Kernel methods on GPUs and applications

Benjamin Charlier (Université de Montpellier)

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Foreword

The word *kernel* may have different meanings

- Mathematical Analysis: a function $X \times X \to Y$ interation between points
- Linear algebra: the null set of a linear operator
- Programming: a short piece of code, a function. Usually intend to be run on GPU. A “cuda kernel”, “openCL kernel”, ...

Overview

Motivations: shapes analysis using kernels

KeOps and symbolic matrices

Autodiff engine

- Introduction
- KeOps autograd

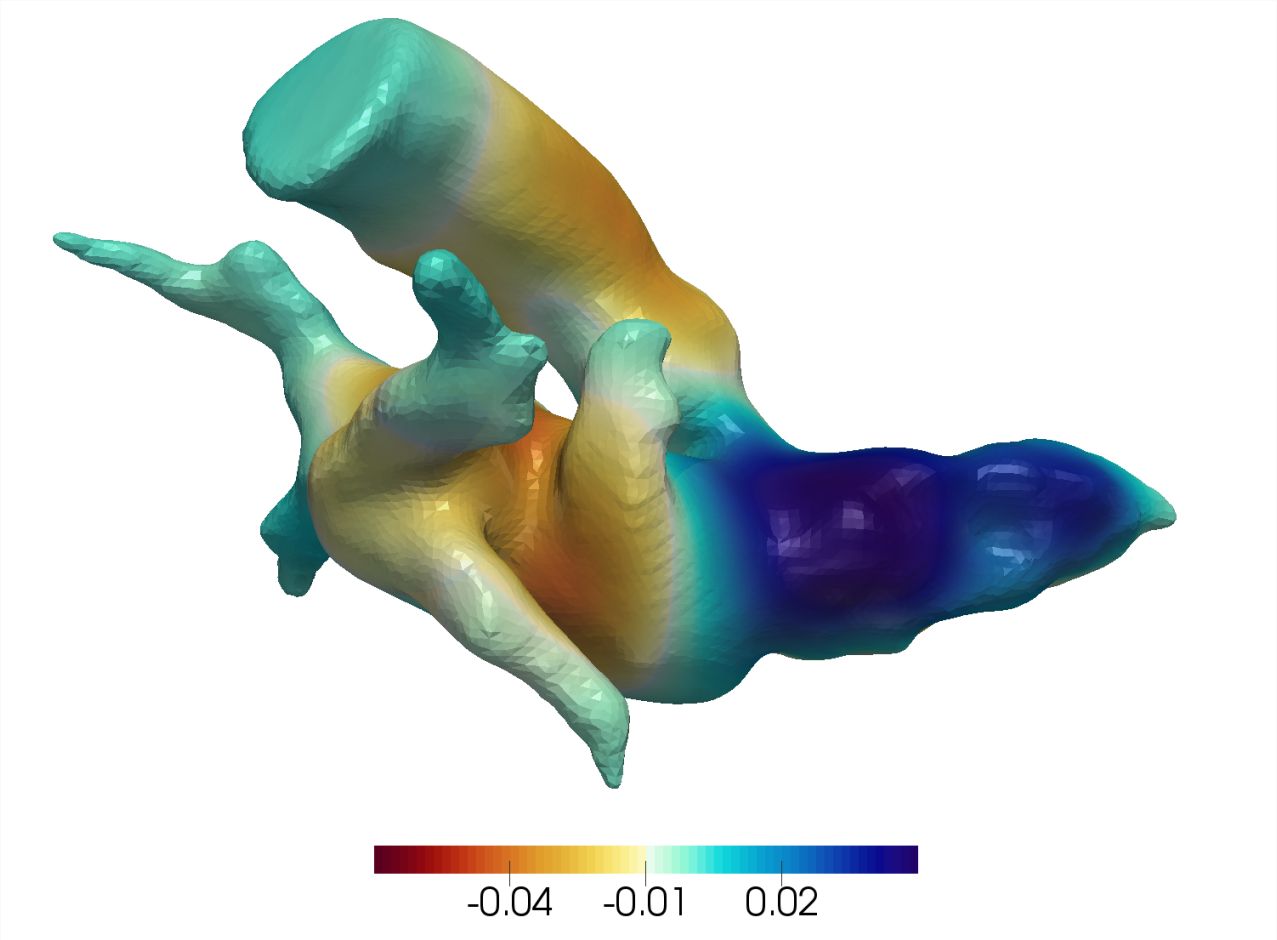
Advanced linear algebra operations

Computation on GPU

- Architecture
- Example: Matrix multiplication
- JIT with cuda: nvrtc

Motivations: shapes analysis using kernels

LDDMM: generate Diffeomorphic deformations



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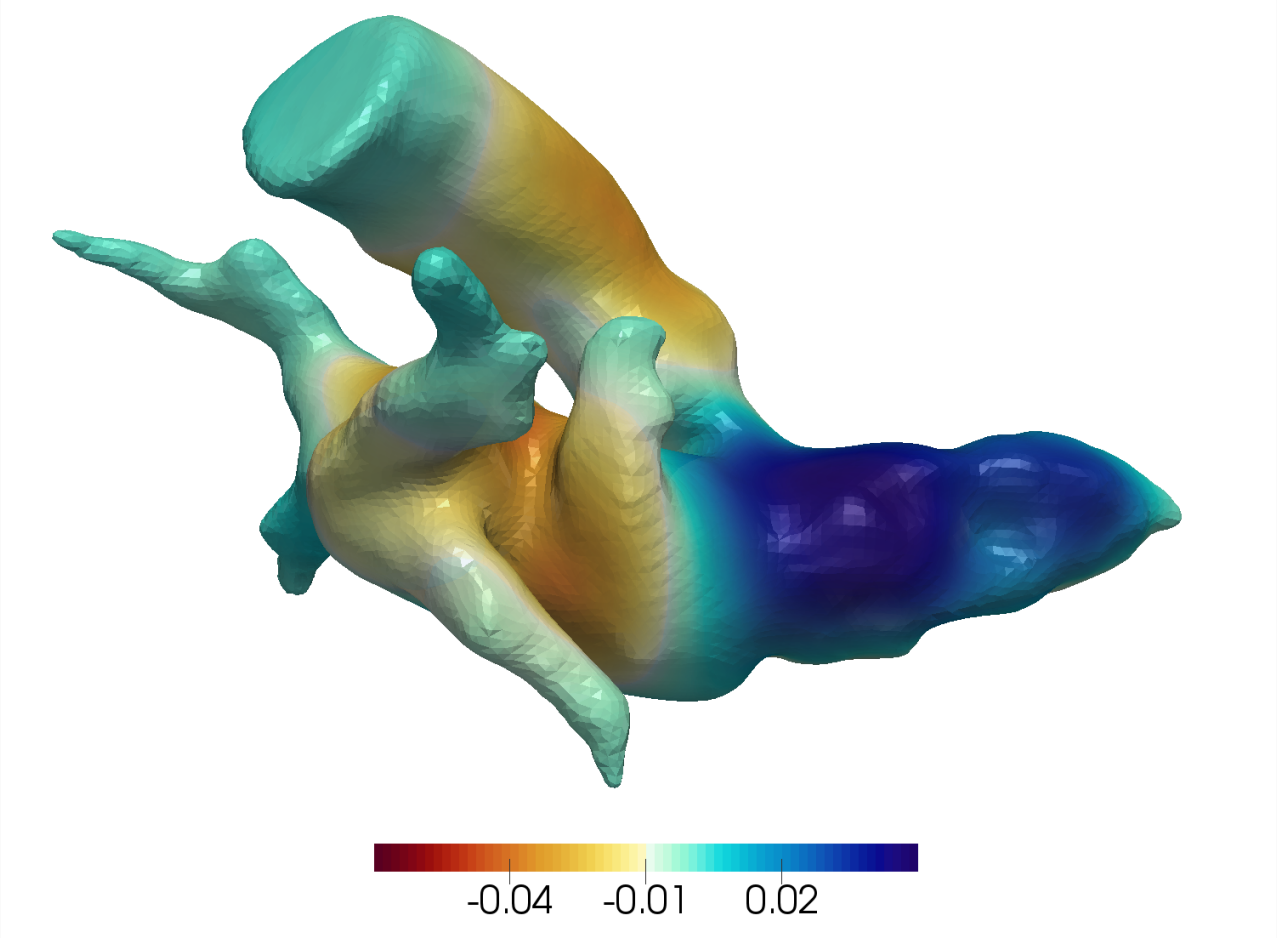

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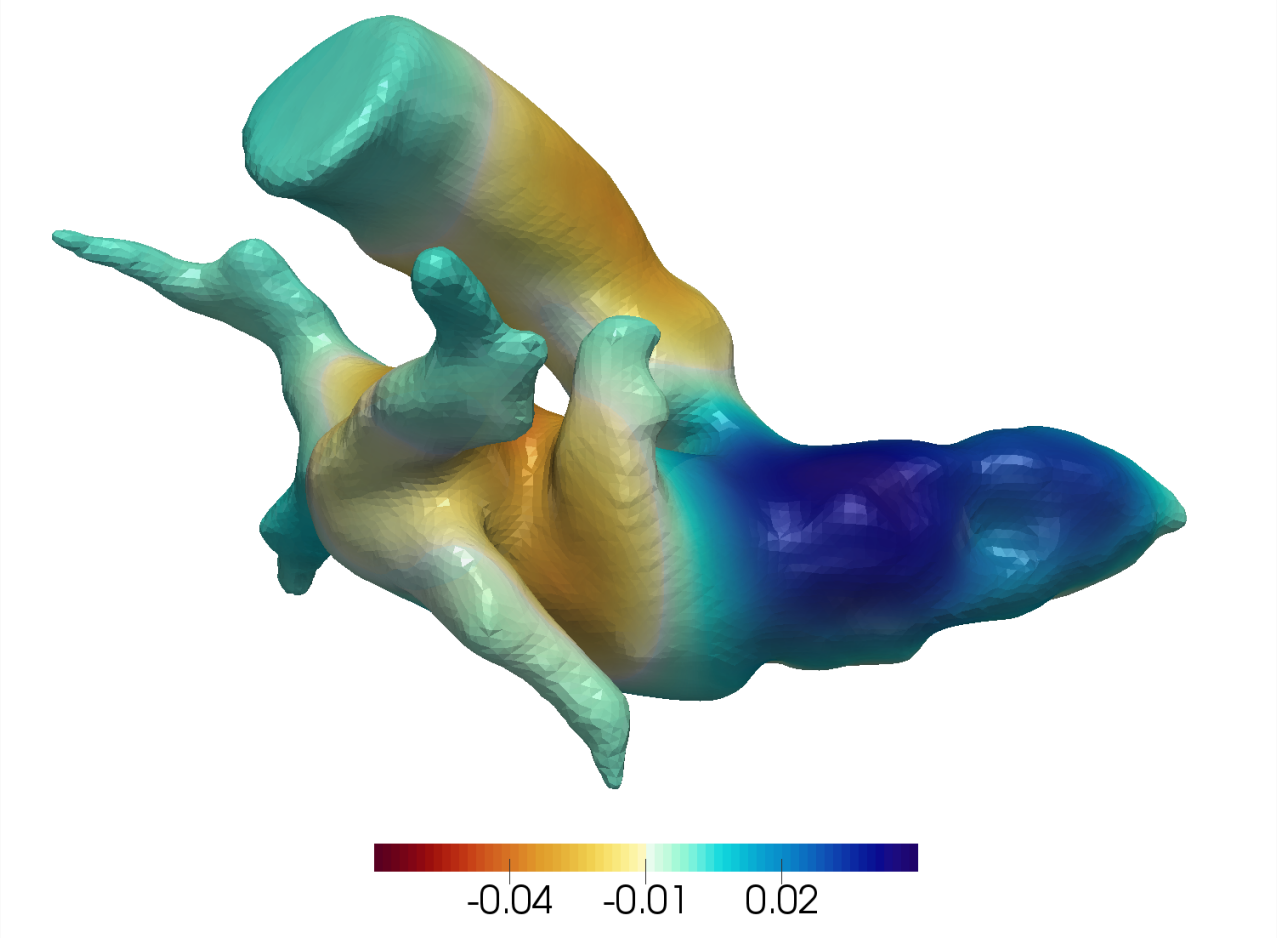

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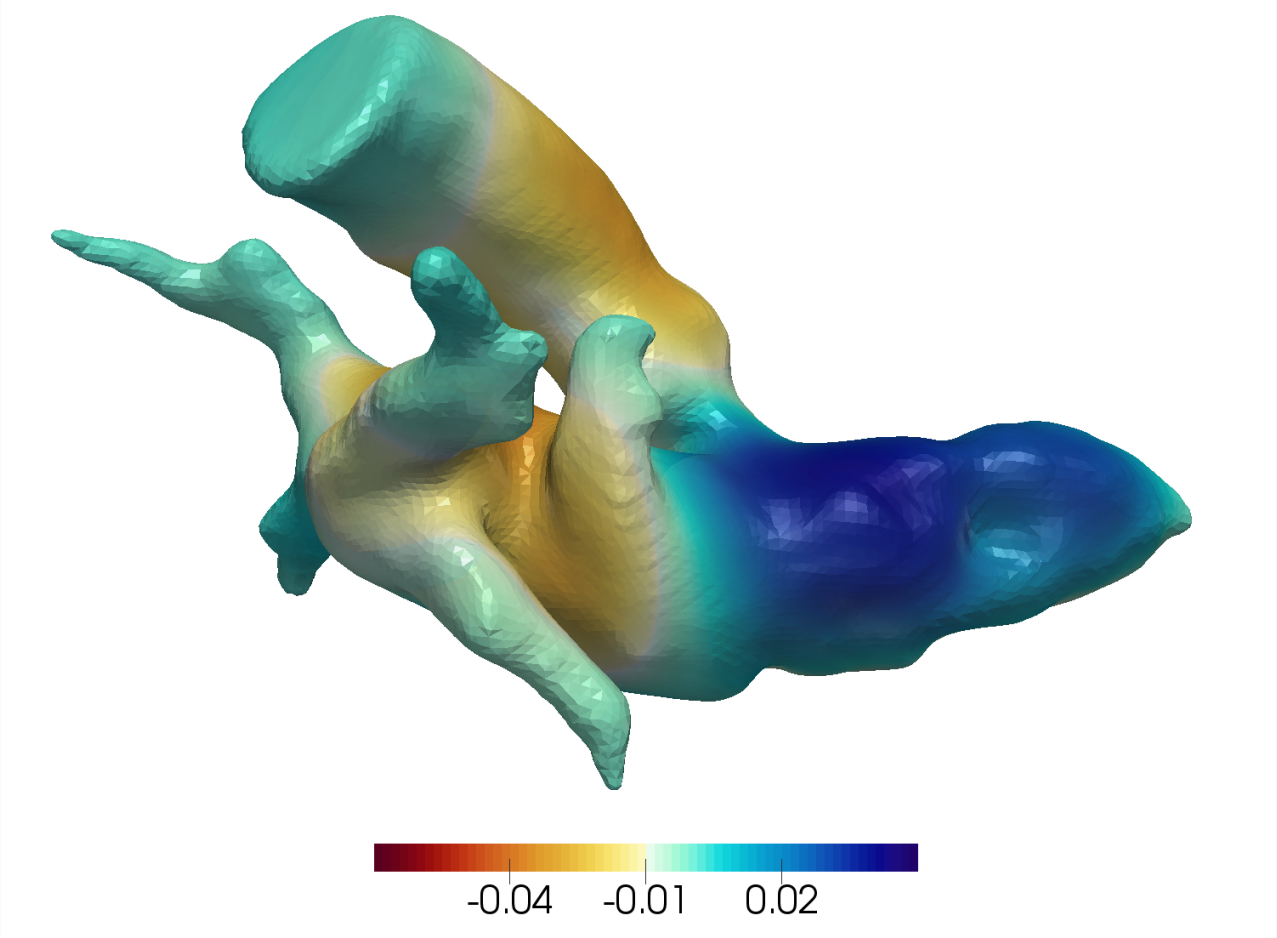

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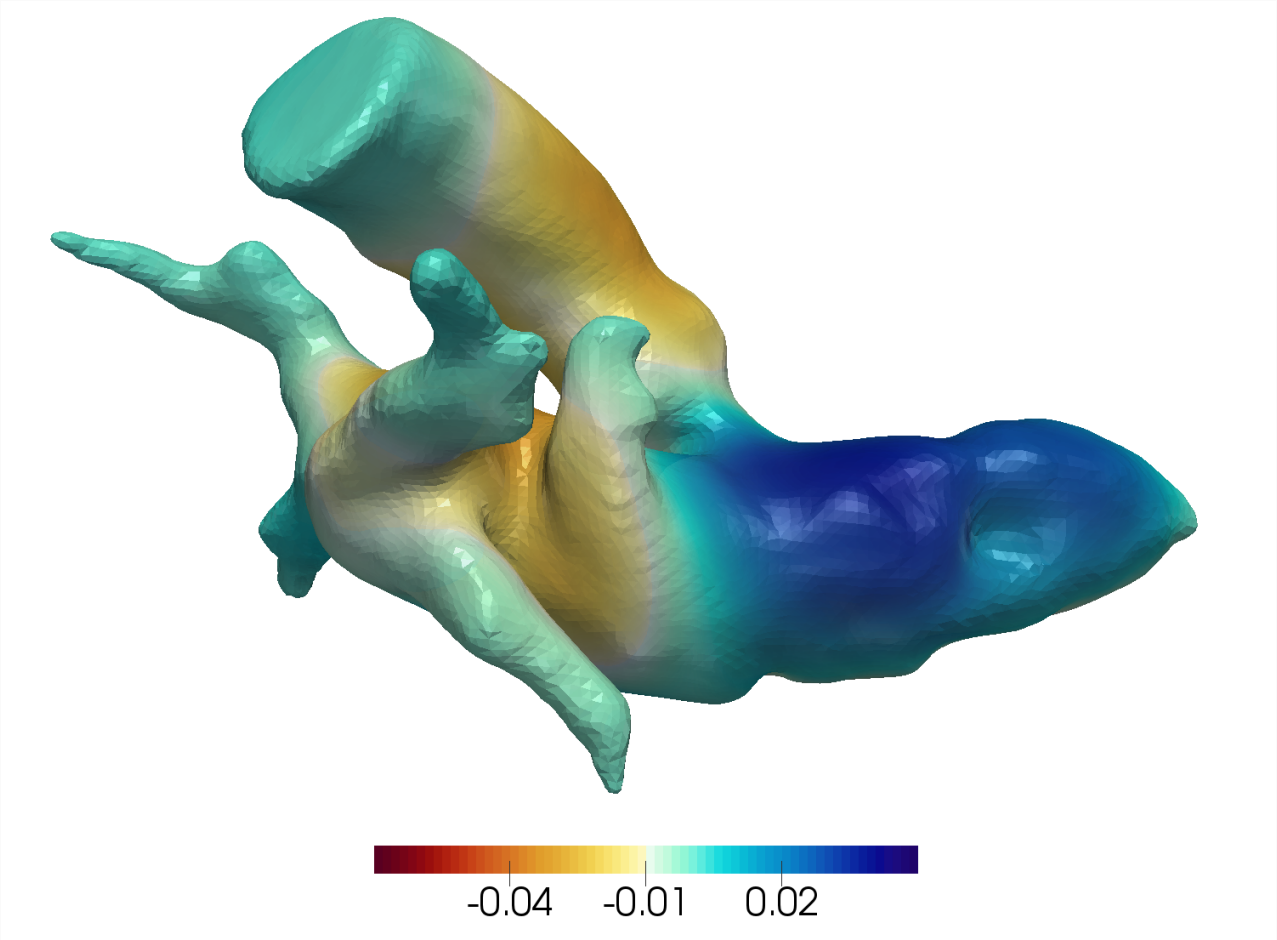

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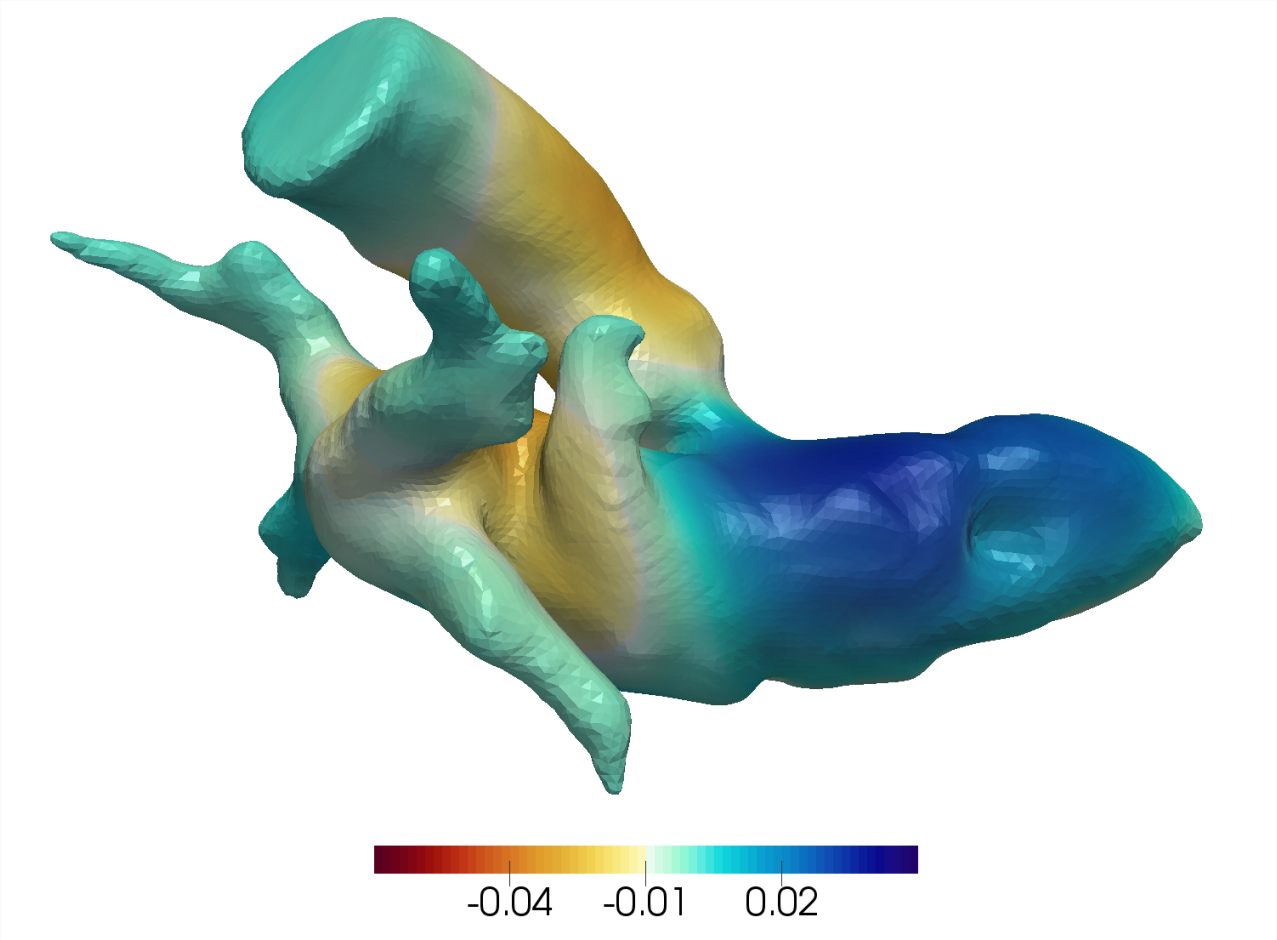

