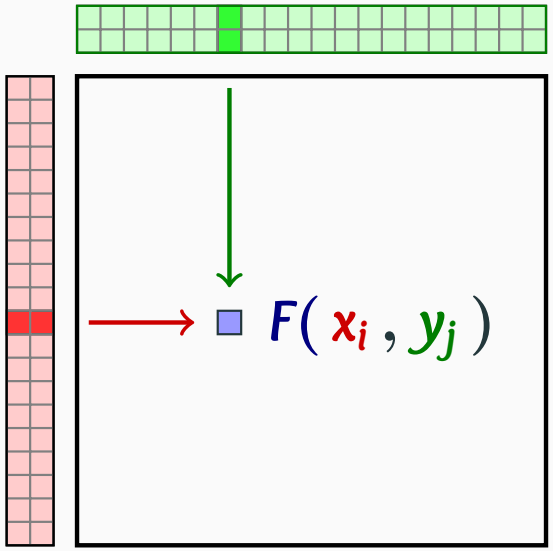
Sparse matrix

Coordinates + coeffs



Symbolic matrix

Formula + data

Distance and **kernel** matrices, **point** convolutions, **attention** layers:

+ **Linear** memory usage: no more **memory** overflows.
+ We can optimize the use of registers for a $\times 10$ - $\times 100$ **speed-up** vs. a standard PyTorch GPU baseline.

We provide support for this "new abstraction" on the GPU

Our library comes with all the perks of a deep learning toolbox:

+ Transparent **array-like** interface.
+ Full support for automatic **differentiation**.
+ Comprehensive collection of **tutorials**, available online.

Under the hood: combines an optimized **C++** engine with high-level binders for **PyTorch**, **NumPy**, Matlab and R (thanks to Ghislain Durif).