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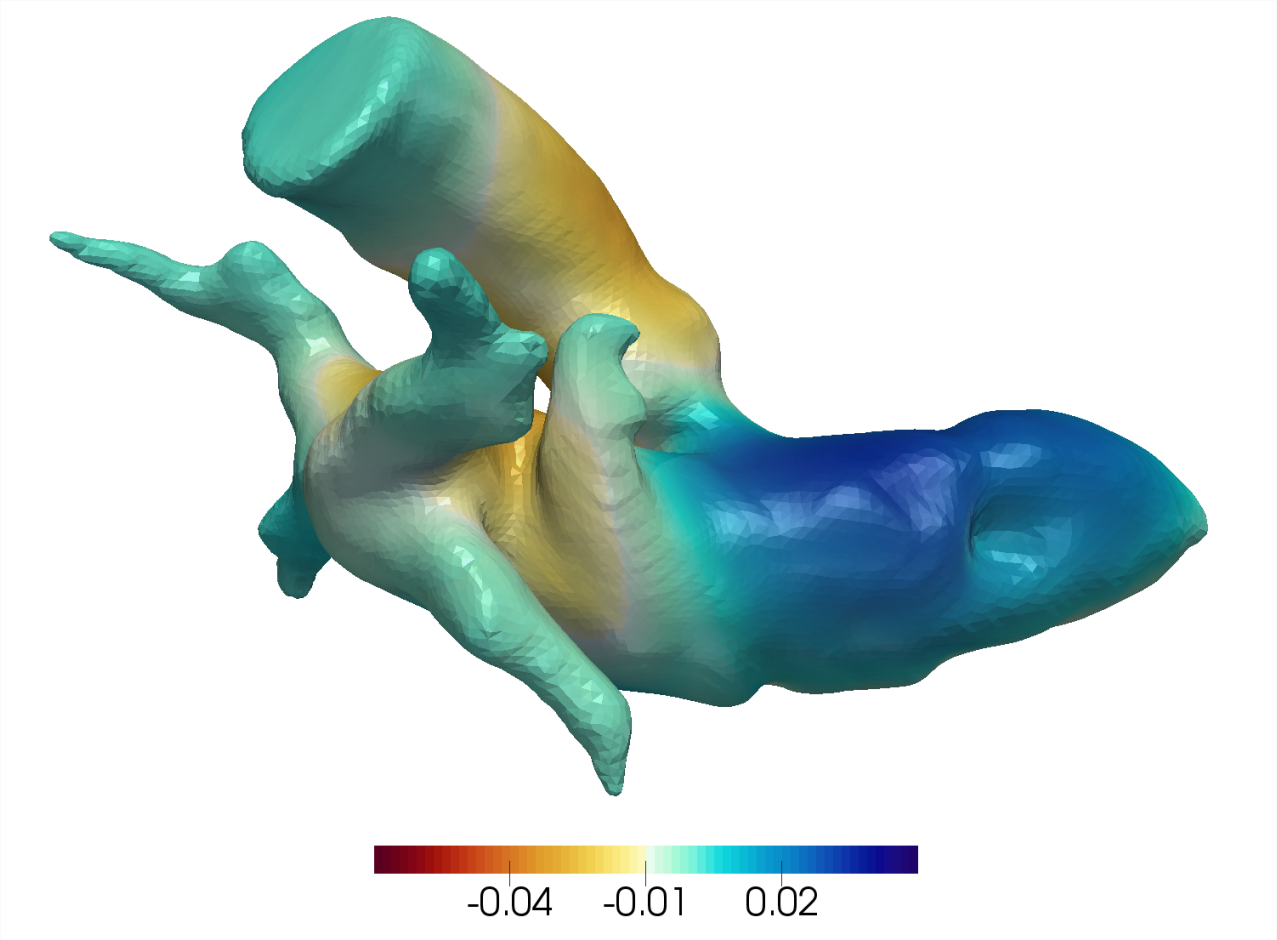

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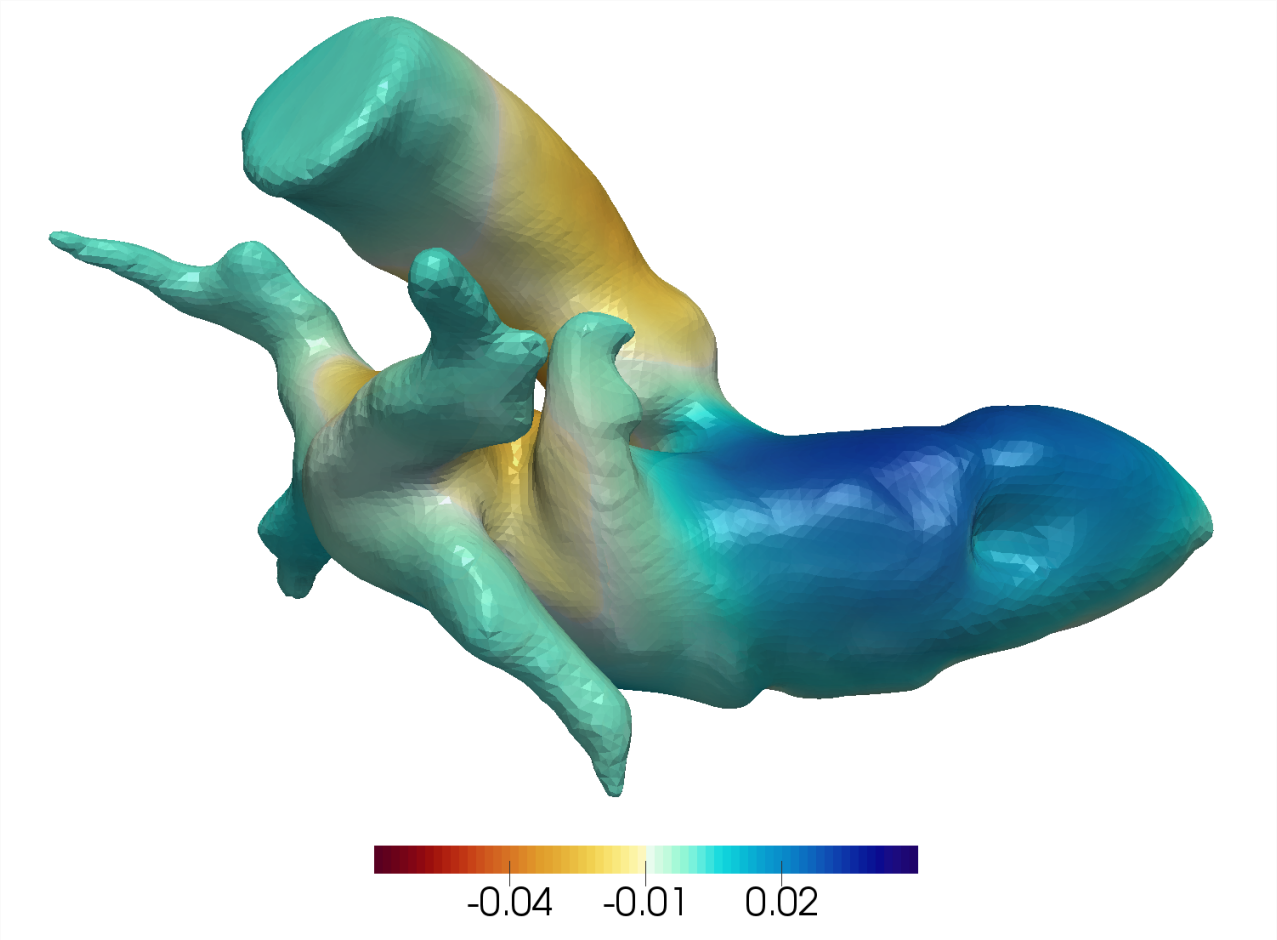

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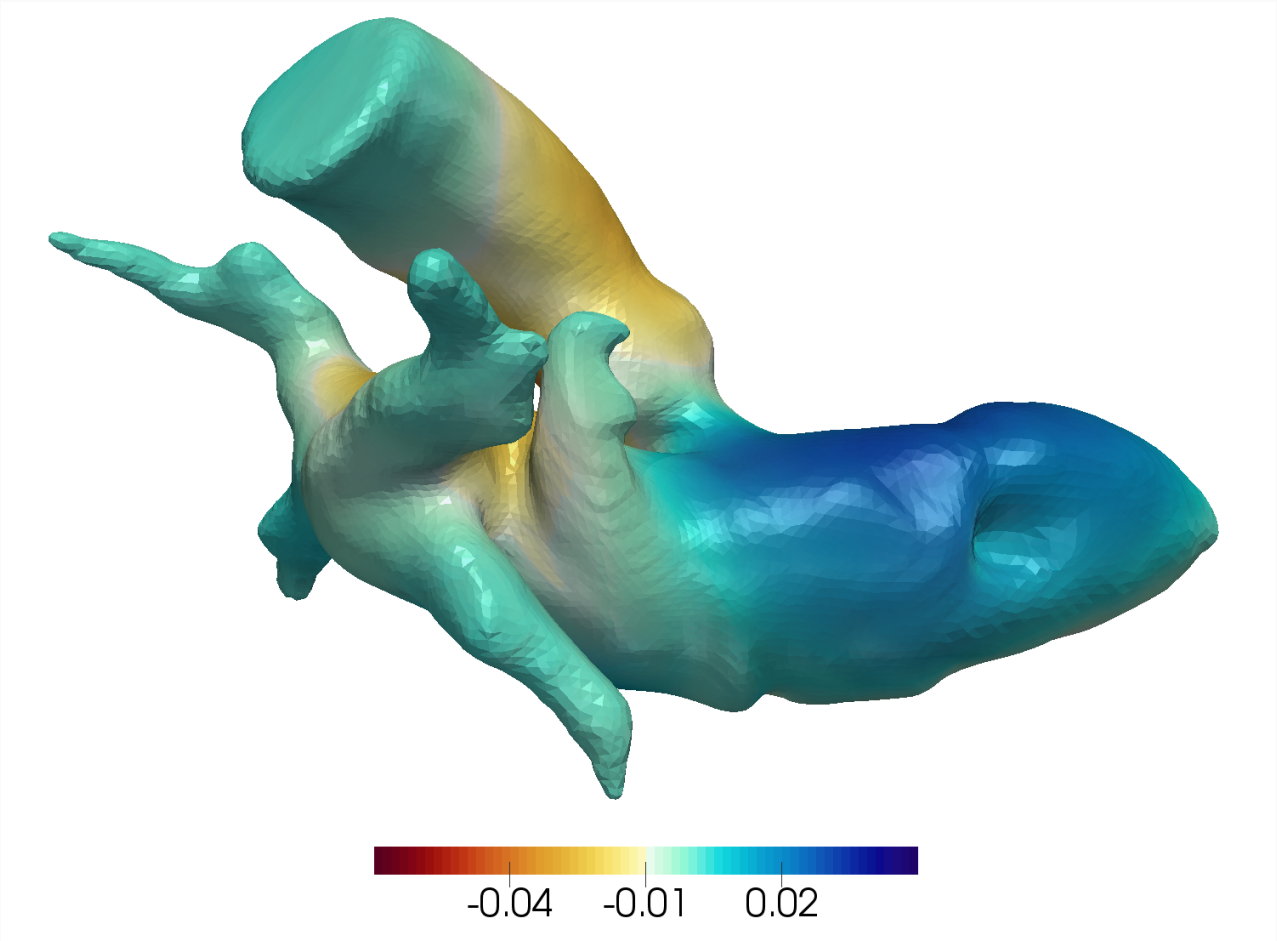

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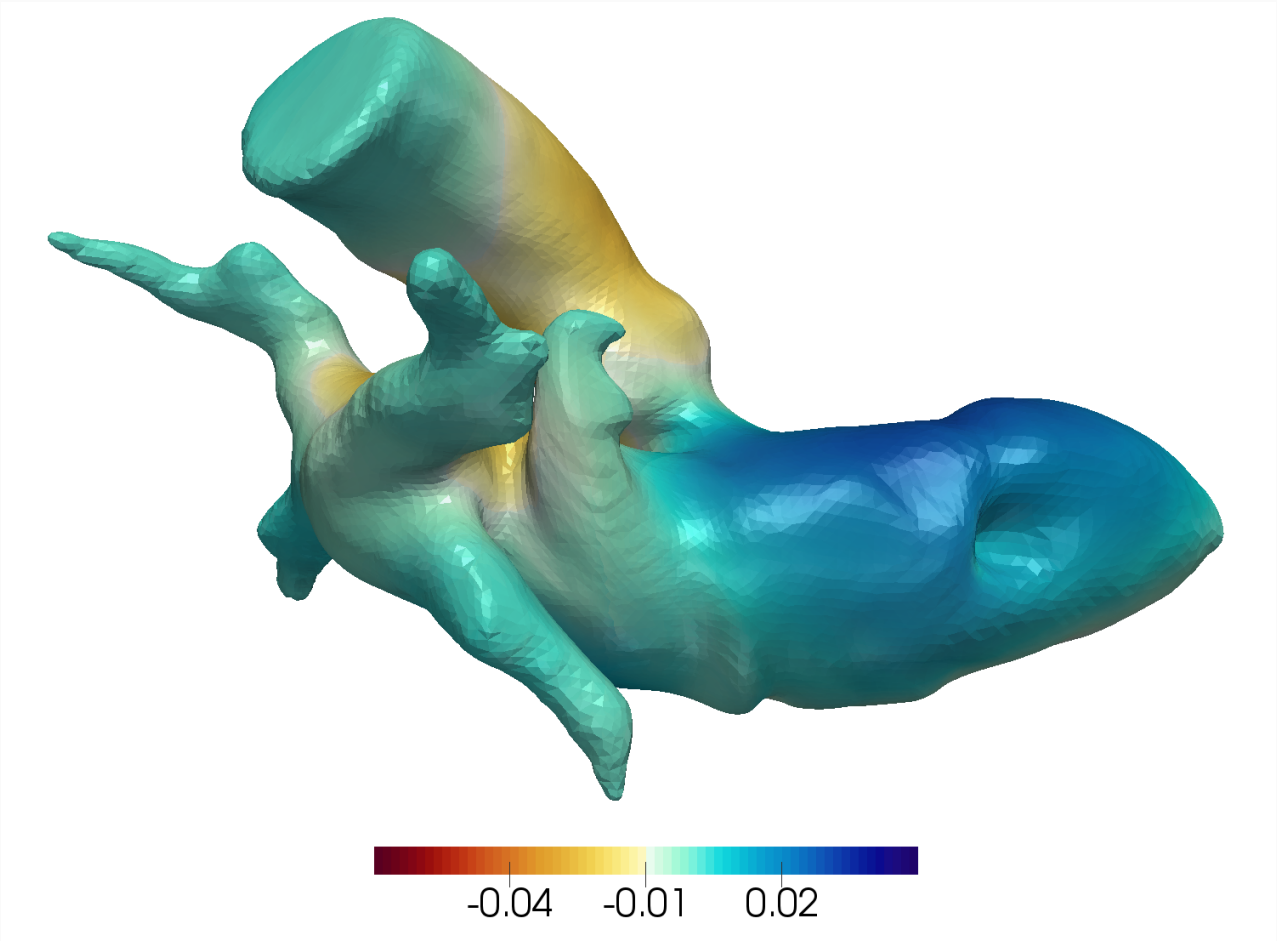

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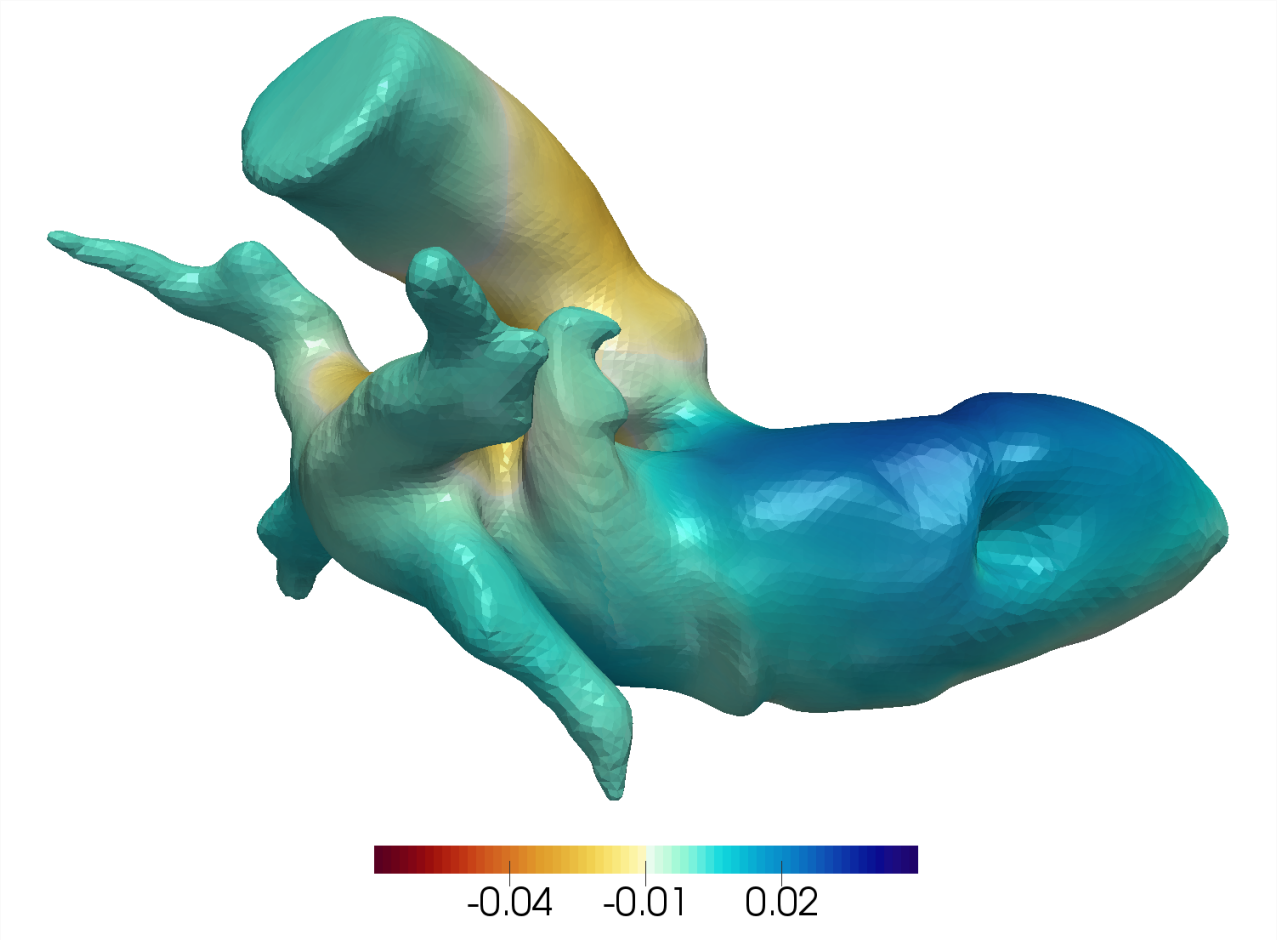

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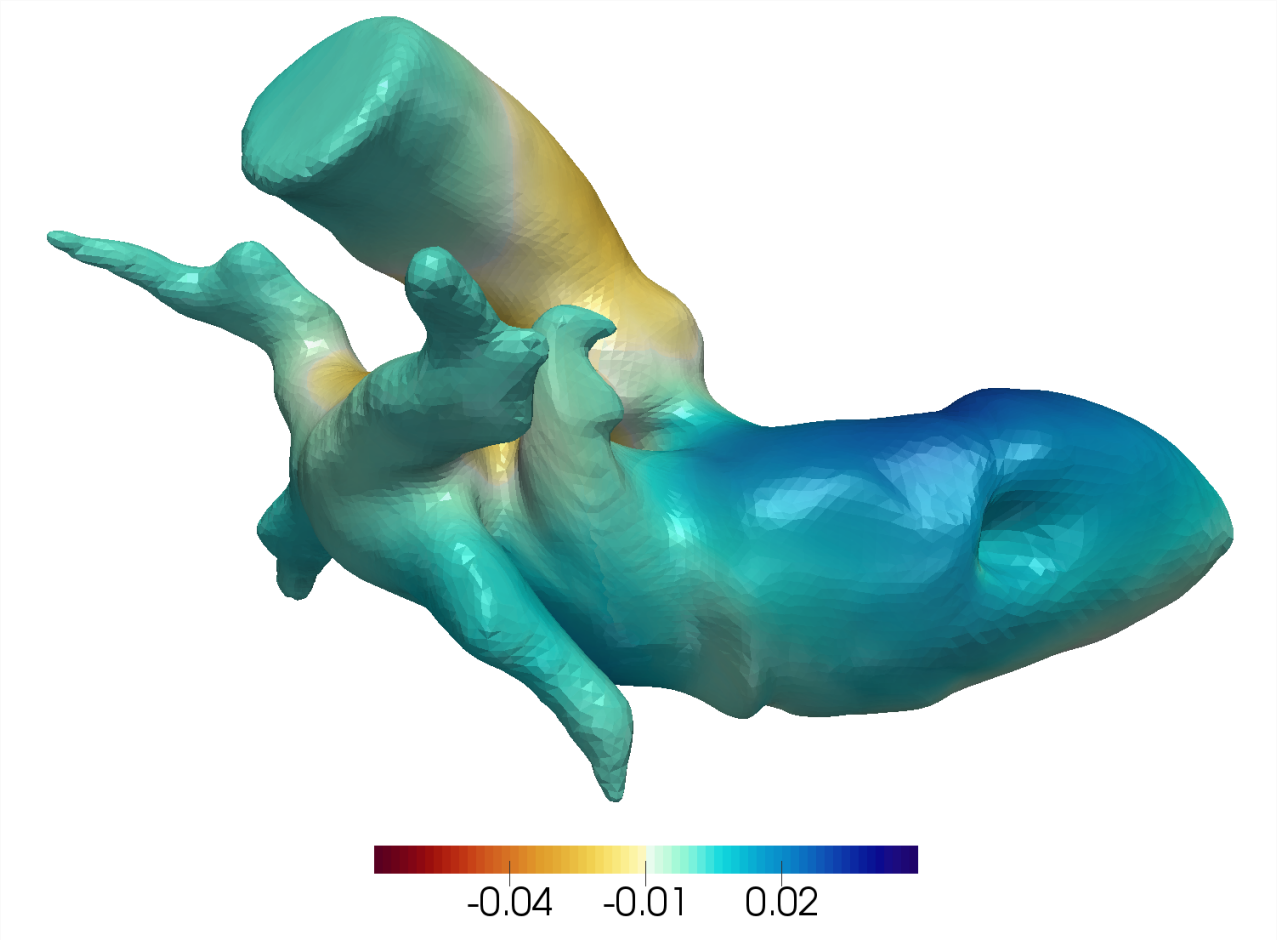

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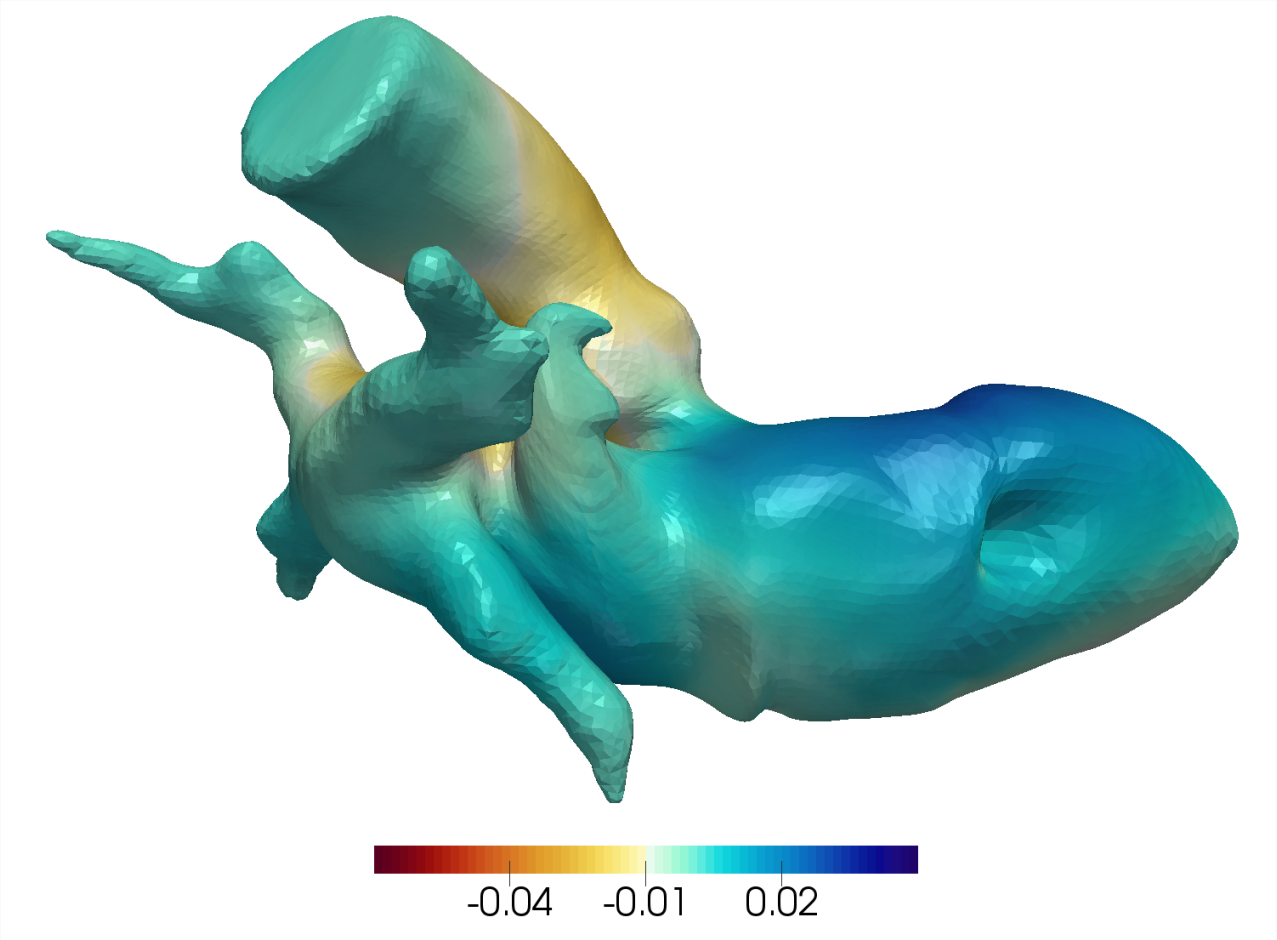

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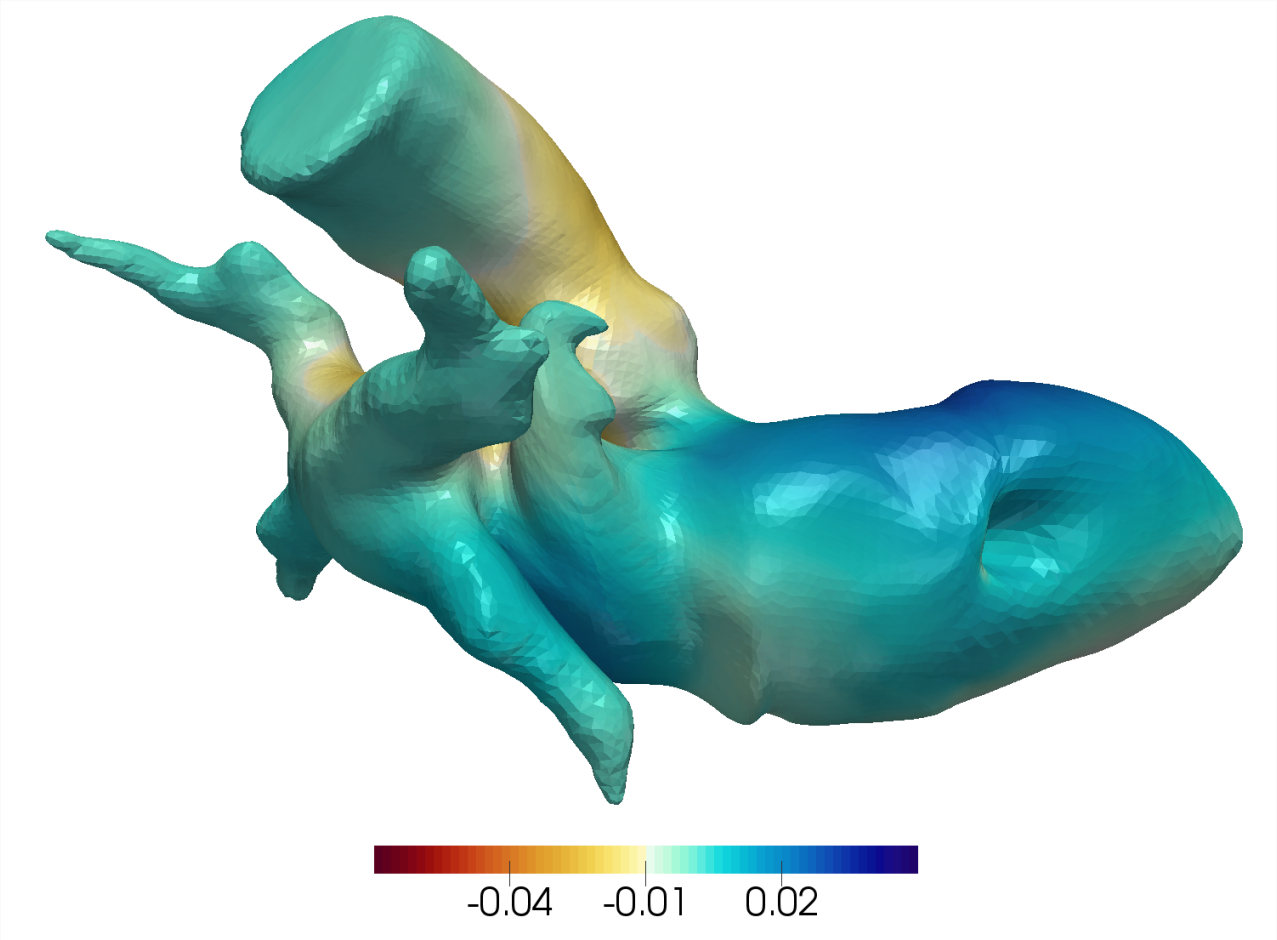

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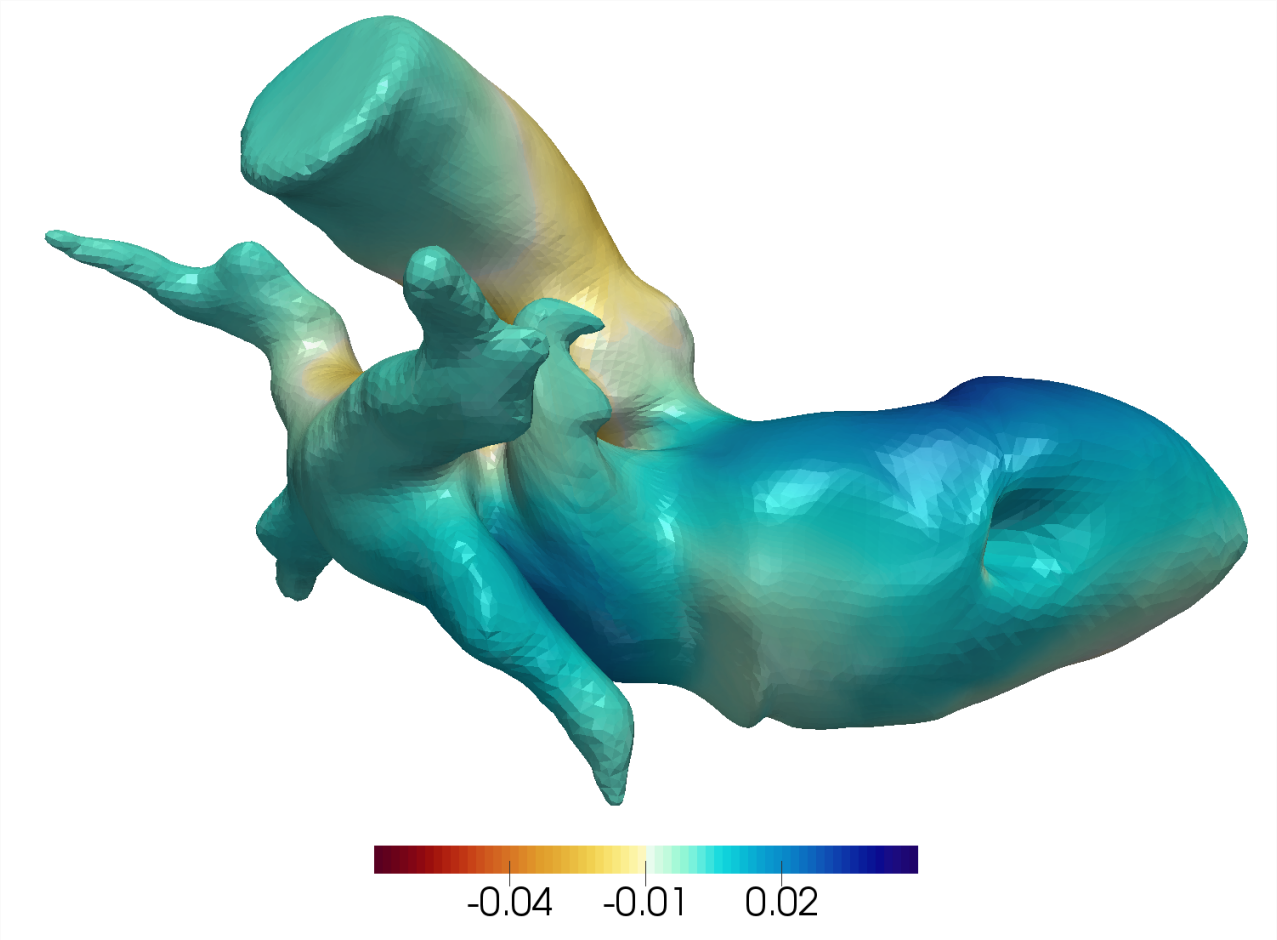

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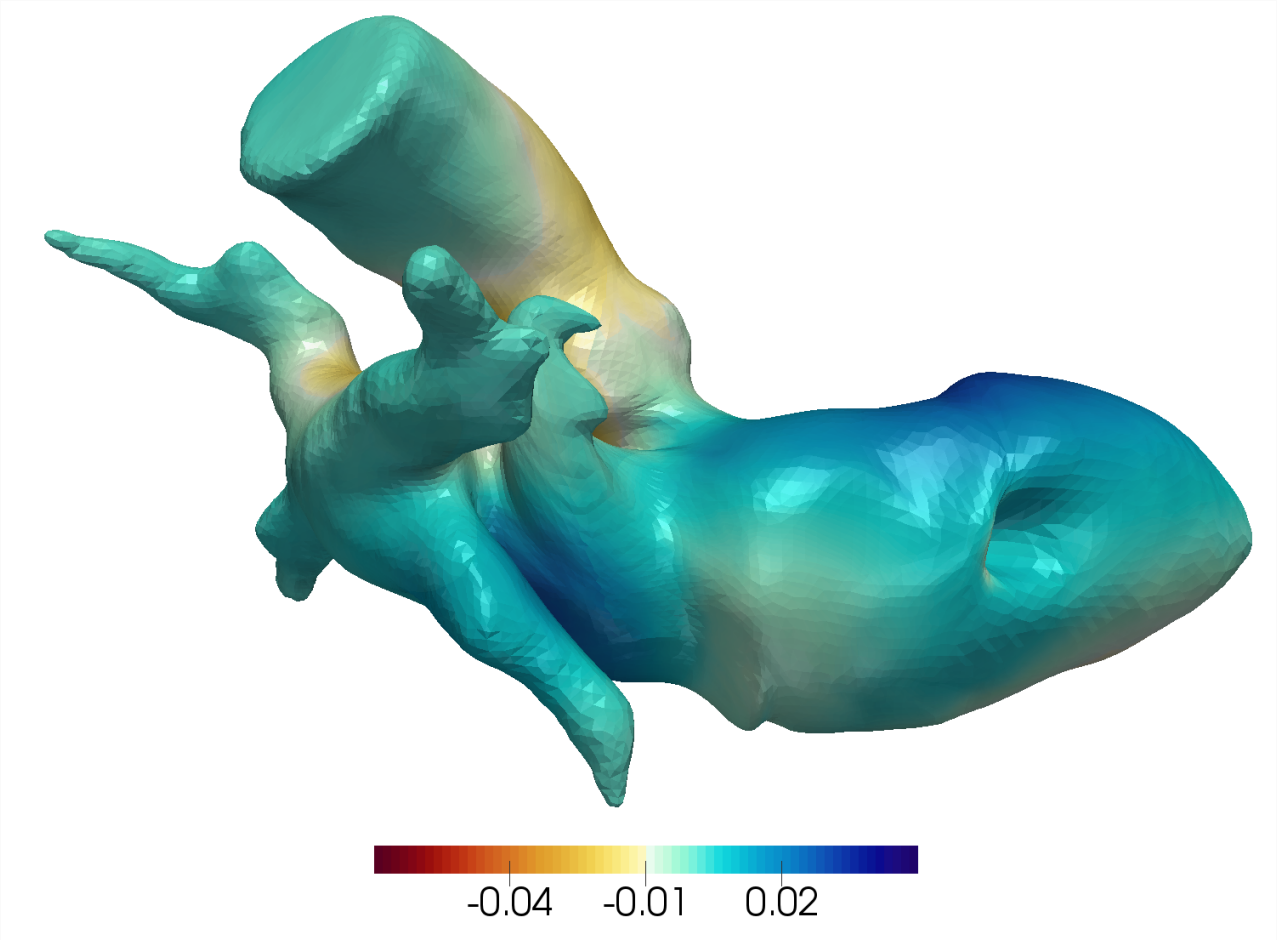

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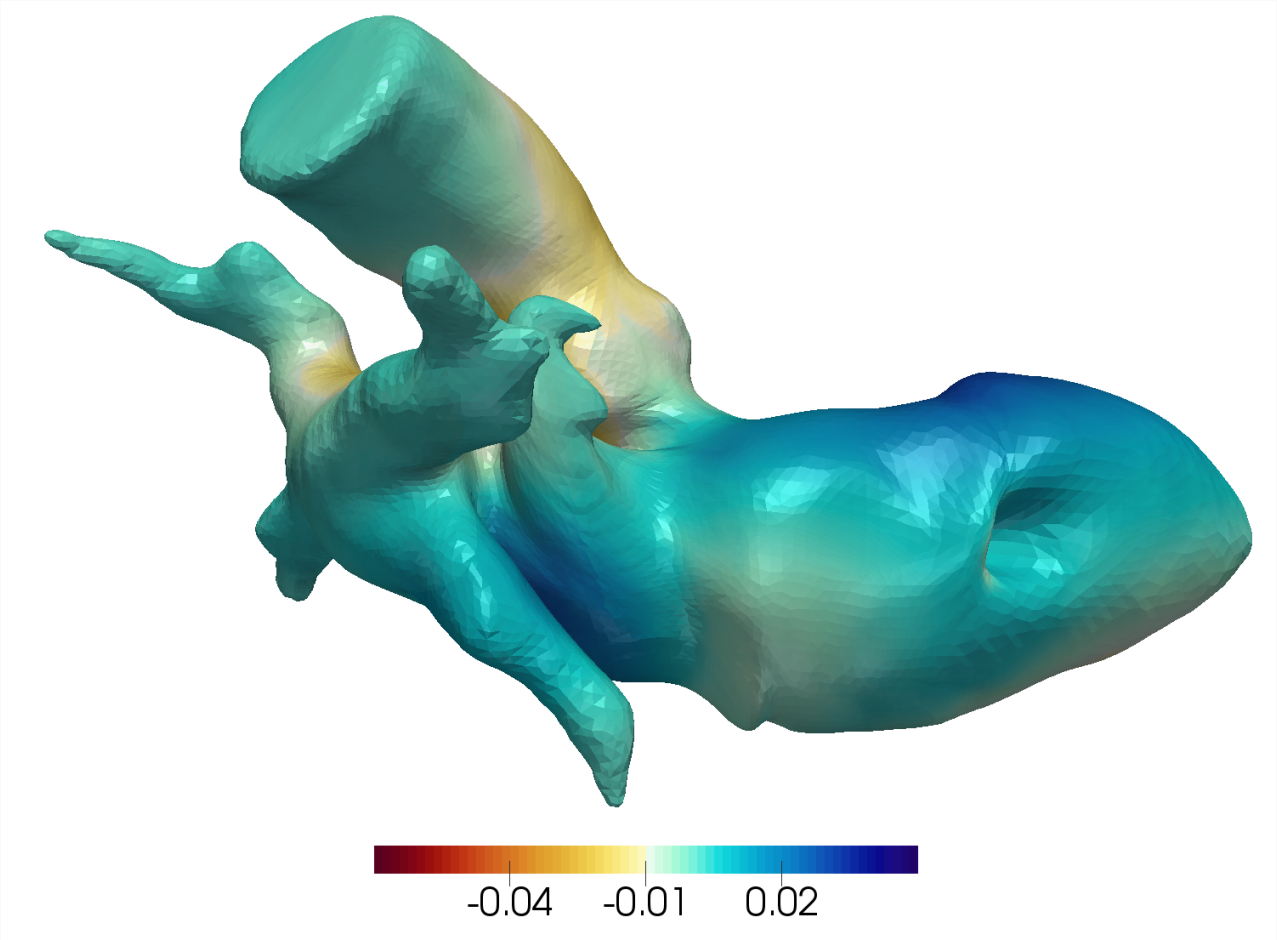

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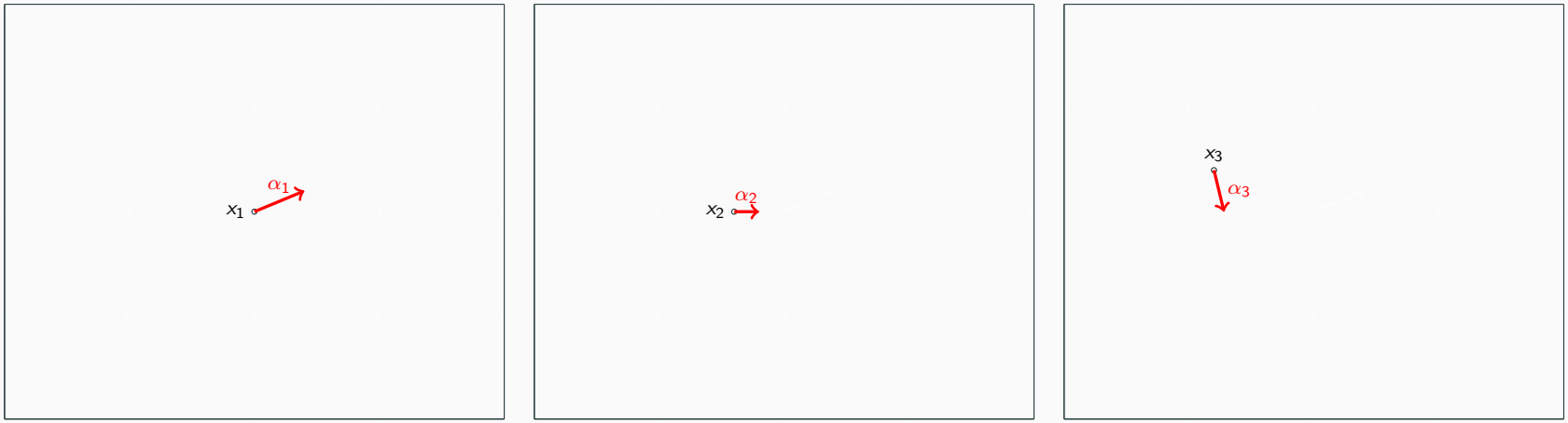
Geometrical deformations: RKHS of vectors fields

- **Space of vectors fields V :** an RKHS of vectors fields (smooth, vanishing at infinity). There exists a kernel $K_s : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}^{D\times D}$ such that

$$\text{Span}\{\delta_x^\alpha = K_s(x,\cdot)\alpha, x \in \mathbb{R}^D, \alpha \in \mathbb{R}^D\}$$

  is dense in V. In practice, $D = 2, 3$ and

$$K_s(x,y) = e^{-\frac{\|x-y\|^2}{\sigma^2}} Id_D.$$



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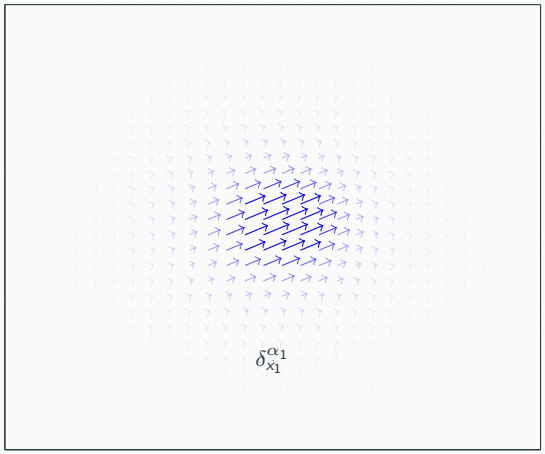

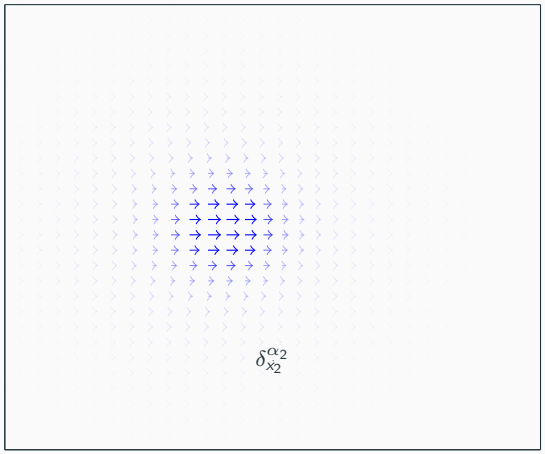

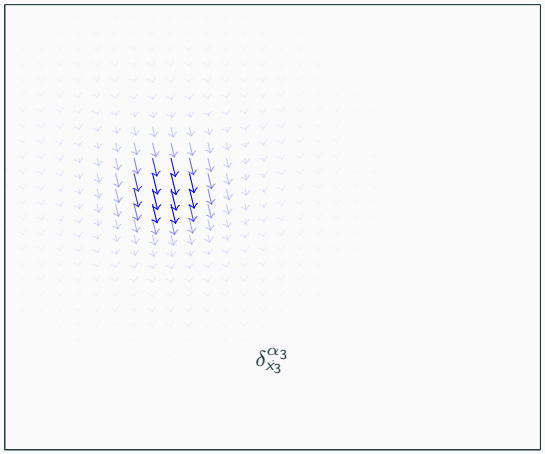

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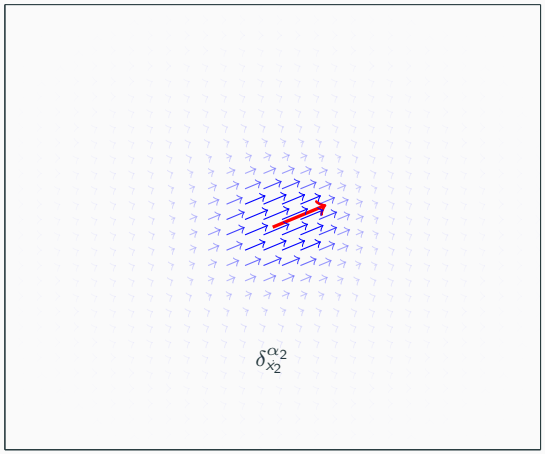
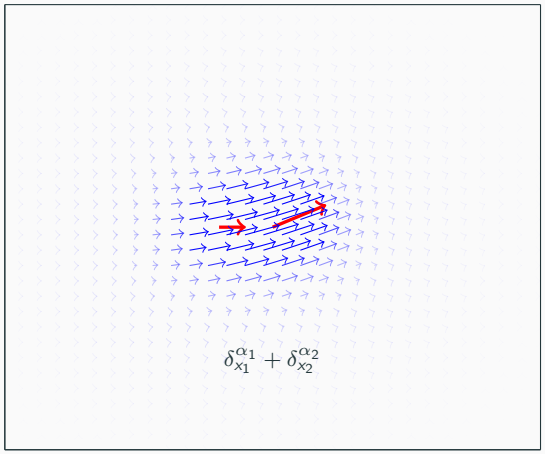
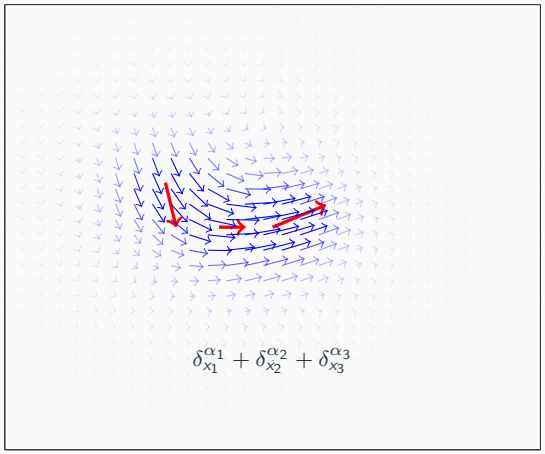