(We welcome **contributors** for JAX, Julia and other frameworks!)

To get started:

$\Longrightarrow$ `pip install pykeops` $\Longleftarrow$

`www.kernel-operations.io`

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
```

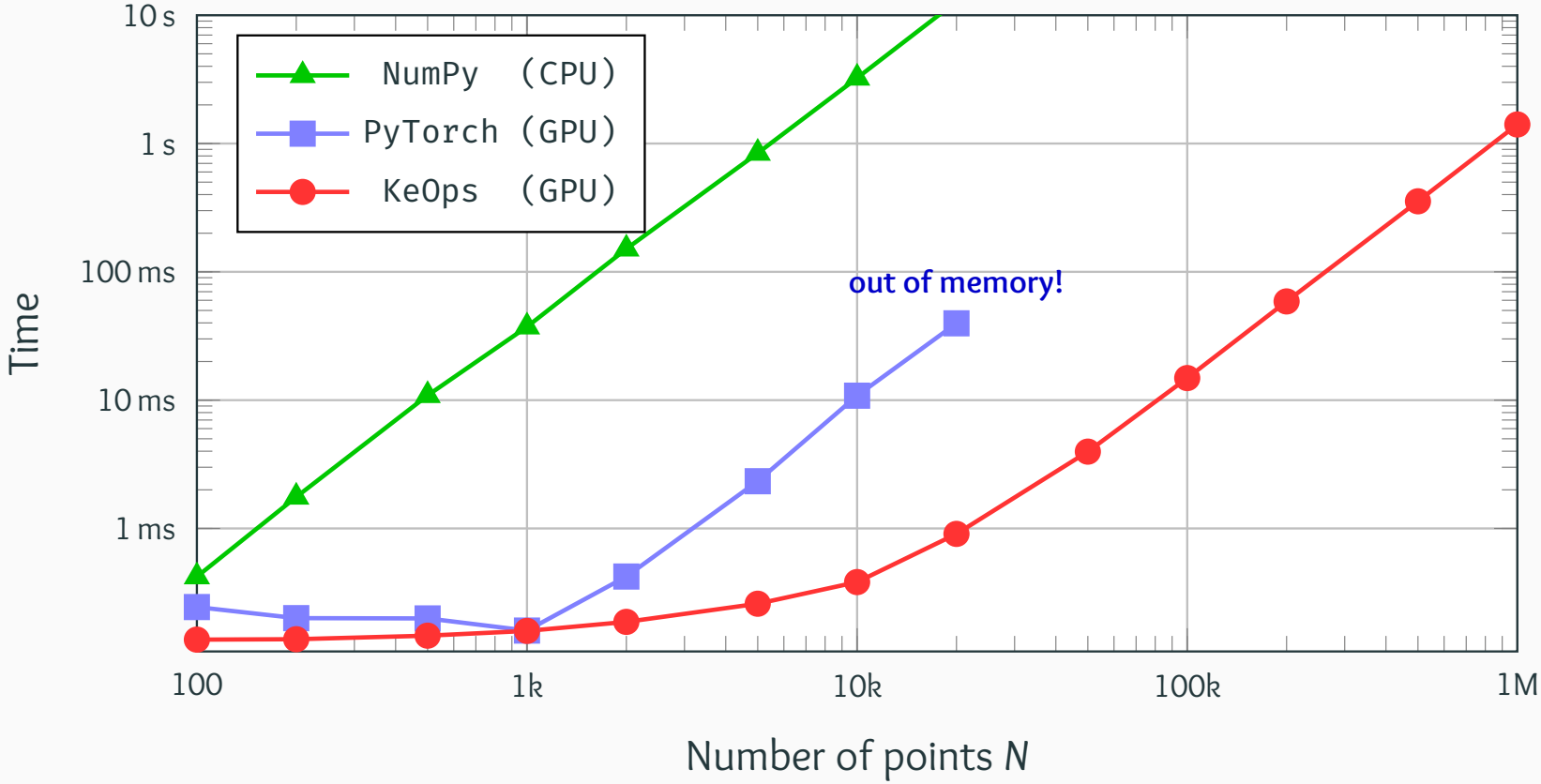
KeOps supports arbitrary **formulas** and **variables** with:

- **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

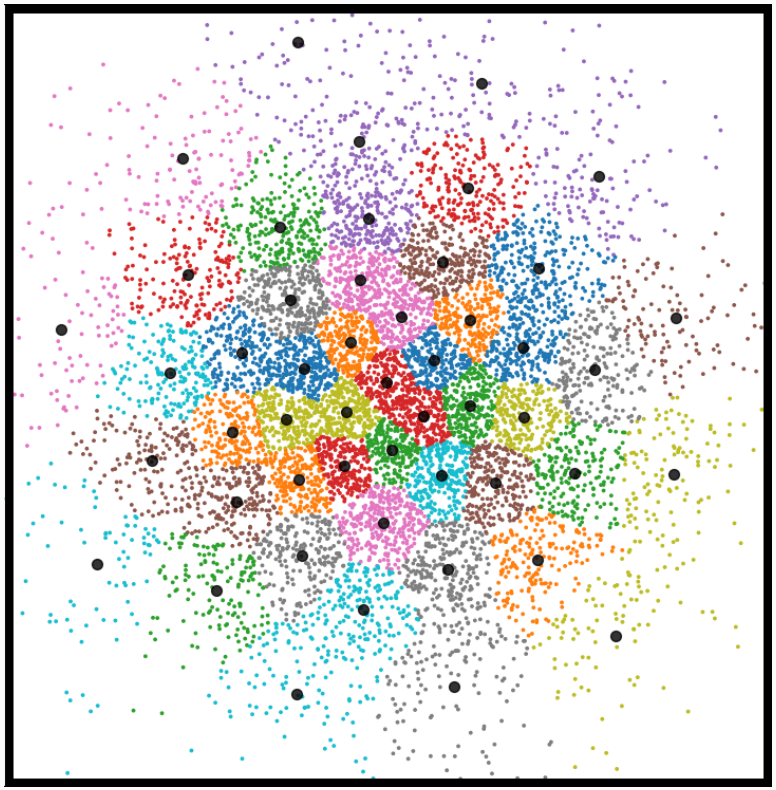
Benchmark of a matrix-vector product with a N-by-N Gaussian kernel matrix between 3D point clouds.

We run NumPy, PyTorch and KeOps on a RTX 2080 Ti GPU.

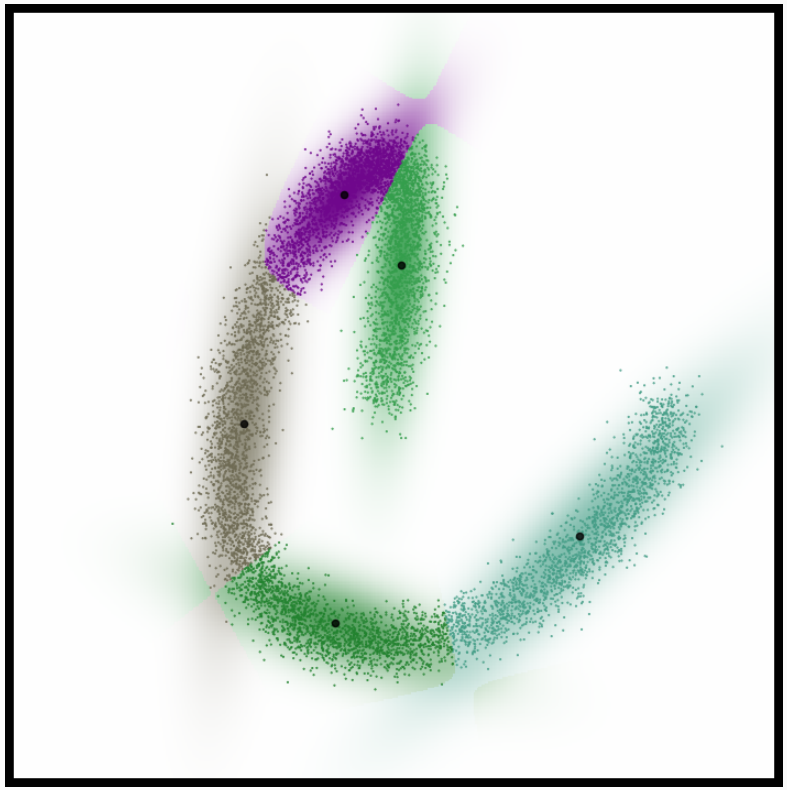


Applications

KeOps is a good fit for machine learning research



K-Means.