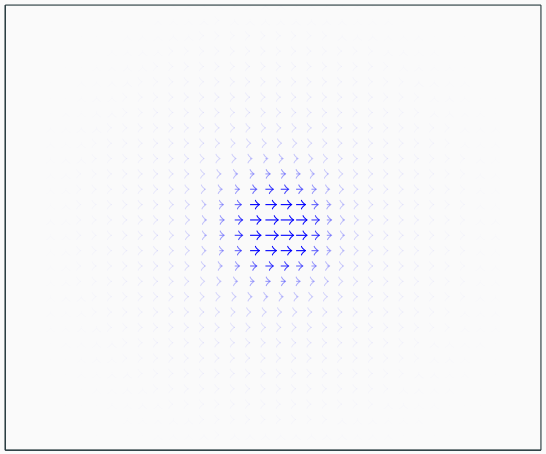


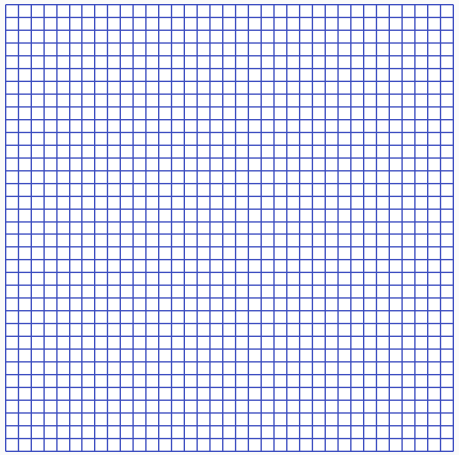


Geometrical deformations: flow of time varying smooth vector field

- **Flow:** let $v = (v_t)_{t\in[0,1]} \in V$ be a time dependant vectors field of $\mathbb{R}^D$. Let $\varphi : [0,1] \times \mathbb{R}^D \to \mathbb{R}^D$:

$$\begin{cases} \dot{\varphi}_t(x) = v_t(\varphi_t(x)) \\ \varphi_0(x) = x. \end{cases} \qquad t \in [0,1] \text{ and } x \in \mathbb{R}^D$$





$t = 0$

Geometrical deformations: flow of time varying smooth vector field

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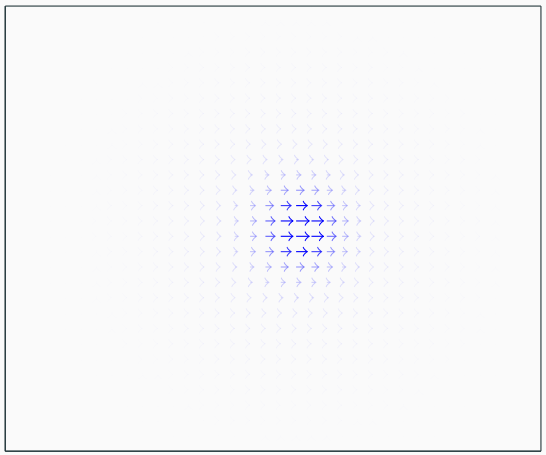

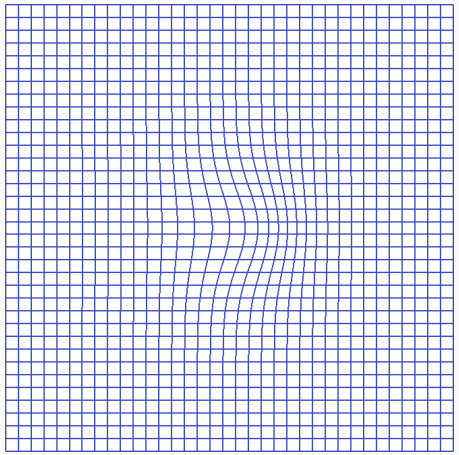

$t = 1/5$

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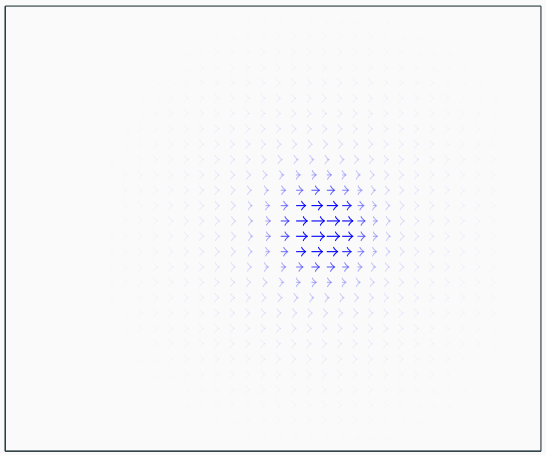

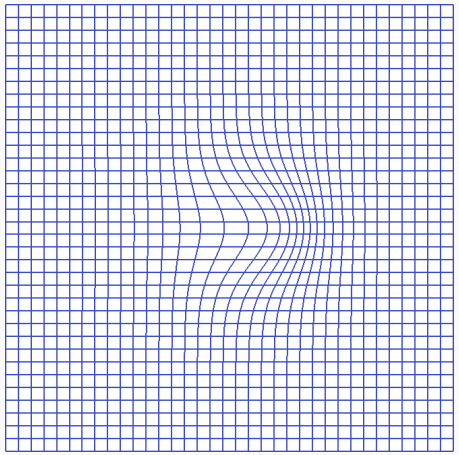

$t = 2/5$

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- **Flow:** let $v = (v_t)_{t\in[0,1]} \in V$ be a time dependant vectors field of $\mathbb{R}^D$. Let $\varphi : [0,1] \times \mathbb{R}^D \to \mathbb{R}^D$:

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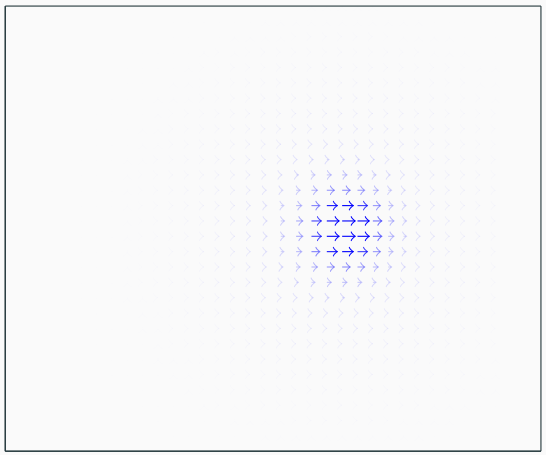

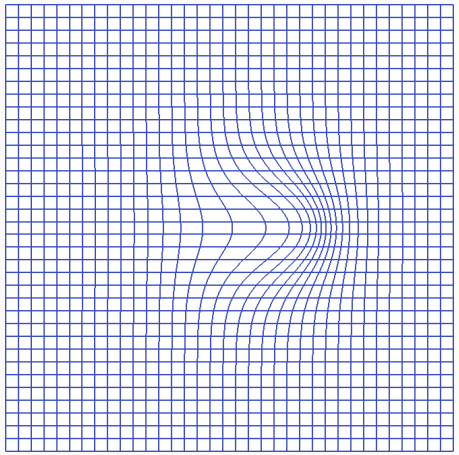

$t = 3/5$

Geometrical deformations: flow of time varying smooth vector field

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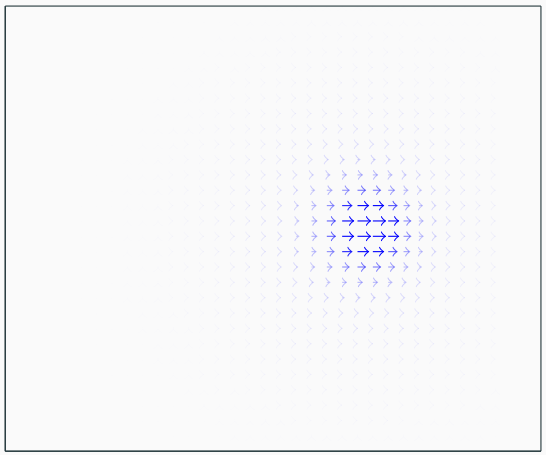

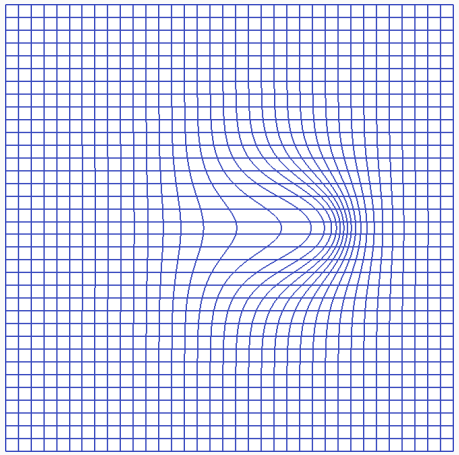

$t = 4/5$

Geometrical deformations: flow of time varying smooth vector field

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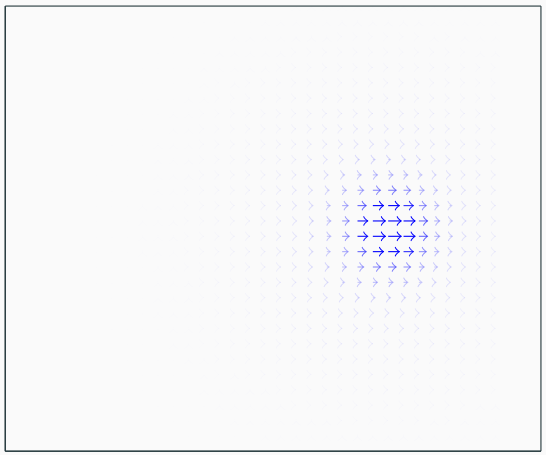

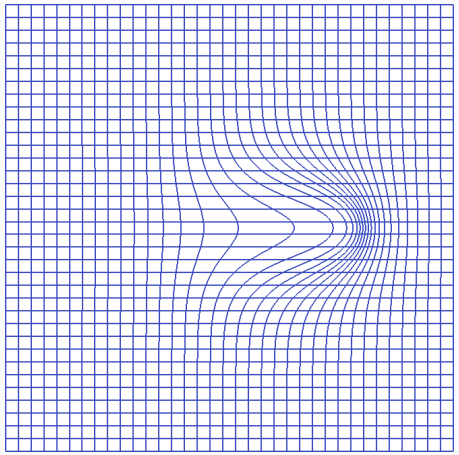

$t = 1$

Geometrical deformations: a group acting on objects

The space V contains smooth vectors fields vanishing at infinity.

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- **Group action :** Let $L^2_V \doteq L^2([0,1], V)$. For all $v \in L^2_V$, $\varphi_1^v(\cdot)$ is a $\mathcal{C}^1$-difféomorphism of $\mathbb{R}^D$. The set

$$G_V = \{\varphi_1^v : \mathbb{R}^D \to \mathbb{R}^D, v \in L^2_V\}$$

  is a group endowed with the (right invariant) distance

$$d^2(\mathrm{Id}, \varphi) = \inf\{\|v\|^2_{L^2_V} \doteq \int_0^1 \|v_t\|^2_V dt, \dot{\varphi} = v \circ \varphi, \varphi_1 = \varphi\}$$

- **Initial momentum :** vectors field $p_0 : \mathbb{R}^D \to \mathbb{R}^D$ generating minimum energy deformations by integrating an Hamiltonian system.

Computing an Hamiltonian

Let $\boldsymbol{q}, \boldsymbol{p} \in \mathbb{R}^{N \times D}$, we need to compute the Hamiltonian (interpreted as a kinetic energy / RKHS norm).

$$H(\boldsymbol{q}, \boldsymbol{p}) = \frac{1}{2} \boldsymbol{p}^t \underbrace{K_s(\boldsymbol{q}, \boldsymbol{q})}_{O(N^2)\text{terms}} \boldsymbol{p} = \frac{1}{2} \sum_i \sum_j p_i^t \underbrace{K_s(q_i, q_j)}_{\exp(-\|q_i - q_j\|^2 / s^2)} p_j$$

. . . and its derivative (up to 2nd order).

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```
import torch

torch.set_default_tensor_type(torch.cuda.FloatTensor)

# Clouds of 1000 points in 3D
N, D = 1000, 3

# Generate arbitrary arrays
q = torch.randn(N, D, requires_grad=True)
p = torch.randn(N, D, requires_grad=True)
s2 = torch.tensor([0.5 * 0.5], requires_grad=False)
```

Computing the Hamiltonian

```
def gaussian_kernel(x, y, sigma2):
    x_i = x[:, None, :]                    # (M, 1, 1)
    y_j = y[None, :, :]                    # (1, N, 1)
    D_ij = ((x_i - y_j) ** 2).sum(-1)      # (M, N) matrix of squared distances
    return (-D_ij / sigma2).exp()          # (M, N) matrix of Gaussian kernel
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K_qq = gaussian_kernel(q, q, s2)
```

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    return (-D_ij / sigma2).exp()          # (M, N) matrix of Gaussian kernel

K_qq = gaussian_kernel(q, q, s2)

v = K_qq @ p                               # mat. mult. (N,N) @ (N,D) = (N,D)
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torch.cuda.OutOfMemoryError:  CUDA out of memory.  [...]
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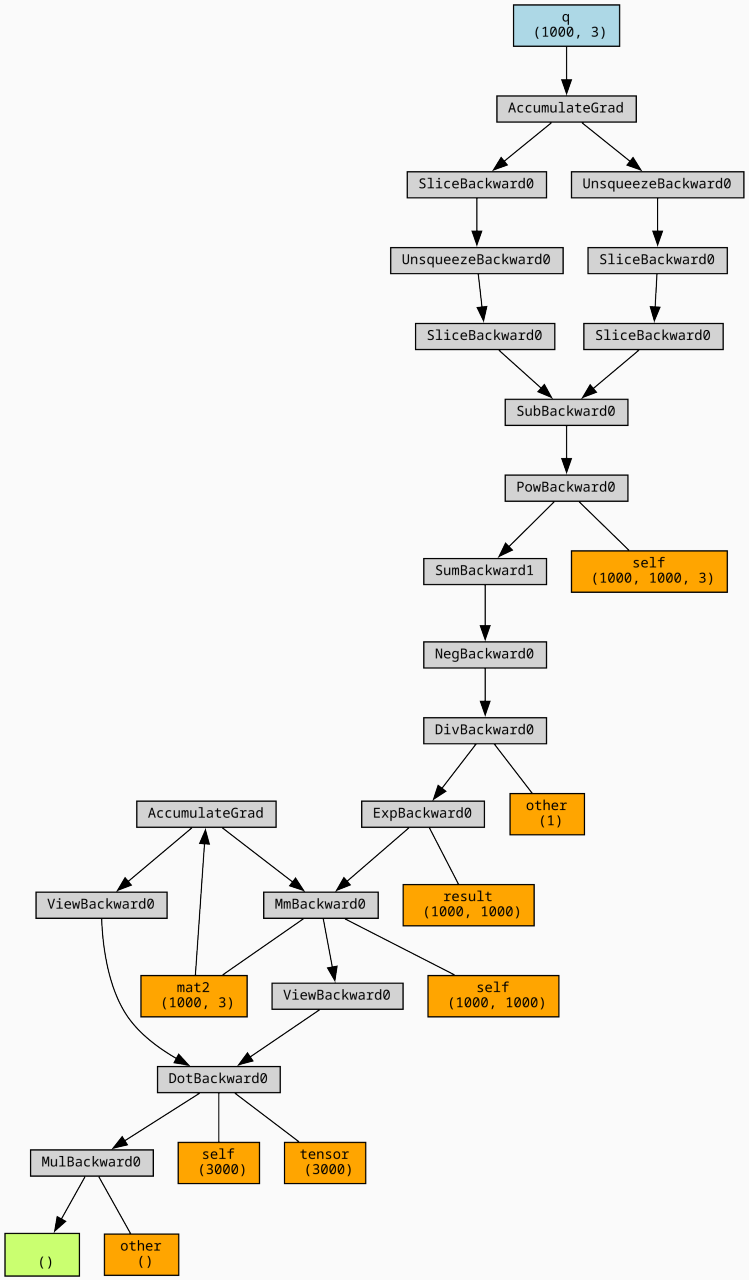
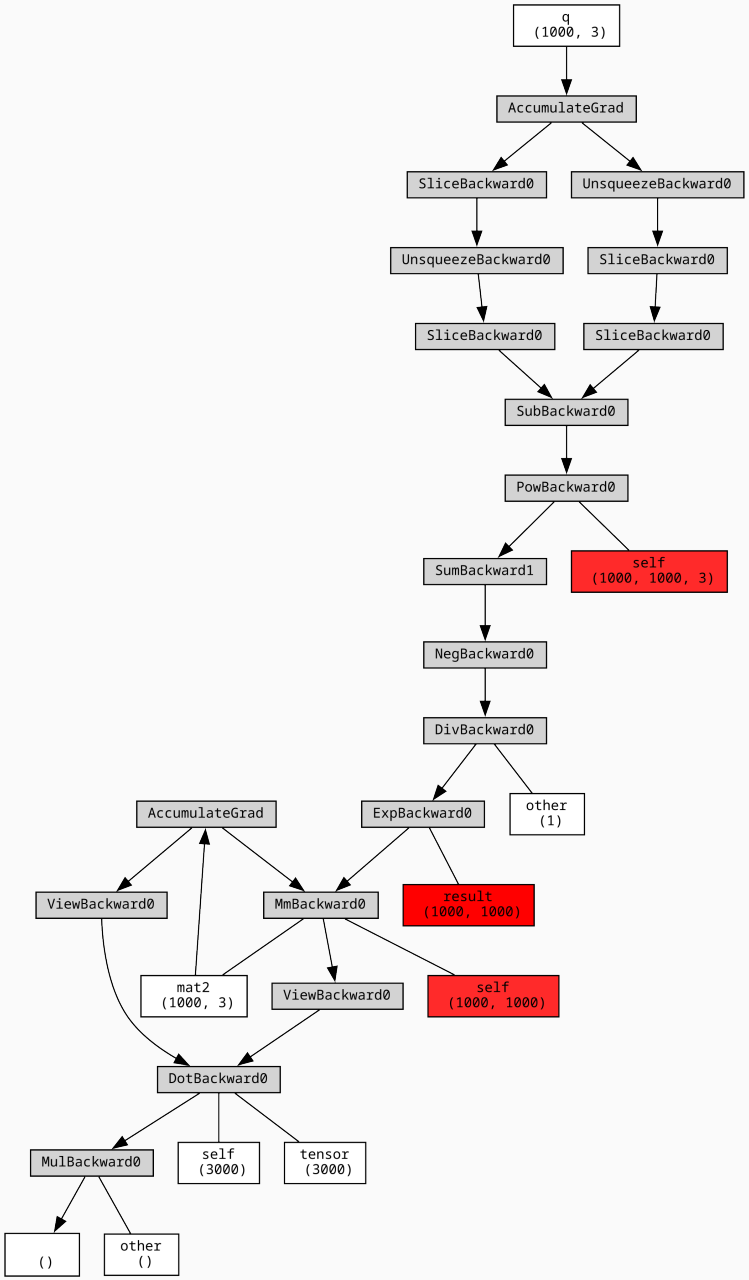
torch.cuda.OutOfMemoryError:  CUDA out of memory.  [...]
```

```
from torchviz import make_dot

# Display -- see next figure.
make_dot(H, {'q':q, 'p':p, 's':s2}, show_saved=True).render(view=True)
```


q
(1000, 3)
AccumulateGrad
SliceBackward0
UnsqueezeBackward0
UnsqueezeBackward0
SliceBackward0
SliceBackward0
SliceBackward0
SubBackward0
PowBackward0
SumBackward1
self
(1000, 1000, 3)
NegBackward0
DivBackward0
AccumulateGrad
ExpBackward0
other
(1)
ViewBackward0
MmBackward0
result
(1000, 1000)
mat2
(1000, 3)
ViewBackward0
self
(1000, 1000)
DotBackward0
MulBackward0
self
(3000)
tensor
(3000)
()
other
()


q
(1000, 3)
AccumulateGrad
SliceBackward0
UnsqueezeBackward0
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SliceBackward0
SliceBackward0
SliceBackward0
SubBackward0
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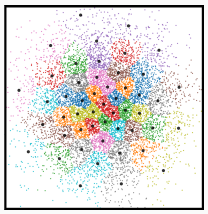
self
(1000, 1000, 3)
NegBackward0
DivBackward0
AccumulateGrad
ExpBackward0
other
(1)
ViewBackward0
MmBackward0
result
(1000, 1000)
mat2
(1000, 3)
ViewBackward0
self
(1000, 1000)
DotBackward0
MulBackward0
self
(3000)
tensor
(3000)
()
other
()

KeOps and symbolic matrices

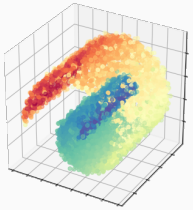
Kernel methods are ubiquitous

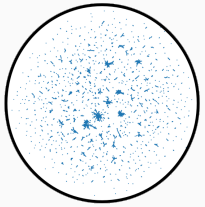
Model dataset with **interacting** particles (*e.g.* through distance or covariance matrix).

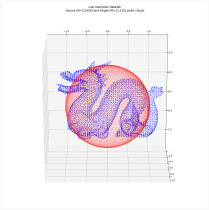

meshes


clustering


Gaussian processes


Spectral methods


Dimension red (UMAP)


Optimal Transport

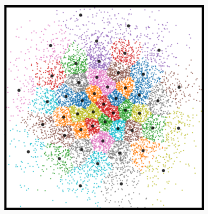
Reproducing Kernel Hilbert spaces

- nice mathematical structures (scalar product, norms, completeness, *etc*. . .)
- from continuous to discrete problems (evaluation is continuous)

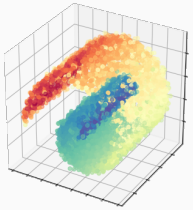
Kernel methods are ubiquitous

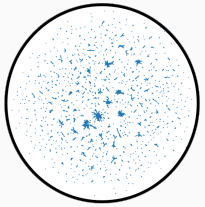
Model dataset with **interacting** particles (*e.g.* through distance or covariance matrix).


meshes


clustering


Gaussian processes


Spectral methods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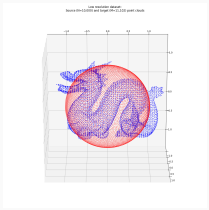

Optimal Transport

Reproducing Kernel Hilbert spaces

- nice mathematical structures (scalar product, norms, completeness, *etc*. . .)
- from continuous to discrete problems (evaluation is continuous)

Since 2017, with J. Glaunès, J. Feydy we are developing  KeOps (kernels on GPU with CUDA)

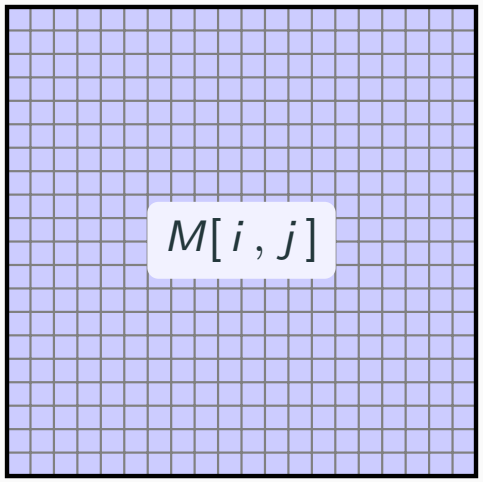
- developped for Deep Learning framework (NeurIPS 2020)
- autodiff with kernels for optimisation (JMLR 2021)

- **Download:** 650k
- **Github stars:** 1k
- **Dependency:** 404
- **Citations:** 170

Prix science ouverte 2023

Ouvrir la science !

Scientific computing libraries represent most objects as tensors

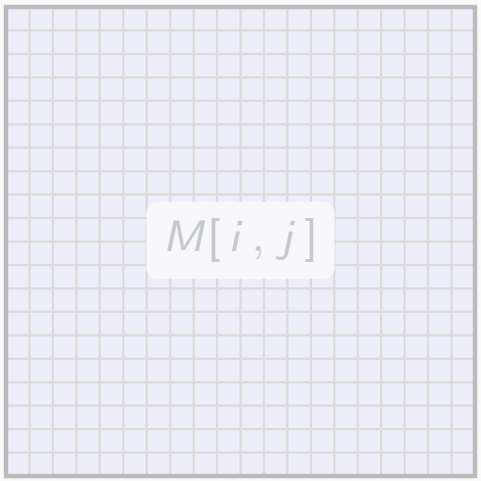


Dense matrix
Coefficients only

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.

Scientific computing libraries represent most objects as tensors



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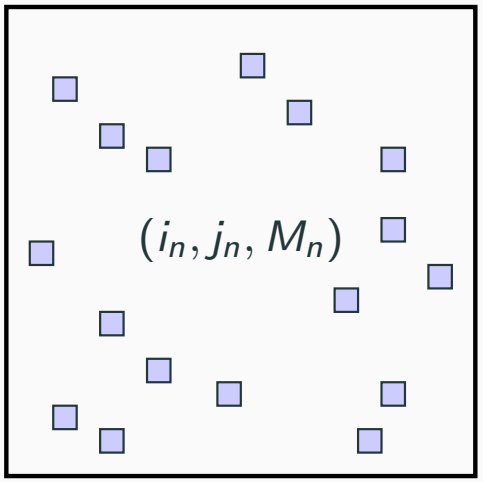
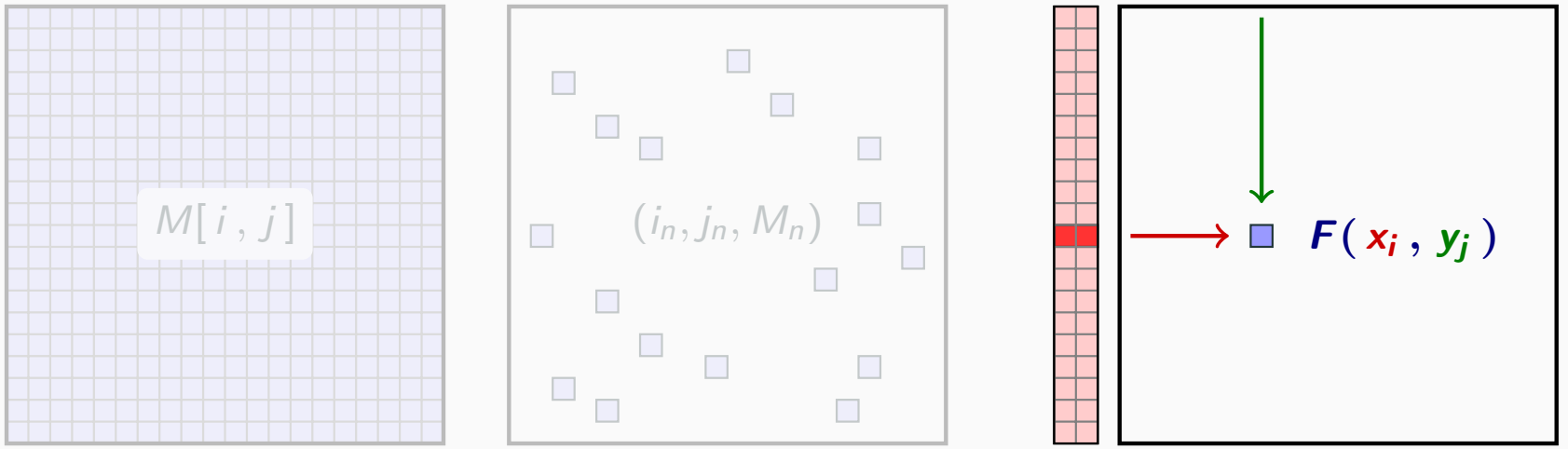


Sparse matrix
Coordinates + coeffs

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.

Scientific computing libraries represent most objects as tensors



Dense matrix
Coefficients only

Sparse matrix
Coordinates + coeffs

Symbolic matrix
Formula + data (think "SIMT")

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.

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

Our library comes with all the perks of a modern numerical computing library:

+ Transparent **array-like** interface (float16, float32, float64).
+ Full support for automatic **differentiation**.
+ Documented and large collection of **tutorials**, available online.

See *www.kernel-operations.io*

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See *www.kernel-operations.io*

Under the hood:

- \+ a meta-programming engine `keopscore` written in `Python` and `Cuda`
- \+ JIT `cuda` code thanks to `nvrtc`
- \+ binders for `PyTorch`, `NumPy` and `R` (thanks to Ghislain Durif).

We welcome **contributors** for `JAX`, `Julia` and other frameworks!

To get started:

```
pip install pykeops
```

Generic reduction in KeOps

Let $1 \leq i \leq N$ and $1 \leq j \leq M$ where $N, M \approx 10^4$ ou 10^6

- A generic case:

$$\left[\sum_j F(\sigma_1, \cdots, \sigma_\ell, X_i^1, \cdots, X_i^k, Y_j^1, \cdots, Y_j^m) \right]_{i=1,\ldots,M} \in \mathbb{R}^M$$

- . . . an even more generic case:

$$\left[\bigstar_j F(\sigma_1, \cdots, \sigma_\ell, X_i^1, \cdots, X_i^k, Y_j^1, \cdots, Y_j^m) \right]_{i=1,\ldots,M} \in \mathbb{R}^M$$

where $\bigstar$ can be any reduction (sum, max, min, logSumExp, *etc.* . .) over a dimension

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
```

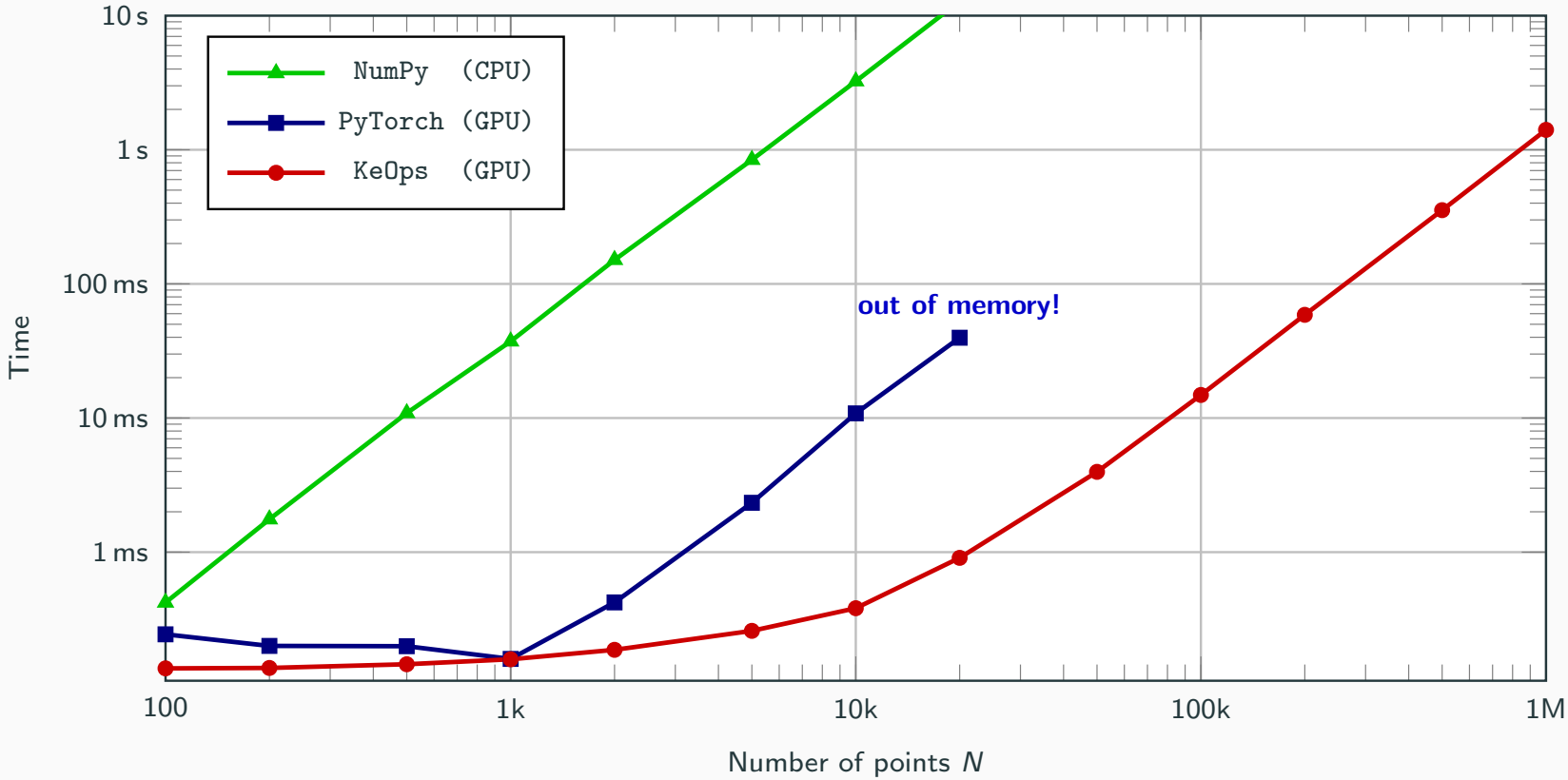
KeOps supports arbitrary **formulas** and **variables** with:

- **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.

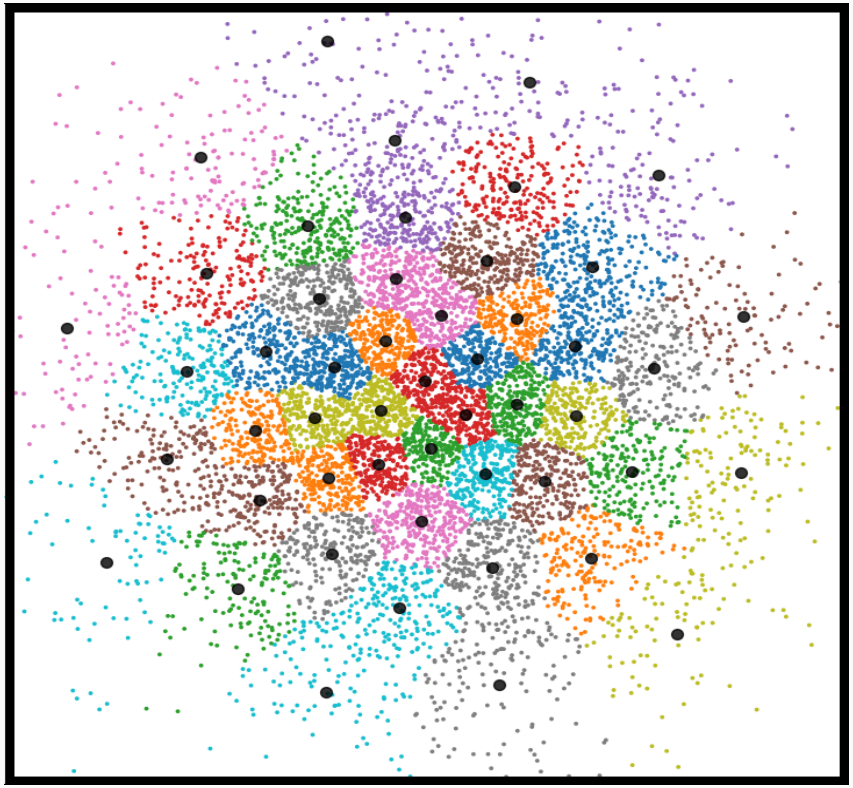
KeOps lets users work with millions of points at a time

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

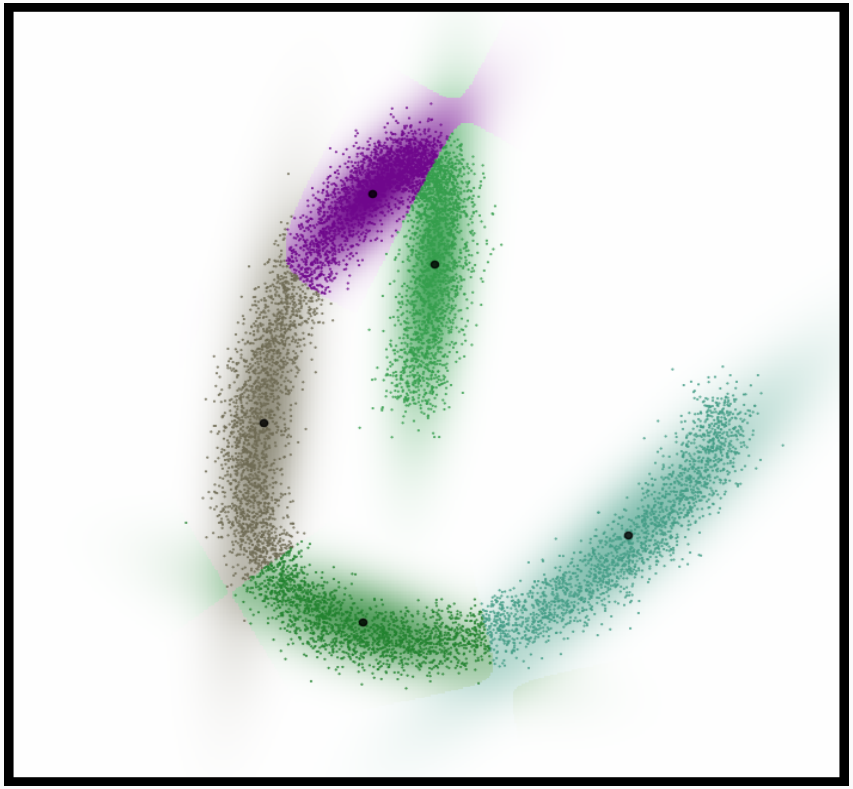
We run NumPy, PyTorch and KeOps on a RTX 2080 Ti GPU.



KeOps is a good fit for various computational fields



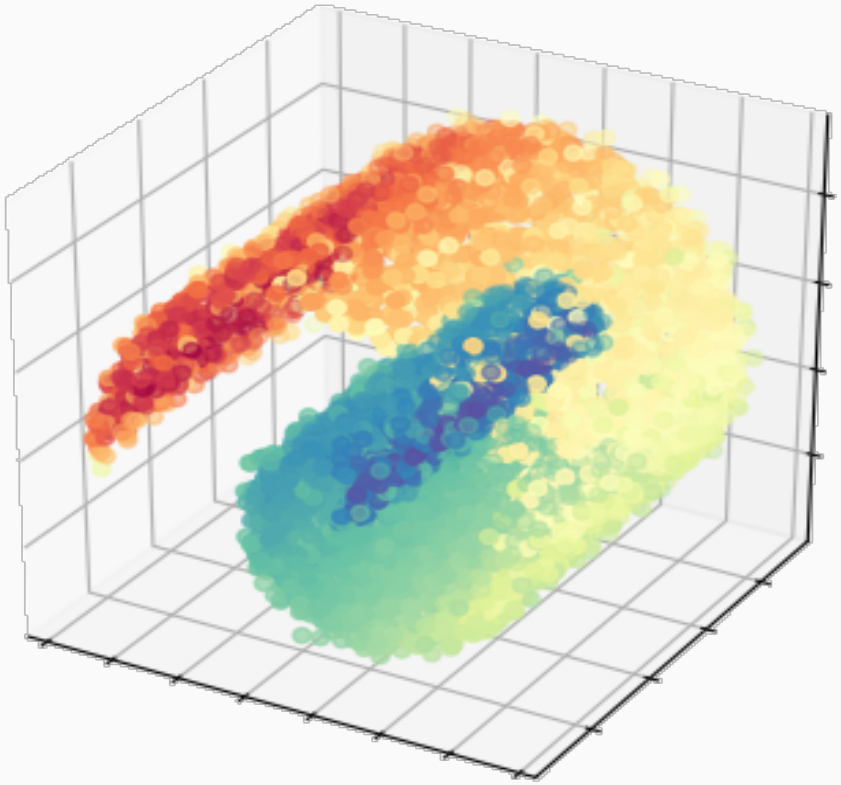
Clustering (K-Means).



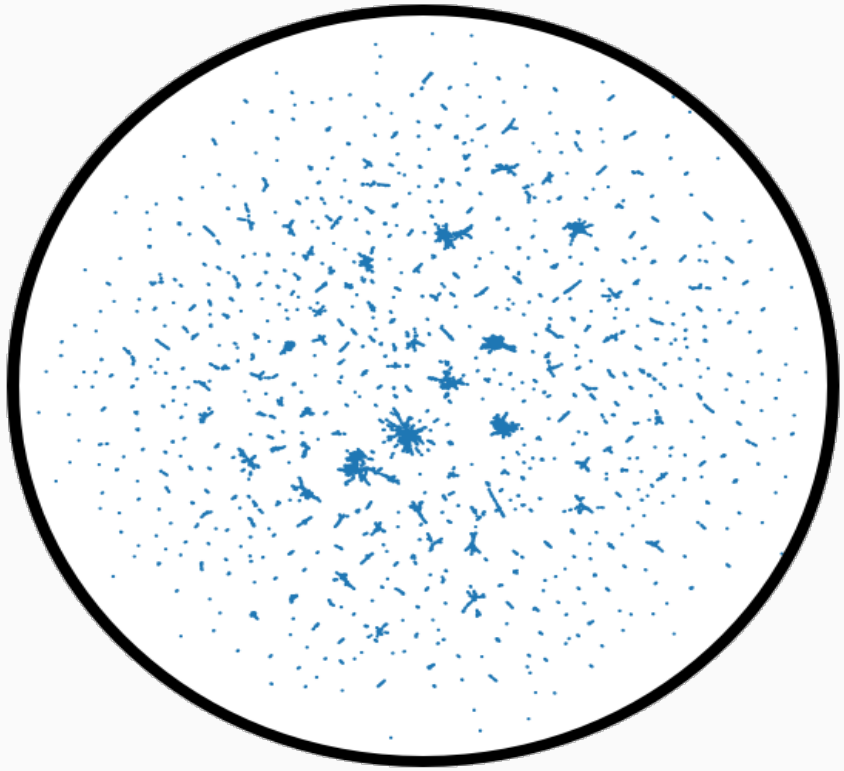
Gaussian Mixture Model.

Use **any** kernel, metric or formula **you** like!

KeOps is a good fit for various computational fields



Spectral analysis.



Dimension reduction (UMAP in hyperbolic space).

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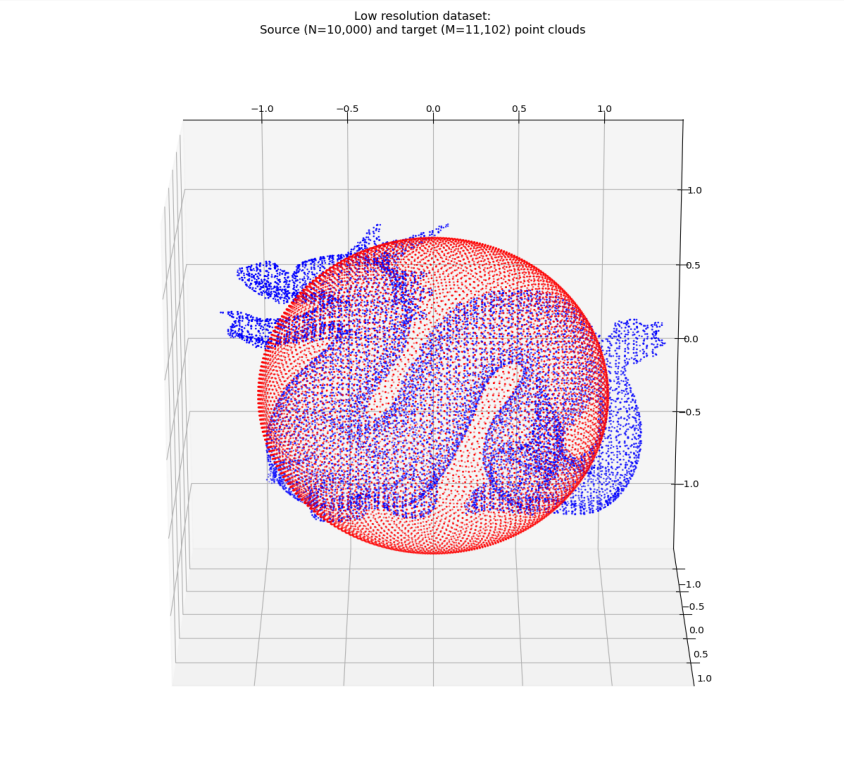
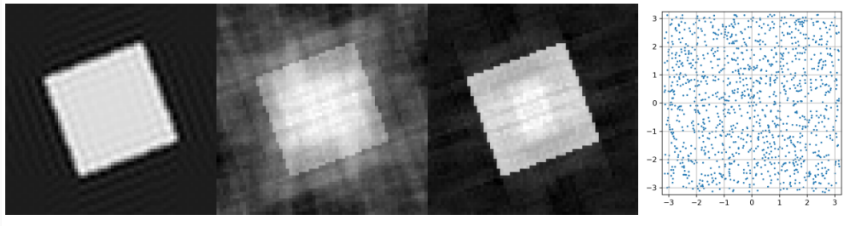


Regularized OT (credit: geomloss).



Inverse problems (NUFT) (credit: A. Gossart, F. de Gourmet, P. Weiss).

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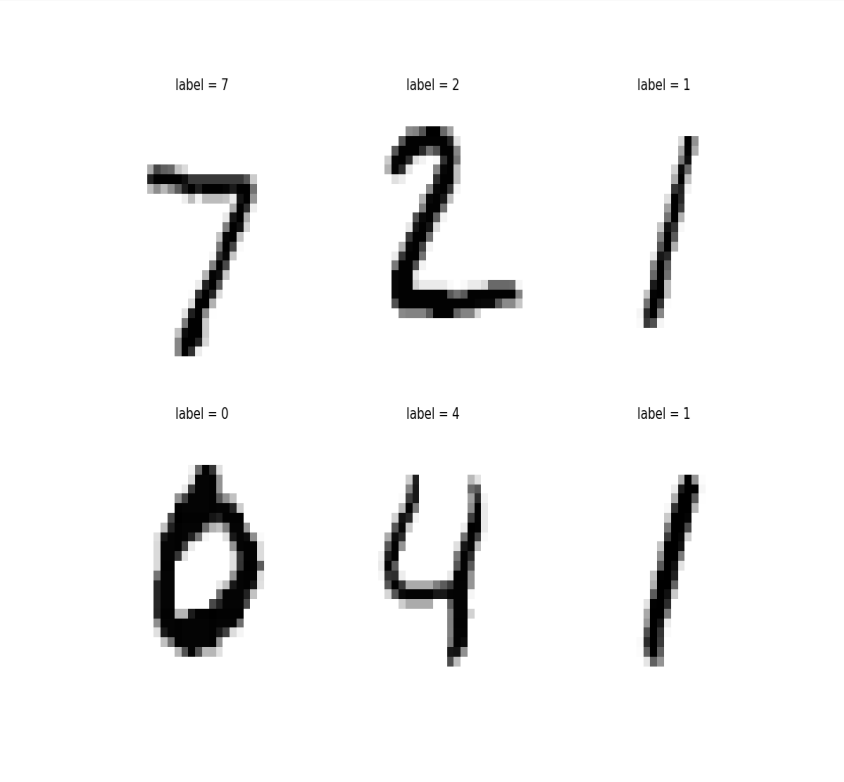
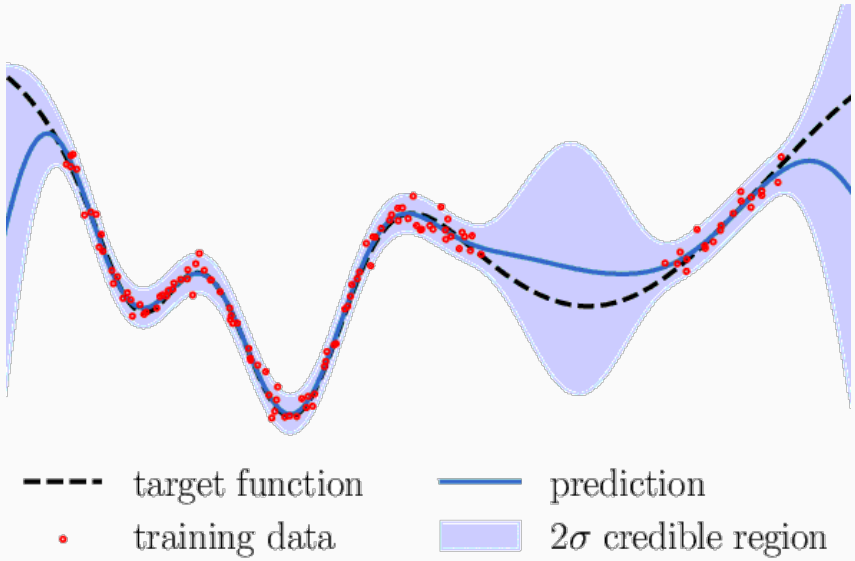


Clustering (k-NN).



Gaussian Processes

Use **any** where are PDEs? Boundary Element Method ?

Similar (yet different!) softwares:

- Triton
- Pytorch jit
- Taichi language
- Tensor comprehension (deprecated)

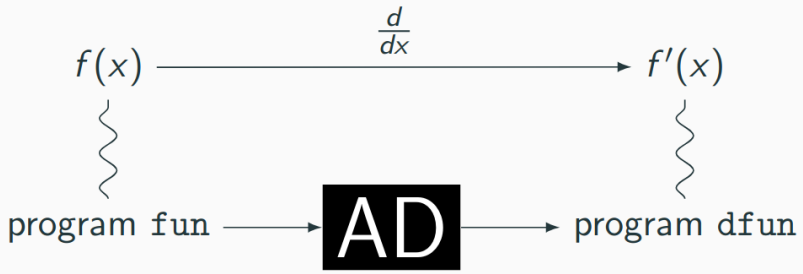
Autodiff engine

Autodiff engine

Introduction

AD as a black box to differentiate

Given a function in a code, how to compute its gradient (when possible, when it makes sens) ?



[1]

composition of augmented programs $\leftrightarrow$ composition of differentiable functions

[1] part of these slide from S. Vaiter and J. Feydy

Finite differences?

Let $F : \mathbb{R}^p \to \mathbb{R}$ be a smooth function. Then:

$$\nabla F(x_0) \quad = \quad \begin{pmatrix} \partial_{x^1} F(x_0) \\ \partial_{x^2} F(x_0) \\ \vdots \\ \partial_{x^n} F(x_0) \end{pmatrix} \quad \simeq \quad \frac{1}{\delta t} \begin{pmatrix} F(x_0 + \delta t \cdot (1, 0, \ldots, 0)) - F(x_0) \\ F(x_0 + \delta t \cdot (0, 1, \ldots, 0)) - F(x_0) \\ \vdots \\ F(x_0 + \delta t \cdot (0, 0, \ldots, 1)) - F(x_0) \end{pmatrix}.$$

Finite differences?

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$\Longrightarrow$ costs **(p+1) evaluations of** F, which is poor.

Computing gradient is costly

Let $f : \mathbb{R}^p \to \mathbb{R}$ a smooth function.

Complexity (number of operations), theoretical bounds are:

- Finite differences: $\text{Cost}(\nabla f) = (p+1)\,\text{Cost}(f)$ (linear in p)
- (reverse) AD: $\text{Cost}(\nabla f) \leq 5\,\text{Cost}(f)$ [Baur - Strassen '83] (constant in p)

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Storage (max buffer size), empirical bounds are:

- Finite differences: $\text{Cost}(\nabla f) \sim \text{Cost}(f)$
- (reverse) AD: $\text{Cost}(\nabla f) \sim 7\,\text{Cost}(f)$

Making your (costly) extra Go of GPU RAM critical...

AD is chain rules

Composition of functions $(f_0 : \mathbb{R}^p = \mathbb{R}^{n_0} \to \mathbb{R}^{n_1}, \ldots, f_3 : \mathbb{R}^{n_3} \to \mathbb{R}^{n_4} = \mathbb{R}^n)$

$$f = f_0 \circ f_1 \circ f_2 \circ f_3 : \mathbb{R}^p \to \mathbb{R}^n$$

Computational graph

Chain rule

$$\frac{\partial y}{\partial x} = \frac{\partial w_1}{\partial w_0}\frac{\partial w_2}{\partial w_1}\frac{\partial w_3}{\partial w_2}\frac{\partial w_4}{\partial w_3} = \mathrm{Jac}_{f_3}(w_3)\mathrm{Jac}_{f_2}(w_2)\mathrm{Jac}_{f_1}(w_1)\mathrm{Jac}_{f_0}(w_0)$$

How to compute these term? Choose your way...

Forward AD

$f = f_0 \circ f_1 \circ f_2 \circ f_3 : \mathbb{R}^p \to \mathbb{R}^n$

Jacobian-vector products (JVPs)

$$\mathrm{Jac}_f(x) = \begin{pmatrix} \mathrm{Jac}_f(x)\mathbf{e}_1 & \cdots & \mathrm{Jac}_f(x)\mathbf{e}_p \end{pmatrix} \implies \text{need } p \text{ JVPs (column-per-column)}$$

Chain rule for JVPs

$$\mathrm{Jac}_f(x)e_k = \underbrace{\mathrm{Jac}_{f_3}(w_3)\left[\mathrm{Jac}_{f_2}(w_2)\left\{\mathrm{Jac}_{f_1}(w_1)\left(\mathrm{Jac}_{f_0}(w_0)e_k\right)\right\}\right]}_{\text{right-to-left multiplication (forward } w_0 \to w_1 \to w_2 \to w_3 \to w_4)}$$

Cost of p JVPs: $p \sum_{i=0}^{3} n_i n_{i+1}$ $\qquad$ $O(p^3)$ if $n_i = p$ for $i \neq 4$

Torch autograd: A first example (part 1)