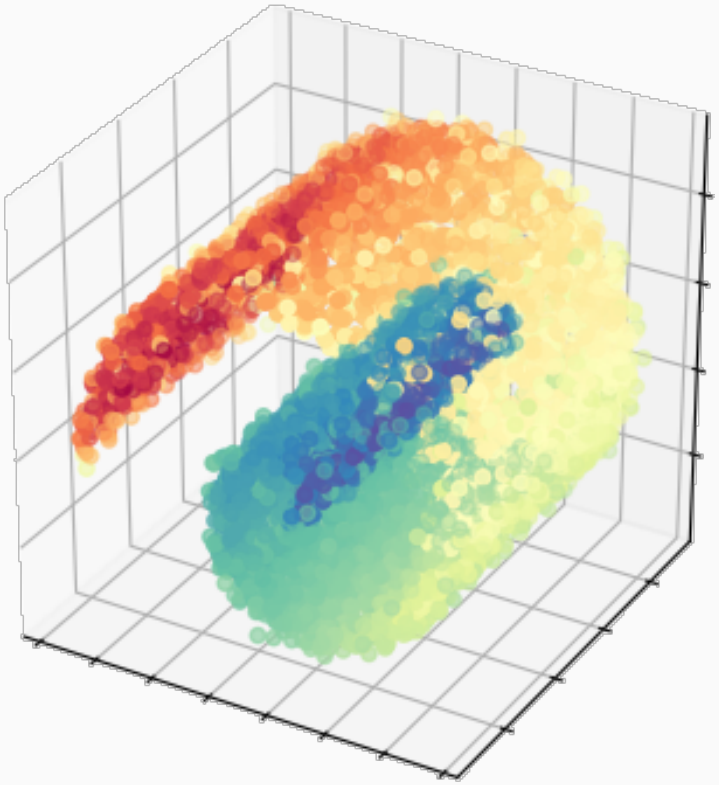


Gaussian Mixture Model.

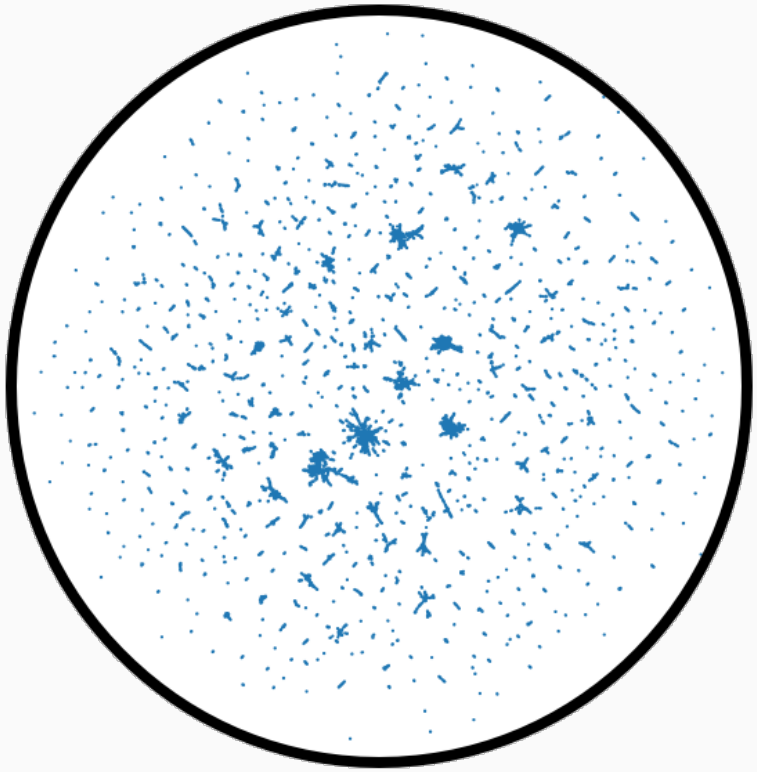
Use any kernel, metric or formula you like!

$\Longrightarrow$ More tutorials coming up soon.

KeOps is a good fit for machine learning research



Spectral analysis.



UMAP in hyperbolic space.

Use any kernel, metric or formula you like!