```
import torch

# function f. Sizes (3, 4) -> (3,)
>>> def func(x):
>>>     return x.exp().sum(dim=1)

>>> inputs = torch.rand(3, 4)  # same size as input of f
>>> v = torch.randn_like(func(inputs))  # same size as output of f
```

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>>> inputs = torch.rand(3, 4)  # same size as input of f
>>> v = torch.randn_like(func(inputs))  # same size as output of f

>>> jac = torch.autograd.functional.jacobian(exp_reducer, inputs) # (3, (3, 4))
# tensor([[[1.6998, 1.1370, 1.7796, 2.6448],
#          [0.0000, 0.0000, 0.0000, 0.0000],
#          [0.0000, 0.0000, 0.0000, 0.0000]],
#
#         [[0.0000, 0.0000, 0.0000, 0.0000],
#          [1.5400, 1.3338, 1.1431, 1.0552],
#          [0.0000, 0.0000, 0.0000, 0.0000]],
#
#         [[0.0000, 0.0000, 0.0000, 0.0000],
#          [0.0000, 0.0000, 0.0000, 0.0000],
#          [2.6941, 2.6420, 1.7159, 2.4825]]])
```

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#          [2.6941, 2.6420, 1.7159, 2.4825]]])

# ... with same entries as exp(inputs)
>>> inputs.exp()
# tensor([[1.6998, 1.1370, 1.7796, 2.6448],
#         [1.5400, 1.3338, 1.1431, 1.0552],
#         [2.6941, 2.6420, 1.7159, 2.4825]])
```

Torch autograd: A first example (part 2)

```
from torch.autograd.functional import vpj, jvp
```

Torch autograd: A first example (part 2)

```
from torch.autograd.functional import vpj, jvp
```

VPJ:

```
# compute f(x), v @ jac_x f: (4,) @ (4, (3, 4)) == (3, 4))
>>> v = torch.randn_like(func(inputs))  # same size as output of f
>>> _, vjp = vjp(exp_reducer, inputs, v)
# tensor([[-0.3657, -0.2446, -0.3829, -0.5690],
#         [-1.6098, -1.3943, -1.1950, -1.1031],
#         [ 4.4814,  4.3948,  2.8542,  4.1294]])

assert torch.allclose(vjp, v @ jac)
# True
```

Torch autograd: A first example (part 2)

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```

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assert torch.allclose(vjp, v @ jac)
# True
```

JVP

```
# tangent vector: same size as x
>>> v2 = torch.randn_like(inputs)
>>> _, jvp = jvp(exp_reducer, inputs, v2)

assert allclose(jvp, (jac.reshape(3, -1) @ v2.reshape(-1,1)).ravel())
# True
```

Backward (or reverse) AD

$f = f_0 \circ f_1 \circ f_2 \circ f_3 : \mathbb{R}^p \to \mathbb{R}^n$

Vector-Jacobian products (VJPs)

$$\mathrm{Jac}_f(x) = \begin{pmatrix} \mathbf{e}_1^\top \mathrm{Jac}_f(x) & \cdots & \mathbf{e}_n^\top \mathrm{Jac}_f(x) \end{pmatrix}^\top \implies \text{need } n \text{ VJPs (row-by-row)}$$

Chain rule for VJPs

$$E_l \, \mathrm{Jac}_f(x) = \underbrace{[\{(E_l \mathrm{Jac}_{f_3}(w_3)) \, \mathrm{Jac}_{f_2}(w_2)\} \, \mathrm{Jac}_{f_1}(w_1)] \, \mathrm{Jac}_{f_0}(w_0)}_{\text{left-to-right multiplication (reverse } w_4 \to w_3 \to w_2 \to w_1 \to w_0)}$$

Cost of n VJPs: $n \sum_{i=0}^{3} n_i n_{i+1}$ $\qquad$ $O(p^2)$ if $n_i = p$ for $i \neq 4$

Torch autograd: A second example

```
import torch
>>> a = torch.randn(5,1, requires_grad=True)
# tensor([[-0.3717],
#         [ 0.1786],
#         [ 0.5572],
#         [-2.5876],
#         [ 0.6250]], requires_grad=True)
```

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```
>>> b = .5 * (a ** 2).sum()
# tensor(3.7833, grad_fn=<MulBackward0>)
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```

```
>>> b = .5 * (a ** 2).sum()
# tensor(3.7833, grad_fn=<MulBackward0>)
```

```
>>> torch.autograd.grad(b, [a], torch.ones(1))
# (tensor([[-0.3717],
#          [ 0.1786],
#          [ 0.5572],
#          [-2.5876],
#          [ 0.6250]]),)
```

Reverse AD

Let $F : (X, \langle \cdot, \cdot \rangle_X) \to (Y, \langle \cdot, \cdot \rangle_Y)$ be a smooth map between be two Hilbert spaces.

Reverse AD

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- the adjoint of the differential is $(\mathrm{d}_x F)^*(x_0) : \alpha \in Y^* \to \beta \in X^*$. Riesz representation theorem gives a map

$$\partial_x F\,(x_0) : a \in Y \ \to b \in X$$

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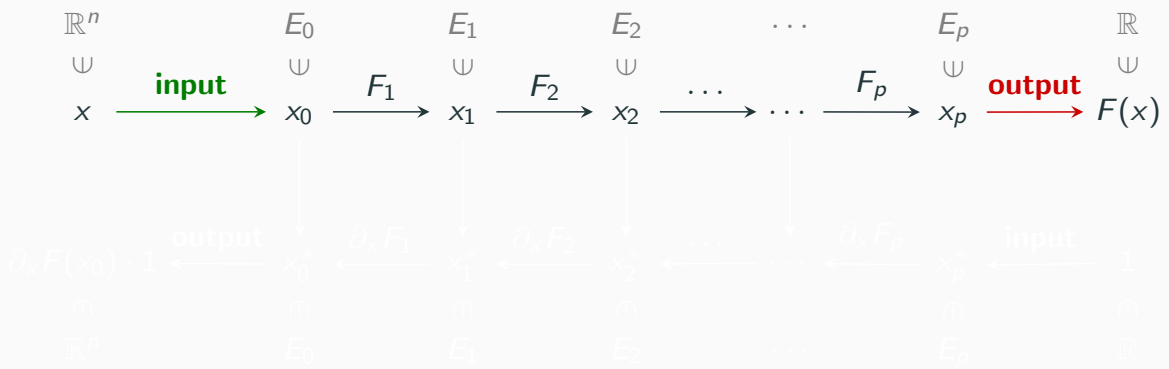
$$\partial_x F\,(x_0) : a \in Y \ \to b \in X$$

  called generalized **gradient**.
- If $X = \mathbb{R}^p$, $Y = \mathbb{R}$ endowed with the Euclidean metric,

$$\mathcal{M}_{\partial_x F(x_0)} = \begin{pmatrix} \partial_{x^1} F(x_0) \\ \partial_{x^2} F(x_0) \\ \vdots \\ \partial_{x^p} F(x_0) \end{pmatrix} = \nabla_x F(x_0)$$

Reverse AD = backpropagating

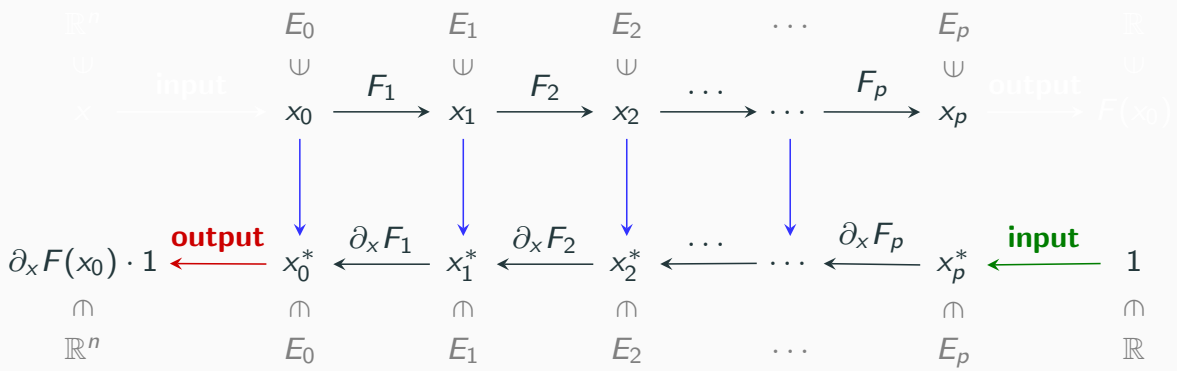


Backpropagating through a computational graph requires:

$$\begin{array}{rcccl} F_i & : & E_{i-1} & \to & E_i \\ & & x & \mapsto & F_i(x) \end{array} \tag{1}$$

encoded as **computer programs**.

Reverse AD = backpropagating

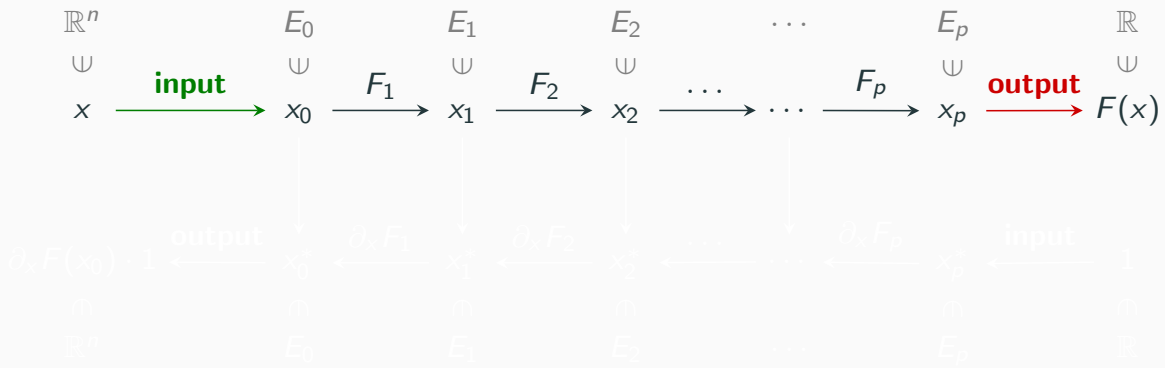


Backpropagating through a computational graph requires:

$$\begin{array}{cccccc} F_i & : & E_{i-1} & \to & E_i \\ & & x & \mapsto & F_i(x) \end{array} \qquad \begin{array}{cccccc} \partial_x F_i & : & E_{i-1} \times E_i & \to & E_{i-1} \\ & & (x_{i-1}, x_i^*) & \mapsto & \partial_x F_i(x_{i-1}) \cdot x_i^* \end{array} \tag{1}$$

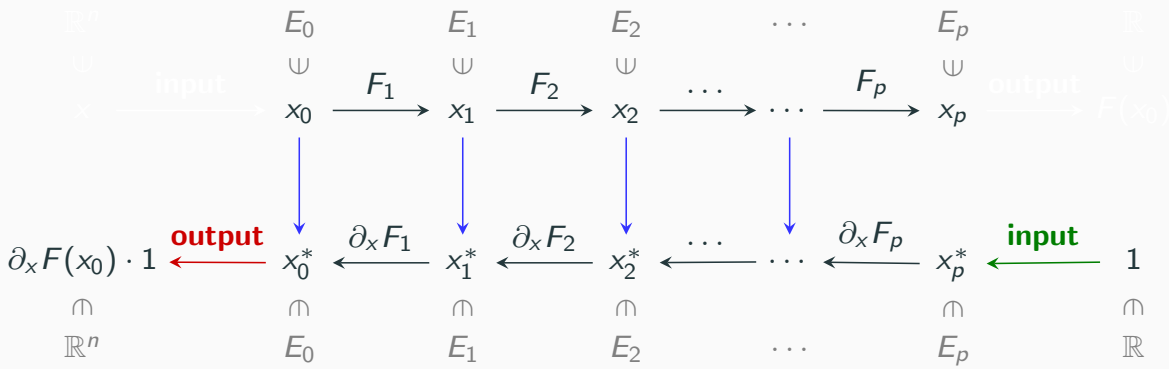
encoded as **computer programs**.

Reverse AD = backpropagating



1. Starting from $x_0 \in \mathbb{R}^n = E_0$, compute and store in memory the successive vectors $x_i \in E_i$. The last one, $x_p = F(x_0) \in \mathbb{R}$.

Reverse AD = backpropagating



1. Starting from $x_0 \in \mathbb{R}^n = E_0$, compute and store in memory the successive vectors $x_i \in E_i$. The last one, $x_p = F(x_0) \in \mathbb{R}$.
2. Starting from the canonical value of $x_p^* = 1 \in \mathbb{R}$, compute the successive dual vectors

$$x_i^* \;=\; \partial_x F_{i+1}(x_i) \cdot x_{i+1}^*. \tag{2}$$

The last one, $x_0^* = \partial_x F(x_0) \cdot 1 = \nabla F(x_0) \in \mathbb{R}^n$, is the gradient.

Autodiff engine

KeOps autograd

KeOps autograd

Let the formula

$$F(x, y) = \left[\sum_{j=1}^{N} \exp(x_i + y_j) \right]_{i=1,\cdots,M}$$

where

- $x \in \mathbb{R}^M$ is a variable indexed by i,
- $y \in \mathbb{R}^N$ is a variable indexed by j

Compute $F : \mathbb{R}^M \times \mathbb{R}^N \to \mathbb{R}^M$ with KeOps:

```
x = torch.rand(4000, 1, requires_grad=True)
y = torch.rand(3000, 1, requires_grad=True)

X = pykeops.torch.LazyTensor(x.reshape(4000, 1, 1))
Y = pykeops.torch.LazyTensor(y.reshape(1, 3000, 1))
Z = (X + Y).exp()  # still LazyTensor

F = Z.sum(1)
# [KeOps] Generating code for formula Sum_Reduction(Exp(Var(0,1,0)+Var(1,1,1)),0)
# ... OK

torch.allclose(torch.exp(x + y.t()).sum(1), F.view(-1))
# True
```

KeOps autograd

Compute the gradient $\mathbb{R}^N \ni y \mapsto F(x,y) \in \mathbb{R}^M$ applied to an arbitrary test vector $e \in \mathbb{R}^M$:

$$[\partial_y F(x,y)](e) = [d_y F^*(x,y)](e) = \left[\sum_{i=1}^{M} \exp(x_i + y_j) e_i \right]_{j=1}^{N}$$

Compute dF with KeOps and `Grad( , , )` operator:

```
e = torch.rand_like(x)

F_grad_y = torch.autograd.grad(F, [y], e)[0]
# [KeOps] Generating code for formula Sum_Reduction(Var(2,1,0)*Exp(Var(0,1,0)+
# Var(1,1,1)),0) ... OK
# [KeOps] Generating code for formula Sum_Reduction(Var(2,1,0)*Exp(Var(0,1,0)+
# Var(1,1,1)),1) ... OK

torch.allclose(torch.exp(x + y.t()).t() @ e,  F_grad_y)
# True
```

KeOps effect on the LDDMM example

```python
from pykeops.torch import LazyTensor

def gaussian_kernel_keops(x, y, sigma2):
    x_i = LazyTensor(x[:, None, :])        # ([M, 1], 1)
    y_j = LazyTensor(y[None, :, :])        # ([1, N], 1)
    D_ij = ((x_i - y_j) ** 2).sum(-1)      # ([M, N]) Symb. mat. of squared distances
    return (-D_ij / sigma2).exp()          # ([M, N]) Symb. mat. of Gaussian kernel
```

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K_qq = gaussian_kernel_keops(q, q, s2)
```

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K_qq = gaussian_kernel_keops(q, q, s2)
v = K_qq @ p                               # mat. mult. ([N,N]) @ (N,D) = (N,D)

# [KeOps] Generating code for formula Sum_Reduction(Exp(-Sum((Var(0,3,0)-
#         Var(1,3,1))**2)/Var(2,1,2))*Var(3,3,1),0) ... OK
```

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# Finally, compute the Hamiltonian H(q,p): .5 * <p,v>
H = .5 * torch.dot(p.view(-1), v.view(-1))
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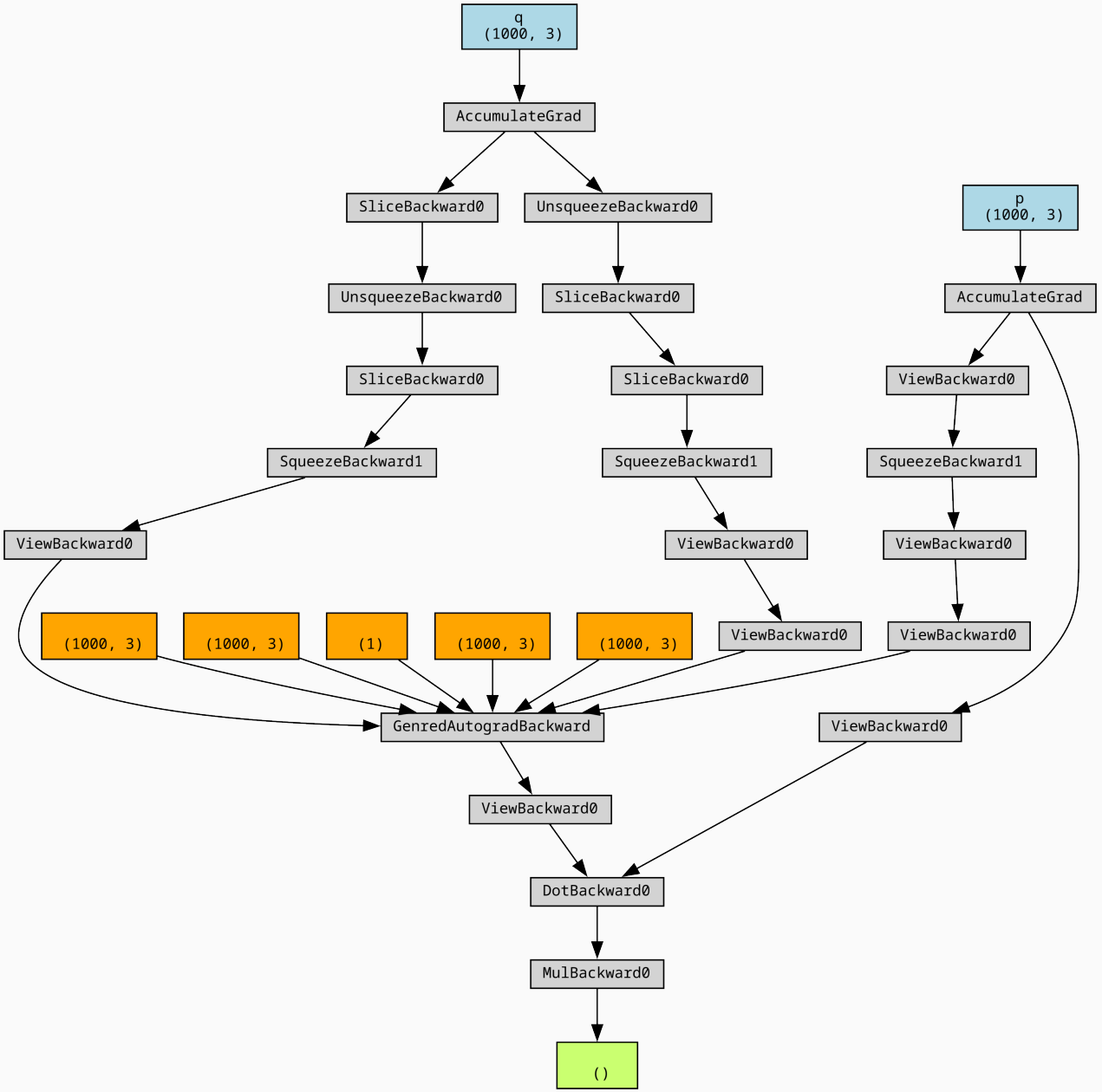
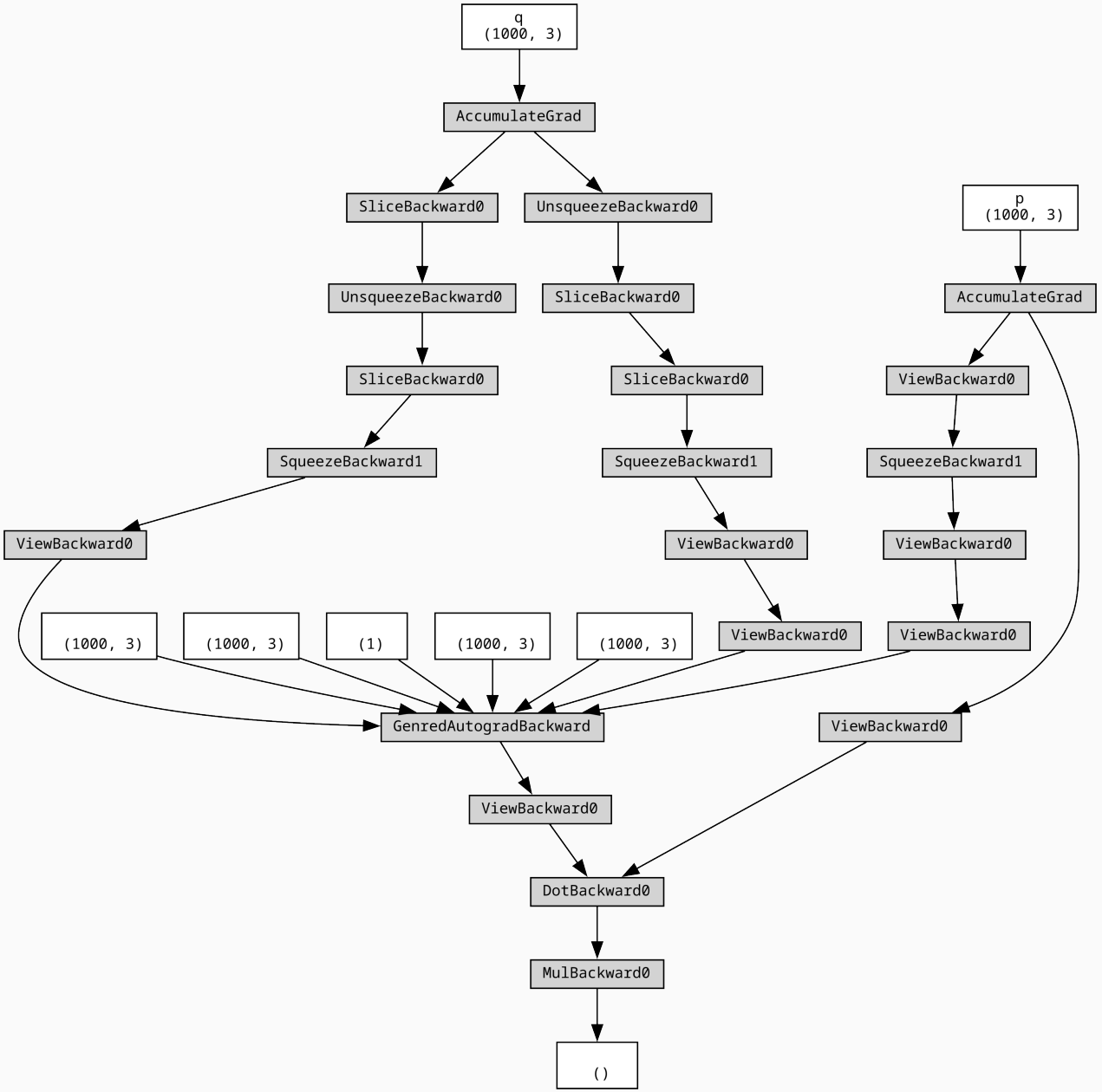
#         Var(1,3,1))**2)/Var(2,1,2))*Var(3,3,1),0) ... OK

# Finally, compute the Hamiltonian H(q,p): .5 * <p,v>
H = .5 * torch.dot(p.view(-1), v.view(-1))

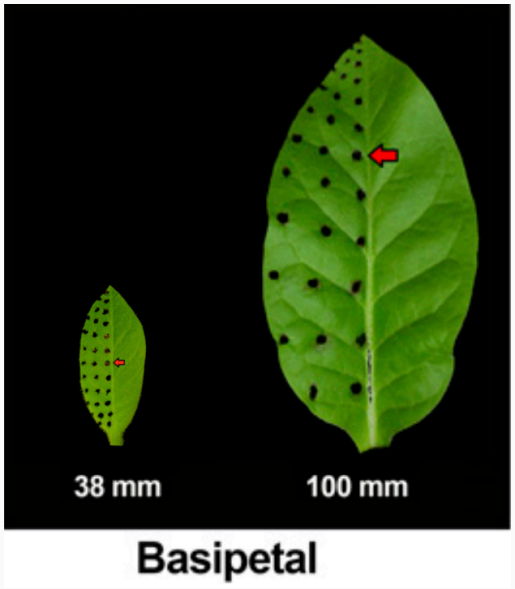
# Automatic differentiation is straitghtforward... and working !
[dq,dp] = torch.autograd.grad(H, [q,p])
```

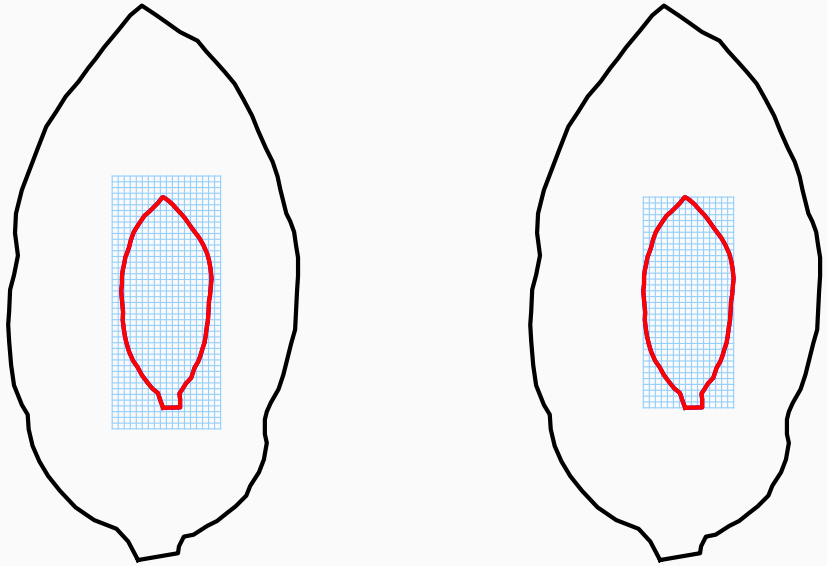

q
(1000, 3)
AccumulateGrad
SliceBackward0
UnsqueezeBackward0
UnsqueezeBackward0
SliceBackward0
SliceBackward0
SliceBackward0
SqueezeBackward1
SqueezeBackward1
ViewBackward0
ViewBackward0
(1000, 3)
(1000, 3)
(1)
(1000, 3)
(1000, 3)
GenredAutogradBackward
ViewBackward0
DotBackward0
MulBackward0
()
p
(1000, 3)
AccumulateGrad
ViewBackward0
SqueezeBackward1
ViewBackward0
ViewBackward0
ViewBackward0
ViewBackward0


q
(1000, 3)
AccumulateGrad
SliceBackward0
UnsqueezeBackward0
p
(1000, 3)
UnsqueezeBackward0
SliceBackward0
AccumulateGrad
SliceBackward0
SliceBackward0
ViewBackward0
SqueezeBackward1
SqueezeBackward1
SqueezeBackward1
ViewBackward0
ViewBackward0
ViewBackward0
(1000, 3)
(1000, 3)
(1)
(1000, 3)
(1000, 3)
ViewBackward0
ViewBackward0
GenredAutogradBackward
ViewBackward0
ViewBackward0
DotBackward0
MulBackward0
()

Advanced linear algebra operations

Motivation: deformation with implicit modules

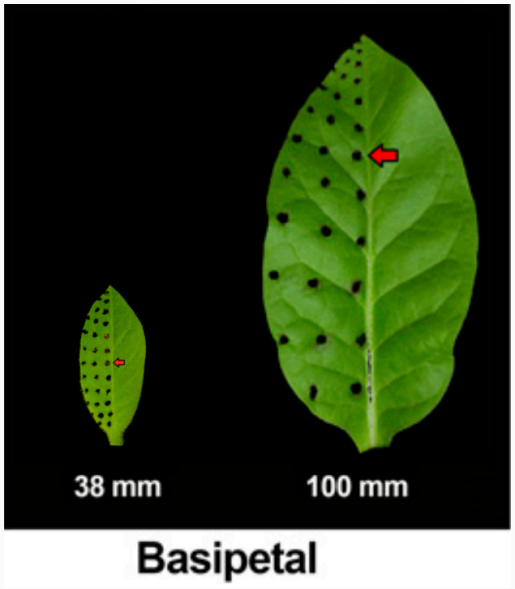


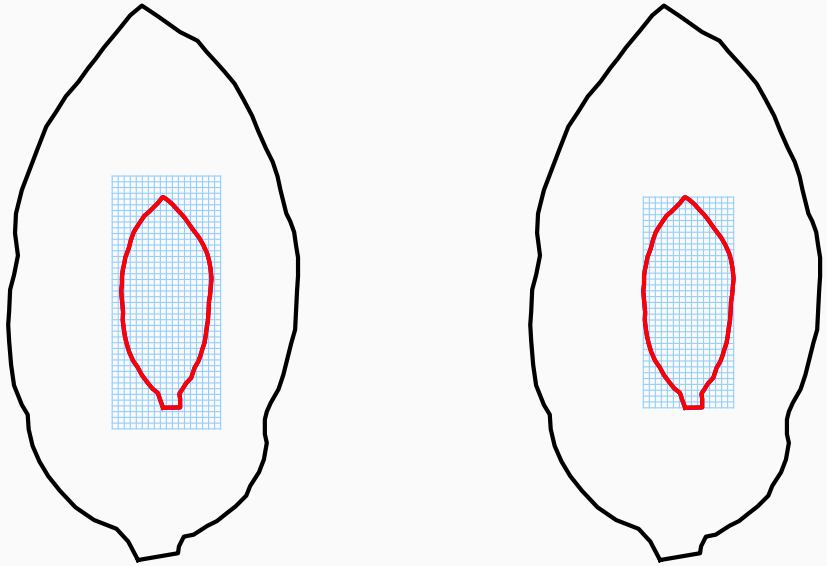


LDDMM IMODAL

L. Lacroix, B. Charlier, A. Trouvé, B. Gris. *IMODAL: creating learnable user-defined deformation models* – CVPR, 2021

Motivation: deformation with implicit modules





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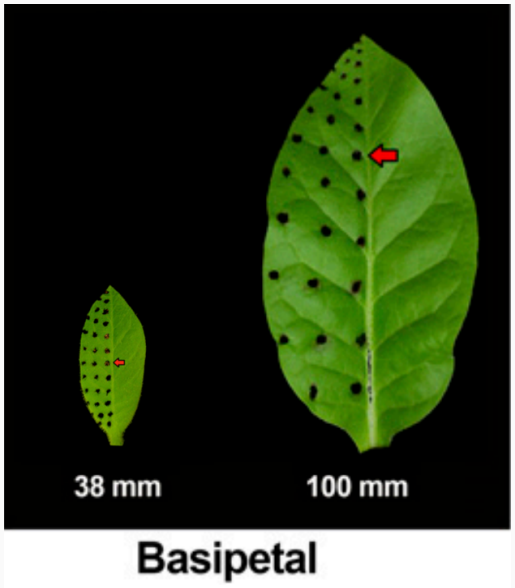

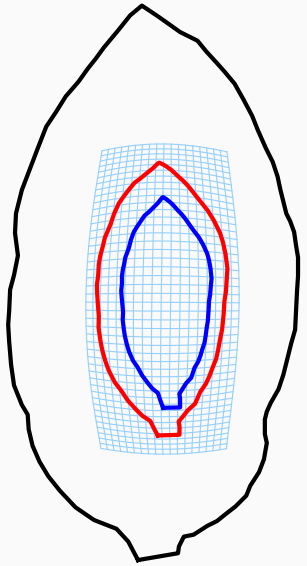

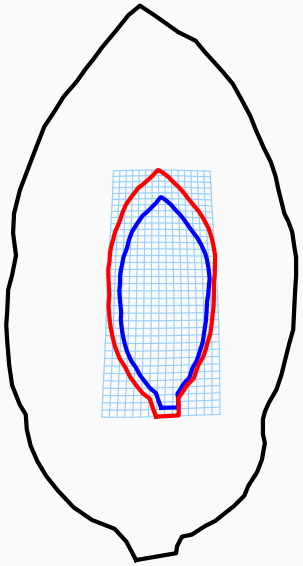

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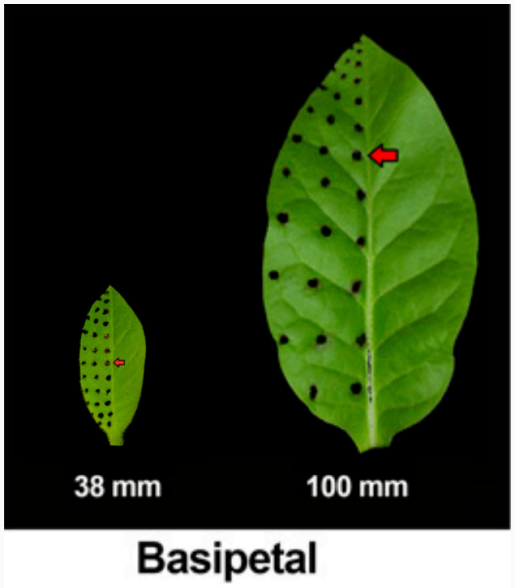

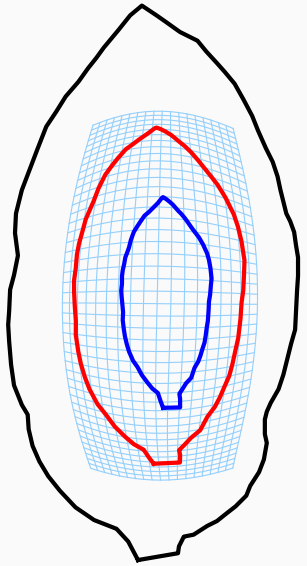

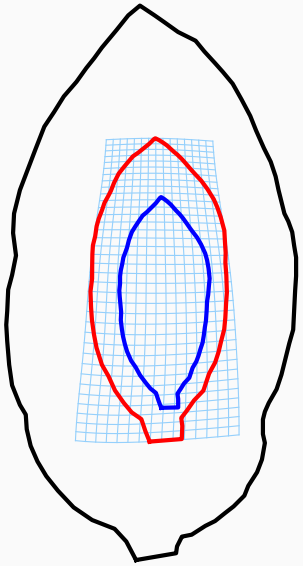

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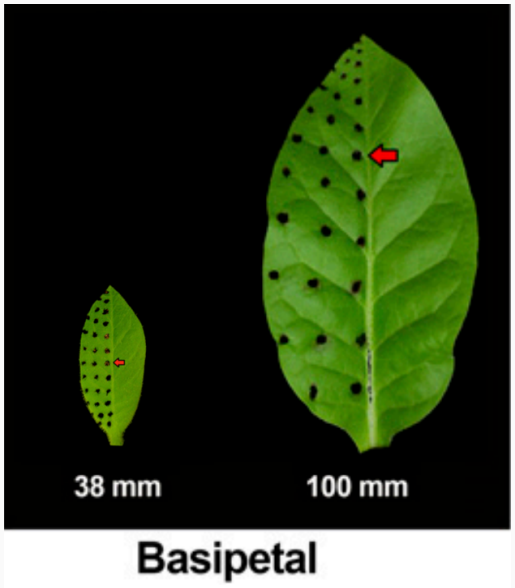

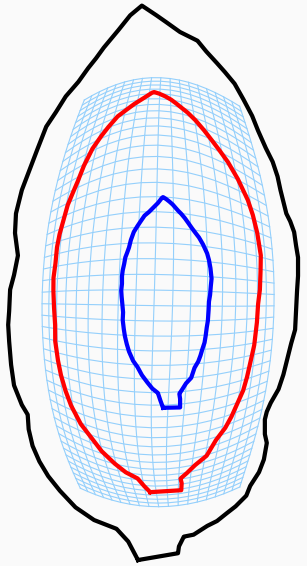

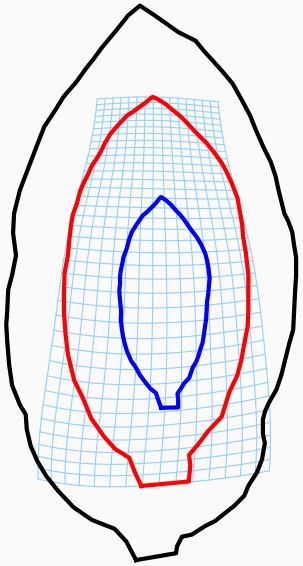

LDDMM IMODAL

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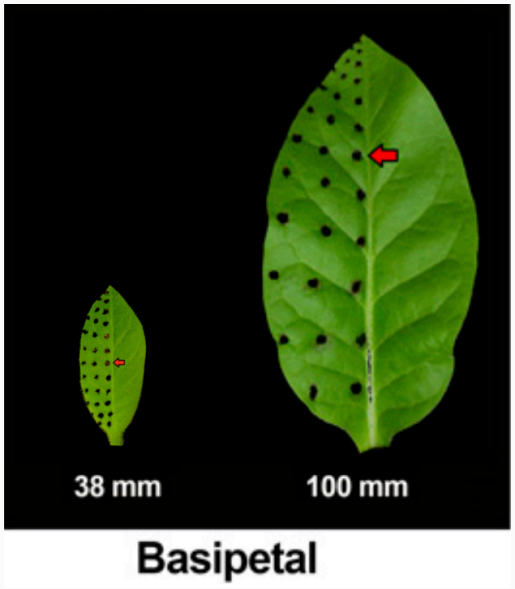

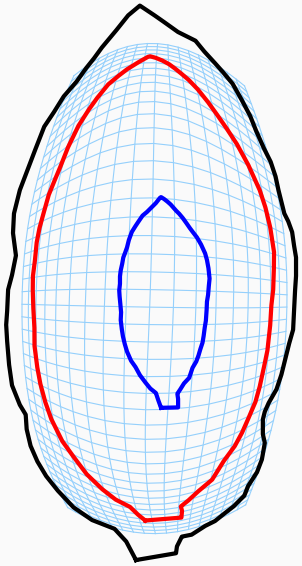

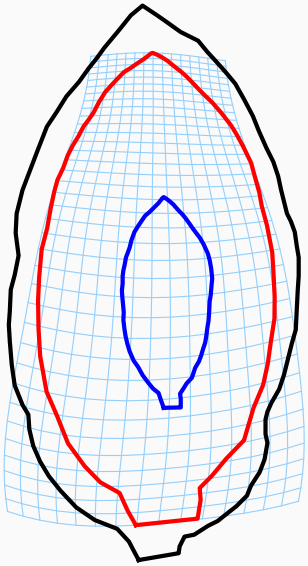

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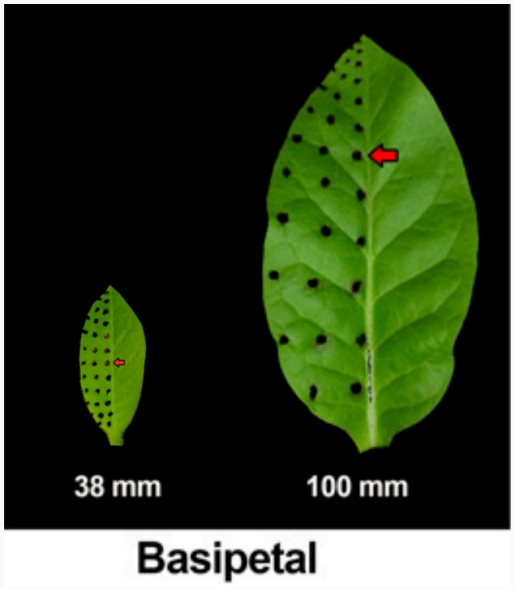

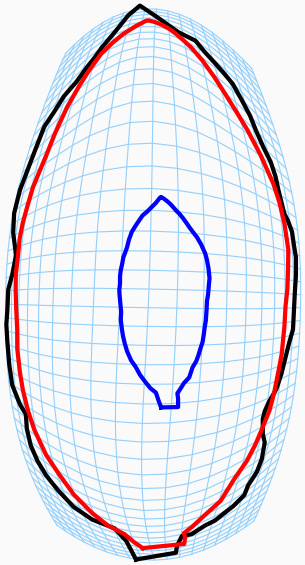

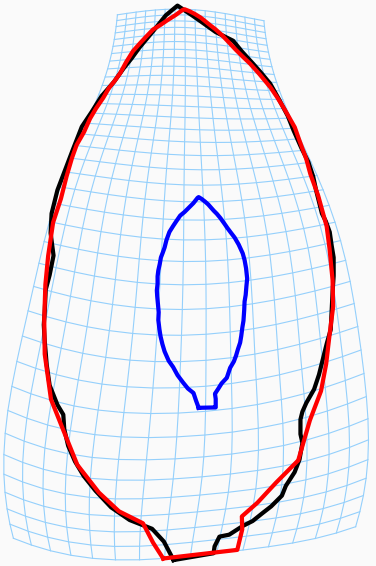

LDDMM IMODAL

L. Lacroix, B. Charlier, A. Trouvé, B. Gris. *IMODAL: creating learnable user-defined deformation models* – CVPR, 2021

Inverse SPD matrix

- Given a symmetric positive definite operator $K = \left[f(|x_i - x_j|/\sigma^2)\right]_{i,j=1}^{n}$ and $a \in \mathbb{R}^n$ we may use KeOps to compute $b \in \mathbb{R}^n$ such that

$$Ka = b$$

  with a sum reduction.

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$$Ka = b \Longleftrightarrow a = K^{-1}b.$$

  ... which is not a reduction.

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$$(K+\alpha Id)a = b \Leftrightarrow a = (K+\alpha Id)^{-1}b.$$

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  ... which is not a reduction.

Possible solutions:

- Gaussian elimination: store n^2 floats; operations: $2n^3/3$ (add, mult, sub, div).
- Conjugate gradient (CG): take advantage of a fast/cheap Matrix-Vector multiplication. Define an iterative procedure to compute an approximate solution x.

Remark: CG may outperform in term of storage and computaiton load.

Krylov spaces

Start with an initial guess $x_0 = b$:

- Take a first approximation to the solution as a multiple of b: $x_1 \in \text{Span}\{b\}$
- Compute Kb and search for an approximation as a linear combination of b and Kb: $x_2 \in \text{Span}\{b, Kb\}$
- $\vdots$
- Continue so that the solution belongs to the Krylov space

$$x_k \in \text{Span}\left\{b, Kb, K^2 b, \ldots, K^{\ell-1} b\right\} \tag{3}$$

Questions:

1. How can good (optimal) approximation from space (3) be computed with a moderate amount of work and storage ? (for Hermitian def pos K: use CG)
2. How good an approximation solution is contained in the space 3 ? (for small ℓ: use a reconditioners)

Conjugate gradient solver

Let $K_\alpha = K + \alpha Id$. We may consider the quadratic problem

$$\underset{a}{\operatorname{argmin}} \frac{1}{2} a^t K_\alpha a - a^t b$$

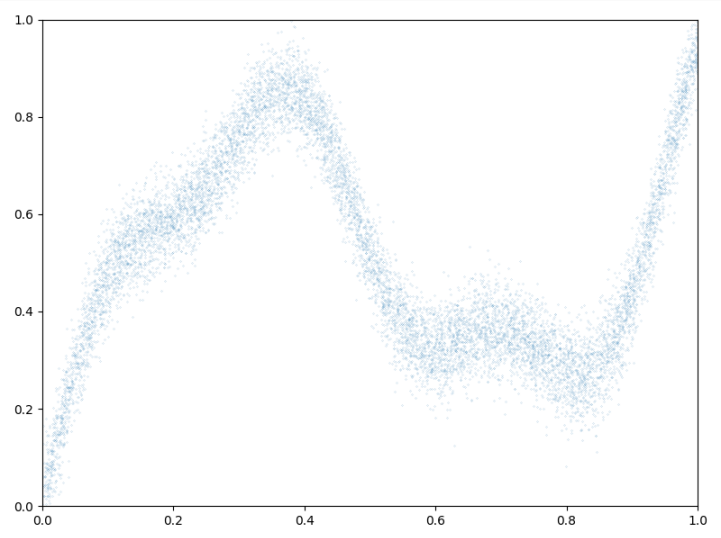
solved for $a = {K_\alpha}^{-1} b$.

- CG approximates the solution with an iterative procedure involving only terms using "$K_\alpha a$"
- Converge in at most n steps... and if we are lucky a good approximation is given in $\ell \ll n$ steps... but, due to round-off errors `maxiter = n*10` in `scipy`
- Convergence speed depends on the distribution of the eigenvaluesof K_α (condition number of K_α is a poor indicator)

Example: Interpolation 1d