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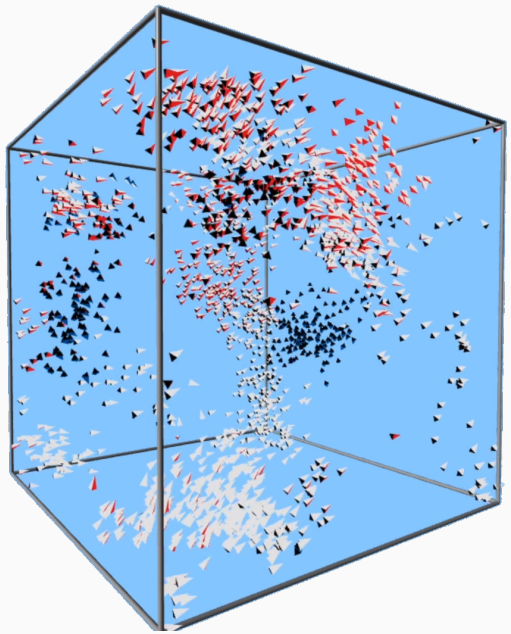
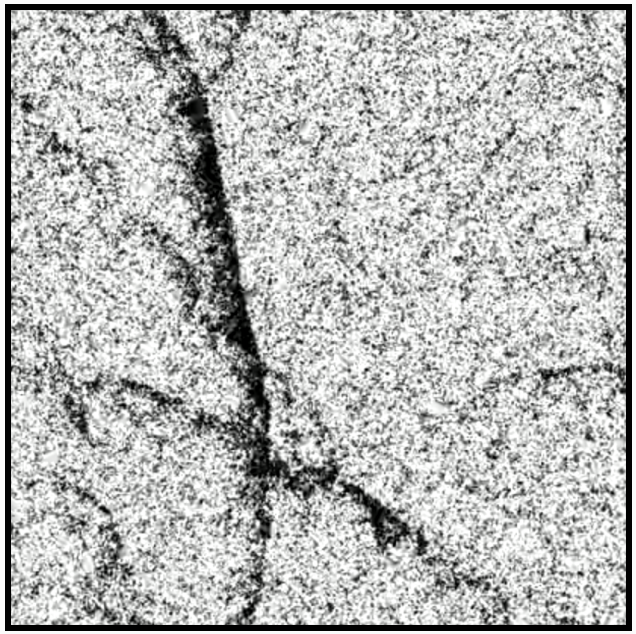
KeOps lets you focus on your models, results and theorems

Some applications to **dynamical systems** [DM08, DFMAT17] and **statistics** [CDF19] with A. Diez, G. Clarté and P. Degond:



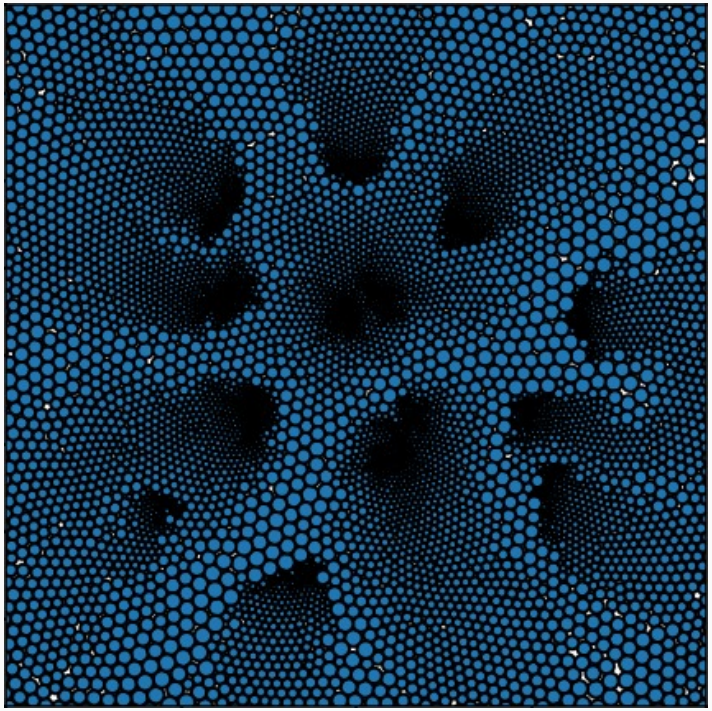
3D Vicsek model with orientation, interactive demo with 2k **flyers**.



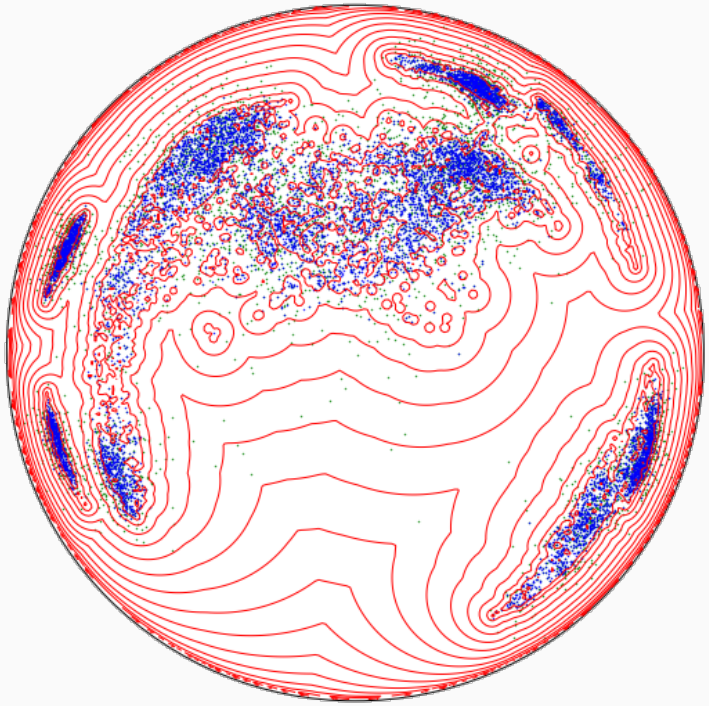
2D Vicsek model on the torus, in real-time with 100k **swimmers**.

KeOps lets you focus on your models, results and theorems

$\Longrightarrow$ Scale up to **millions/billions of agents** with Python scripts.



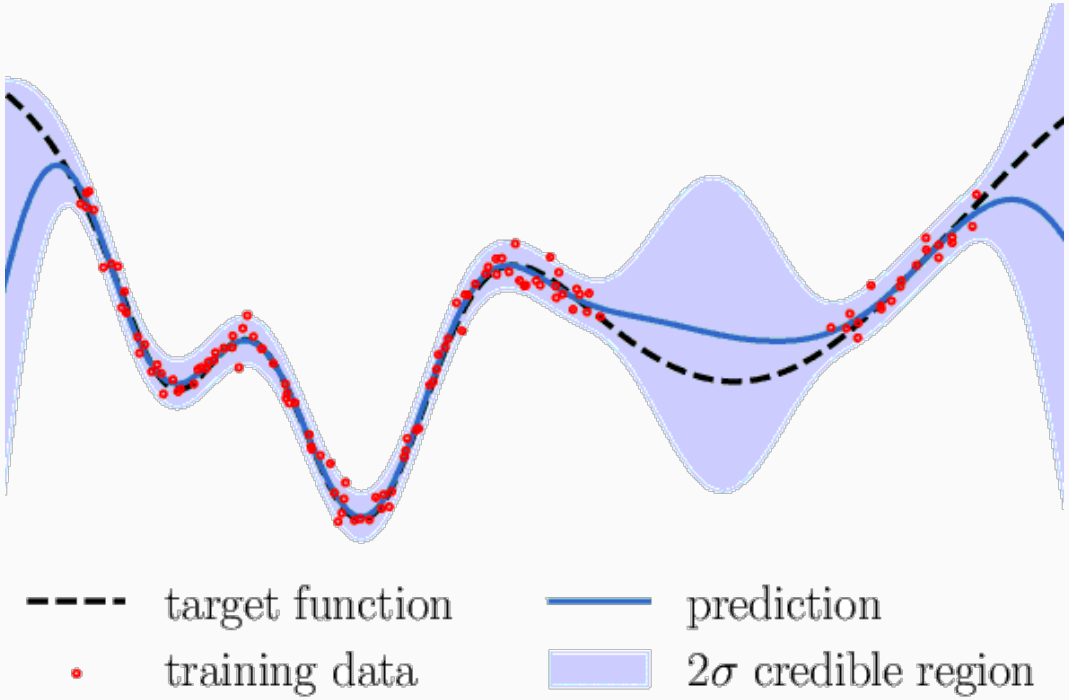
Packing problem in 2D
with 10k repulsive balls.



Collective Monte Carlo **sampling**
on the hyperbolic Poincaré disk.

Applications to Kriging, spline, Gaussian process, kernel regression

A standard tool for regression [Lec18]:



Under the hood, solve a **kernel linear system:**

$$(\lambda\,\mathrm{Id} + K_{xx})\,a \;=\; b \qquad \text{i.e.} \qquad a \;\leftarrow\; (\lambda\,\mathrm{Id} + K_{xx})^{-1} b$$

where $\lambda \geqslant 0$ and $(K_{xx})_{i,j} = k(x_i, x_j)$ is a positive definite matrix.

Applications to Kriging, spline, Gaussian process, kernel regression

KeOps symbolic tensors:

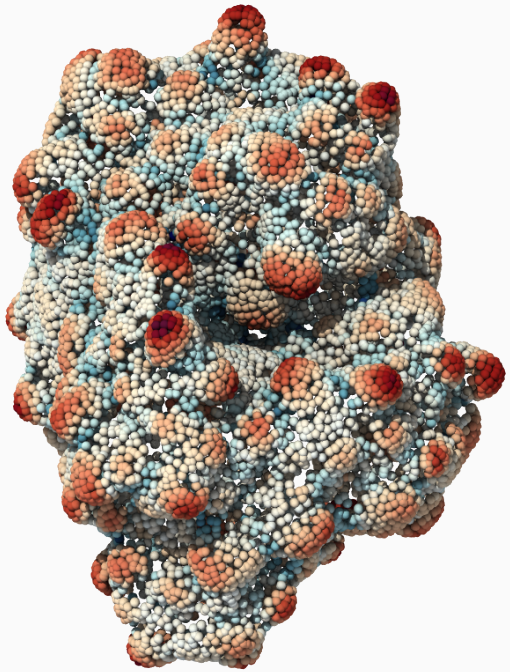
- Can be fed to **standard solvers**: SciPy, GPytorch, etc.
- GPytorch on the 3DRoad dataset ($N = 278k$, $D = 3$):

  7h with 8 GPUs $\quad\rightarrow\quad$ **15mn** with 1 GPU.

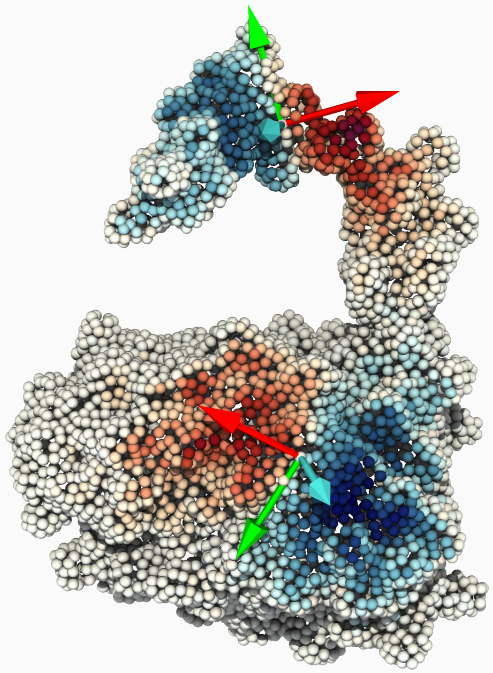
- Provide a **fast backend for research codes**: see e.g.
  Kernel methods through the roof: handling ***billions of points*** *efficiently*, by G. Meanti, L. Carratino, L. Rosasco, A. Rudi (2020).

Data-driven methods on **point clouds** and **proteins** [SFCB20]:

+ **Fast K-NN search:** local interactions.
+ **Fast N-by-N computations:** global interactions.
+ Heterogeneous **batches**, Octree-like acceleration.



Curvatures at all scales.



Quasi-geodesic **convolutions**.

Fast, scalable and robust optimal transport solvers

How should we solve the OT problem?

Key dates for discrete optimal transport with N points:

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

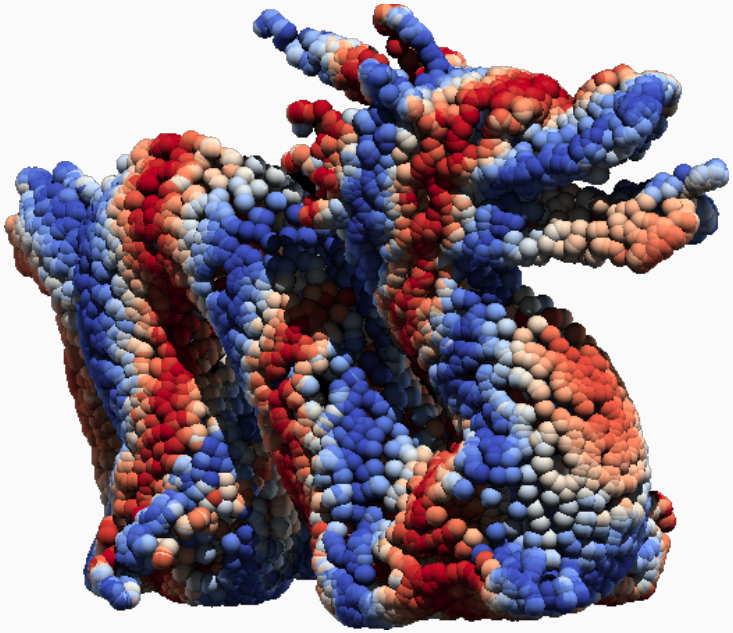
$\Longrightarrow$ Generalized **QuickSort** algorithm.

Scaling up optimal transport to anatomical data

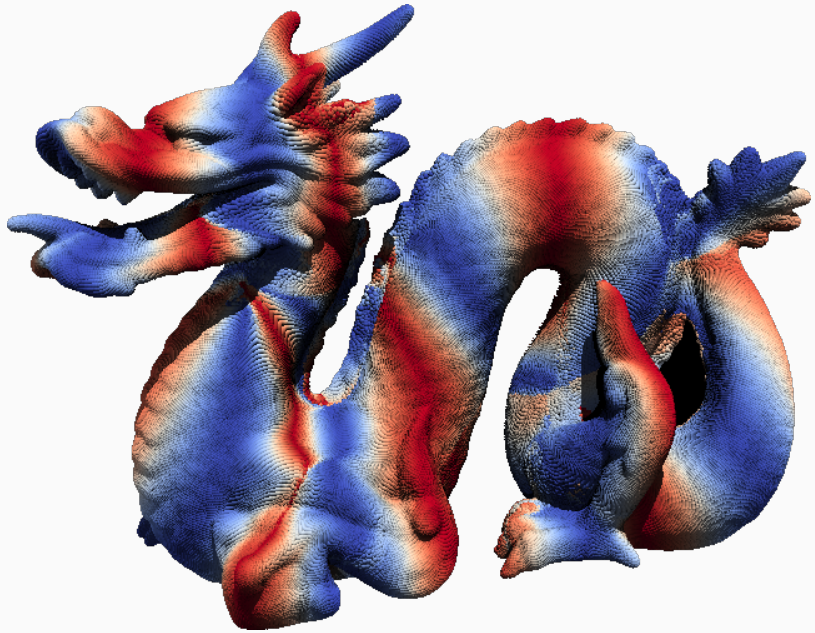
Progresses of the last decade add up to a $\times 100$ - $\times 1000$ **acceleration:**

Sinkhorn GPU $\xrightarrow{\times 10}$ + KeOps $\xrightarrow{\times 10}$ + Annealing $\xrightarrow{\times 10}$ + Multiscale

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



10k points in 30-50ms



100k points in 100-200ms

Geometric Loss functions for PyTorch

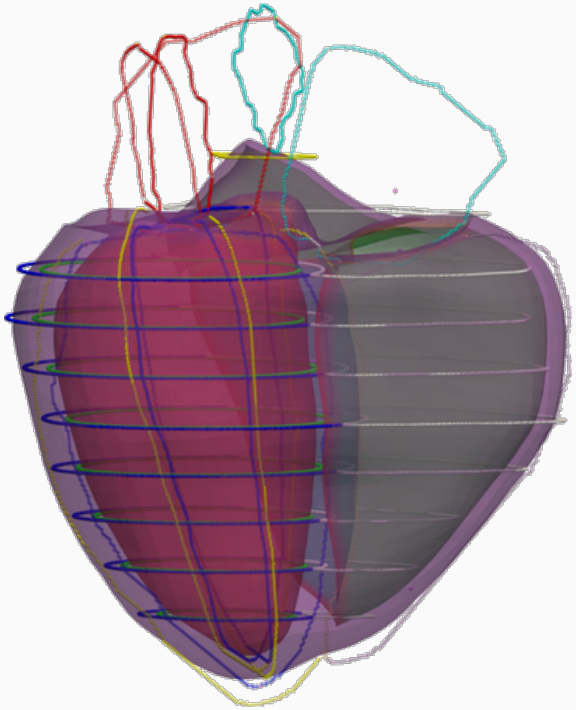
Our website: `www.kernel-operations.io/geomloss`

$\Longrightarrow$ `pip install geomloss` $\Longleftarrow$

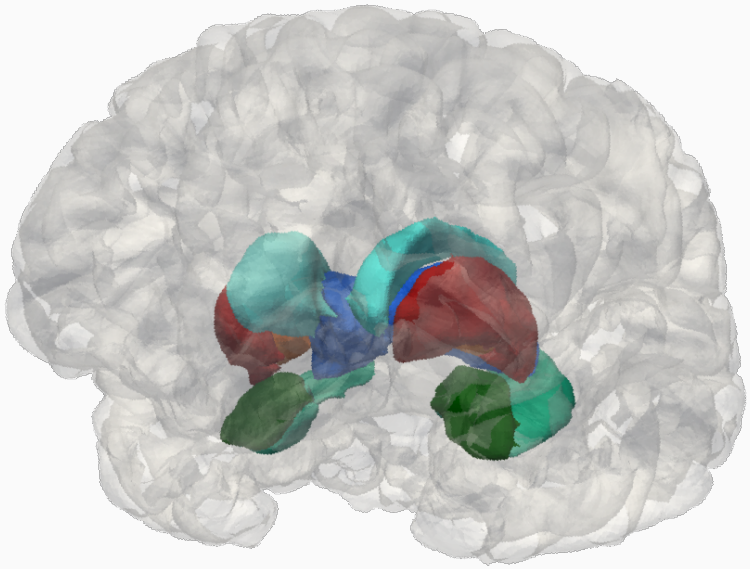
```
# Large point clouds in [0,1]^3
import torch
x = torch.rand(100000, 3, requires_grad=True).cuda()
y = torch.rand(200000, 3).cuda()

# Define a Wasserstein loss between sampled measures
from geomloss import SamplesLoss
loss = SamplesLoss(loss="sinkhorn", p=2)
L = loss(x, y)  # By default, use constant weights
```

Soon: efficient support for **images**, **meshes** and generic metrics.

My first motivation: computational anatomy



Fast OT-based registration with
S. Joutard, X. Hao, A. Young from KCL,
Z. Shen, M. Niethammer from UNC.



Diffeomorphic and spline registration
e.g. Deformetrica LDDMM software
with the Aramis Inria team.

Future improvements

KeOps and GeomLoss are:

- \+ **Fast:** $\times 10$ -$\times 1{,}000$ speedup vs. naive GPU implementations.
- \+ **Memory-efficient:** $O(\mathrm{N})$, not $O(\mathrm{N}^2)$.
- \+ **Versatile, with a transparent interface:** freedom!
- \+ **Powerful and well-documented:** research-friendly.
- − Slow with **large vectors** of dimension $\mathrm{D} > 100$.

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First half of 2021:

- → **Approximation strategies** (Nyström, etc.) in KeOps.
- → Wasserstein **barycenters** and **grid images** in GeomLoss.

An ongoing research project

Roadmap for KeOps + GeomLoss:

2017–18 **Proof of concept** with conference papers, online codes.
Get first feedback from the community.

2019–20 **Stable library** with solid theorems, a well-documented API.
KeOps backends for high-level packages.

2021–22 **Mature library** with focused application papers, full tutorials.
Works out-of-the-box for students and engineers.

2022+ **A standard toolbox**, with genuine clinical applications?
That's the target!

Conclusion

Key points

- **Symbolic** matrices are to **geometric** ML what
  sparse matrices are to **graph** processing:
  $\longrightarrow$ KeOps, **x30 speed-up** vs. PyTorch, TF and JAX.
  $\longrightarrow$ Useful in a wide range of settings.

- Optimal Transport = **generalized sorting**:
  $\longrightarrow$ Geometric gradients.
  $\longrightarrow$ Super-fast $O(N \log N)$ solvers.

- These tools open **new paths** for geometers and statisticians:
  $\longrightarrow$ 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.

Conclusion

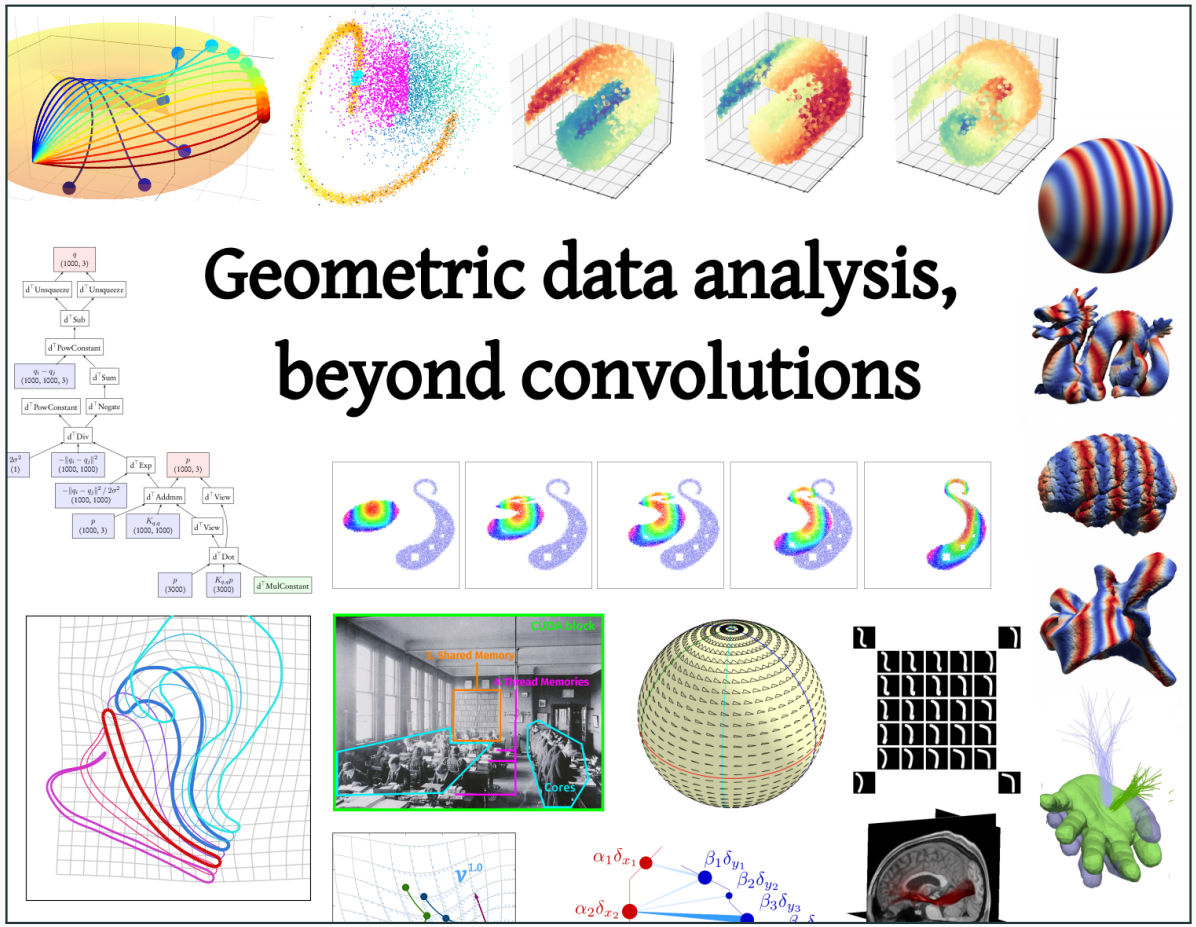
We believe that **KeOps** and **GeomLoss** will stimulate research on:

- **Clustering** methods: fast K-Means and EM iterations.
- Data **representation**: UMAP, fast KNN graphs with any metric.
- **Kernel** methods: kernel matrices.
- **Gaussian** processes: covariance matrices.
- **Geometric** deep learning: point convolutions.
- Geometric **statistics**: going beyond Euclidean models.
- Natural **language** processing: transformer networks?

What do you think?

Documentation and tutorials are available online

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



www.jeanfeydy.com/geometric_data_analysis.pdf

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