```
N = 10000
# Sampling locations:
x = np.random.rand(N, 1)
# Some random-ish 1D signal:
b = x + .5 * np.sin(6 * x) + .1 * np.sin(20 * x) + .05 * np.random.randn(N, 1)

sigma = .1  # Kernel radius
alpha = 1.  # Ridge regularization
```



Example: Interpolation 1d

Let V be a RKHS with radial Gaussian Kernel. We want to solve

$$\underset{v \in V}{\operatorname{argmin}} \|v\|_V^2 + \frac{1}{\alpha}\|v(x_i) - b_i\|_2^2$$

```
def gaussian_kernel(x, y, sigma=0.1):
    x_i = LazyTensor(x[:, None, :])  # (M, 1, 1)
    y_j = LazyTensor(y[None, :, :])  # (1, N, 1)
    D_ij = ((x_i - y_j) ** 2).sum(-1)  # (M, N) symbolic matrix of squared distances
    return (-D_ij / (2 * sigma**2)).exp()  # (M, N) symbolic Gaussian kernel matrix
```

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# Instantiate KeOps routine
K_xx = gaussian_kernel(x, x)
```

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# Instantiate KeOps routine
K_xx = gaussian_kernel(x, x)
# Performe the computations
a = K_xx.solve(b, alpha=alpha)
```

Example: Interpolation 1d

```
# Extrapolate on a uniform sample:
t = np.reshape(np.linspace(0, 1, 1001), [1001, 1]).astype(dtype)

K_tx = gaussian_kernel(t, x)
mean_t = K_tx @ a
```

Example: Interpolation 1d

```
# Extrapolate on a uniform sample:
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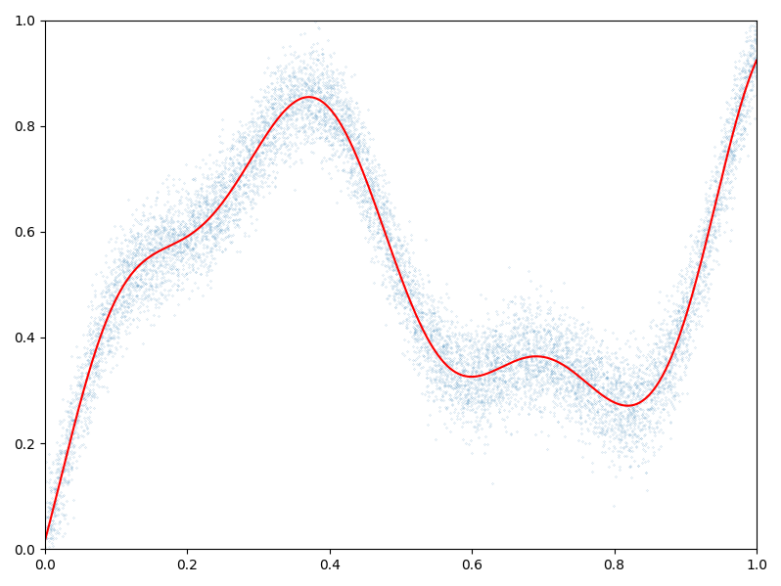
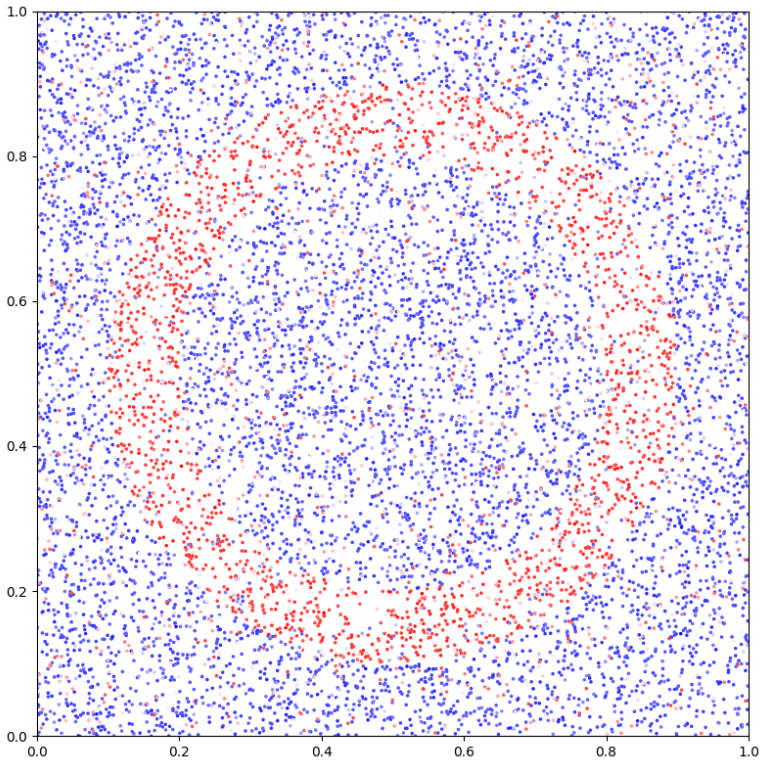
K_tx = gaussian_kernel(t, x)
mean_t = K_tx @ a

plt.scatter(x[:, 0], b[:, 0], s=100 / len(x))  # Noisy samples
plt.plot(t, mean_t, "r")
```



Example: Interpolation 2d

```python
def laplacian_kernel(x, y, sigma=0.1):
    x_i = LazyTensor(x[:, None, :])  # (M, 1, 1)
    y_j = LazyTensor(y[None, :, :])  # (1, N, 1)
    D_ij = ((x_i - y_j) ** 2).sum(-1)  # (M, N) symbolic matrix of squared distances
    return (-D_ij.sqrt() / sigma).exp()  # (M, N) symbolic Laplacian kernel matrix
```



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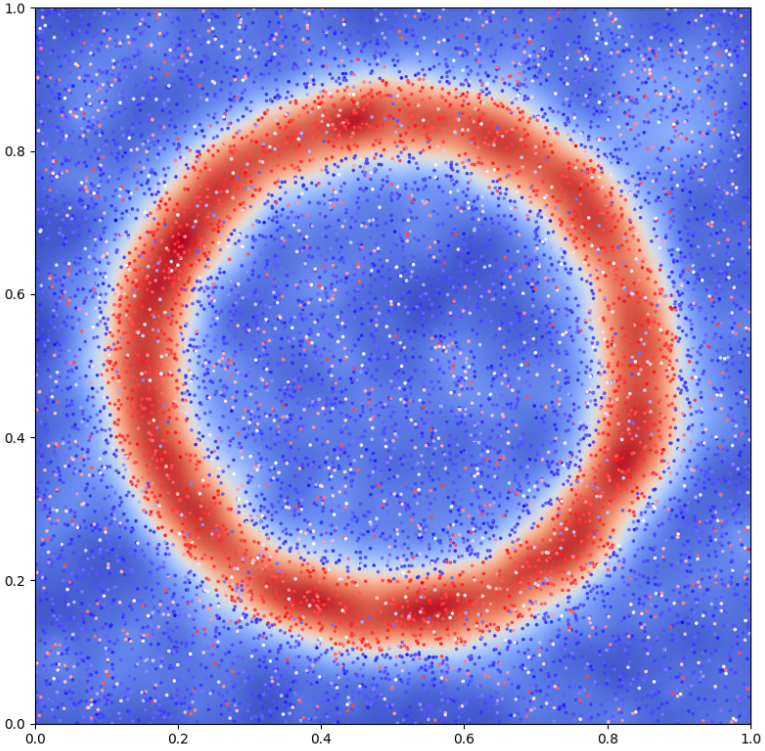
```



Using Scipy LinAlg routines

Create a toy dataset:

```
import numpy as np
N = 10000
x = np.random.randn(N,2)
```

Turn it into a KeOps `LazyTensor`:

```
from pykeops.numpy import LazyTensor
x_i, x_j = LazyTensor(x_[:, None, :]), LazyTensor(x_[None, :, :])
K_xx = (- ((x_i - x_j) ** 2).sum(2) / 2).exp()  # Symbolic (N,N) Gaussian kernel matrix
```

Using a `sum` reduction we may compute a Gaussian convolution...

Using Scipy LinAlg routines

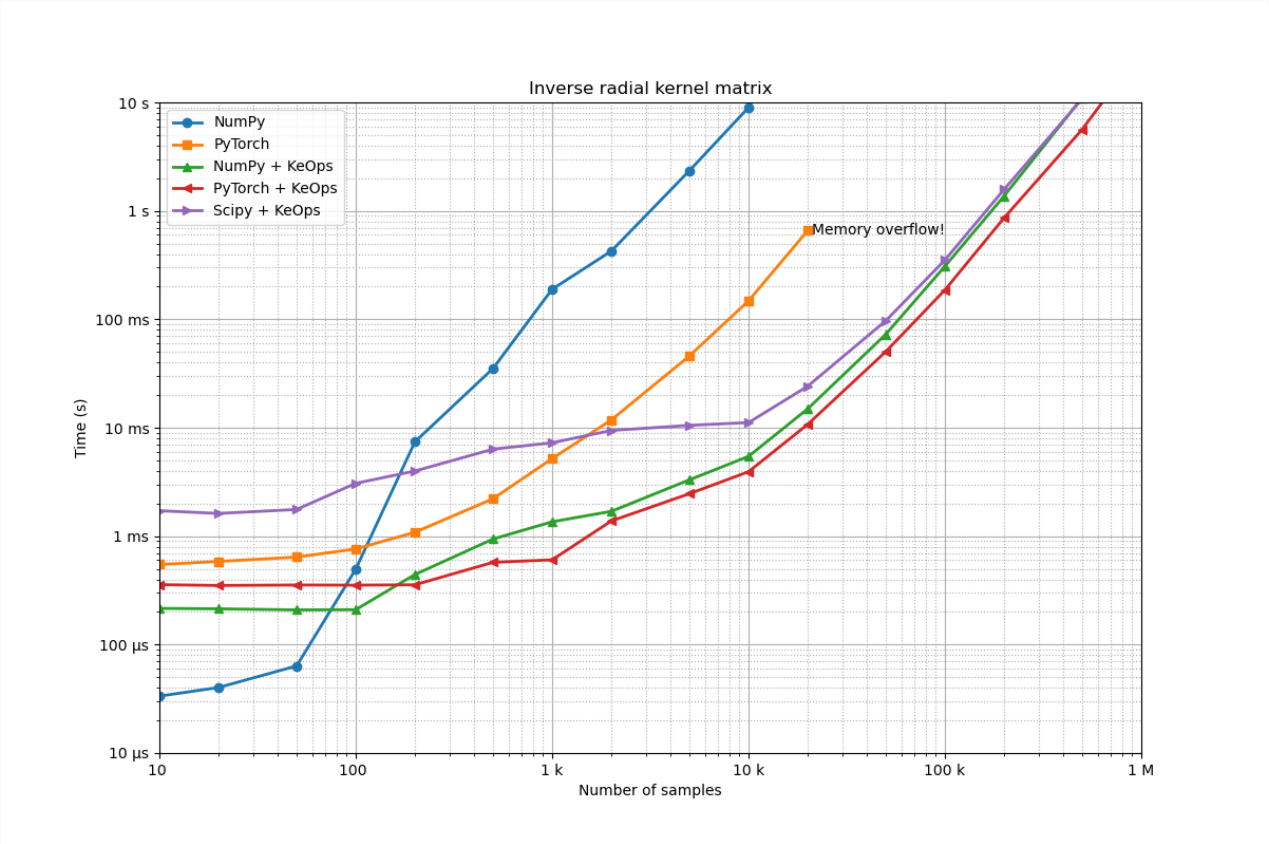
. . . instead, K_{xx} can be directly understood as a `LinearOperator`:

```
from scipy.sparse.linalg import aslinearoperator
K = aslinearoperator(K_xx)

from scipy.sparse.linalg import eigsh
eigenvalues, eigenvectors = eigsh(K, k=5)  # Largest 5 eigenvalues/vectors

# Largest eigenvalues: [ 626.59143  639.14667  663.38983  747.5554  1438.2162 ]
# Eigenvectors of shape: (10000, 5)
```

Benchmark for KernelSolve (Gaussian kernel, dimension 3)



see `http://www.kernel-operations.io/keops/_auto_benchmarks/plot_benchmark_invkernel.html`

Computation on GPU

Computation on GPU

Architecture

The GPU Market by Nvidia

Target:

- Gamers: GeForce Series (300 – 2000€)

- Scientific computing: Quadro, AXX Series (3000 – 20000€)

- Under the hood: similar chipsets with some enhancements (ECC, float64, unlocked driver features...). More RAM (recent A100 up to 80Go)

Nvidia has early developped a integrated software and hardware solution:

+ fast computing
– expensive cards
+ documentation, integration and contribution to open sources solutions (LLVM, C/C++, etc...)
– proprietary ecosystem: cuda code is non portable, buggy driver on Linux

GPU = massively parallel architecture

Figure 1: Nividia GTX XXXX architecture

A GPU architecture

→ scalable array of multithreaded *Streaming Multiprocessors* (*SM*s)

→ each single processor (called a *thread*) is able to execute an independent set of instructions.

1000's of cores inside a single GPU

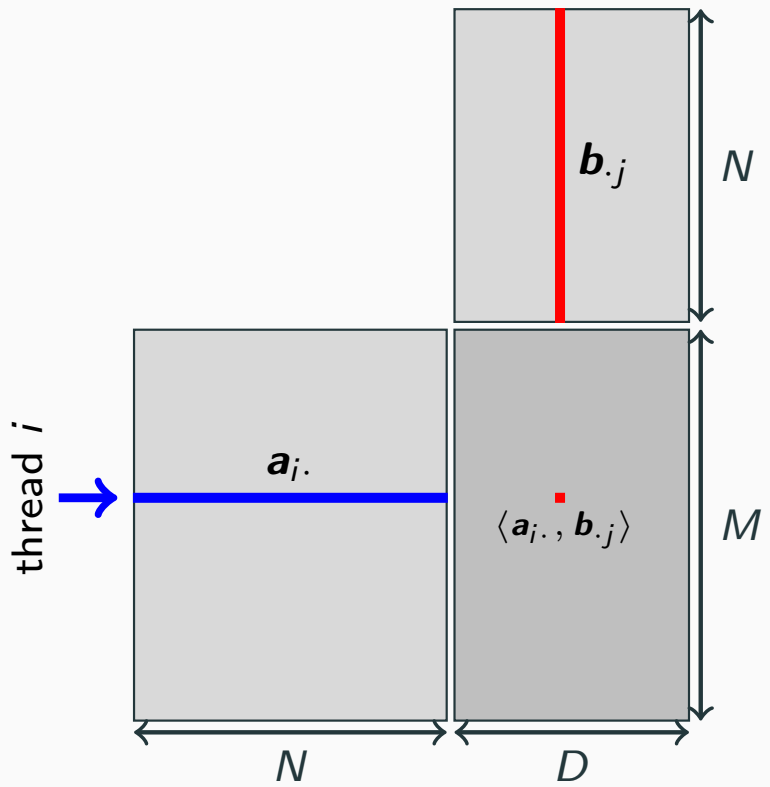
(multi-CPU architecure = at best 10's – 100's of cores)

Computation on GPU

Example: Matrix multiplication

MatMult: A first naive implementation

$\mathbf{A} \in \mathbb{R}^{M \times N}$ and $\mathbf{B} \in \mathbb{R}^{N \times D}$



A matrix multiplication

$$\mathbf{A}\,\mathbf{B} = \left[\sum_k a_{ik}\, b_{kj} \right]_{M \times D}$$

$\rightarrow$ a set of $N \times D$ scalar products

Parallel computing

- each thread computes D scalar products, i.e. $\langle \mathbf{a}_{i\cdot}, \mathbf{b}_{\cdot j} \rangle$ for all j

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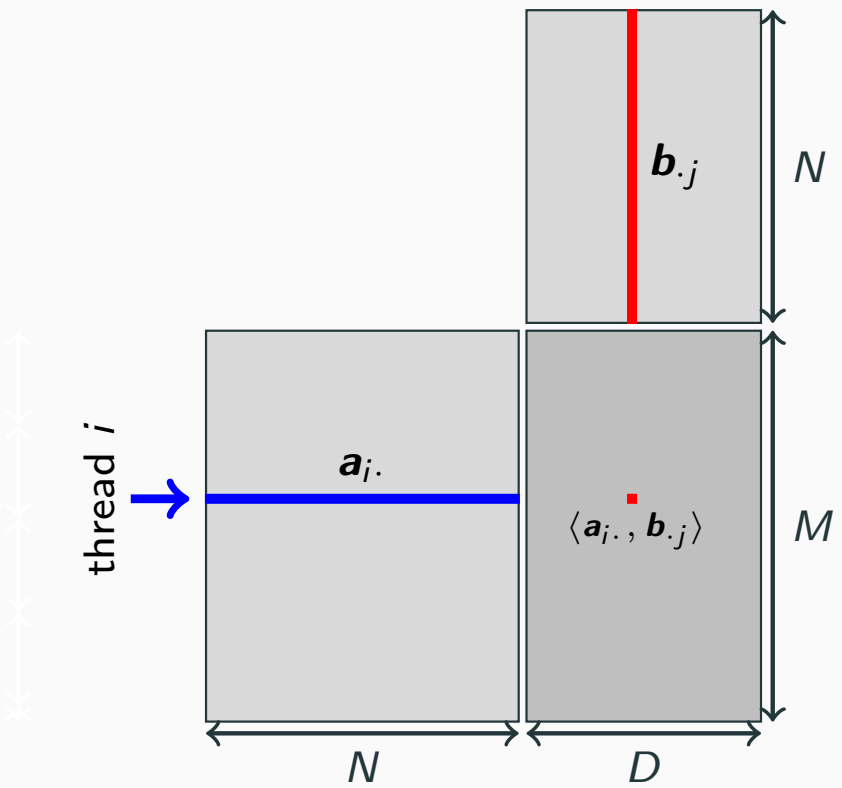

Thread i needs to access

- row $\mathbf{a}_{i\cdot} \in \mathbb{R}^N$
- all columns $(\mathbf{b}_{\cdot j})_{j=1,\dots,D}$ i.e. the full matrix $\mathbf{B}$

$\rightarrow$ potential memory overflow

$\rightarrow$ no mutual memory access between threads

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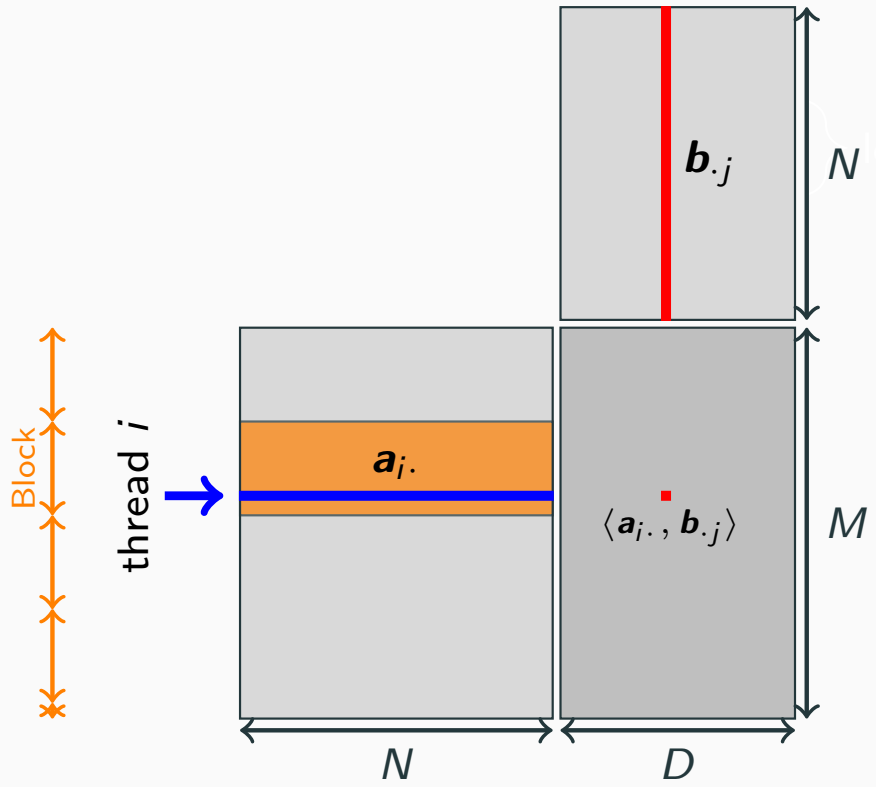
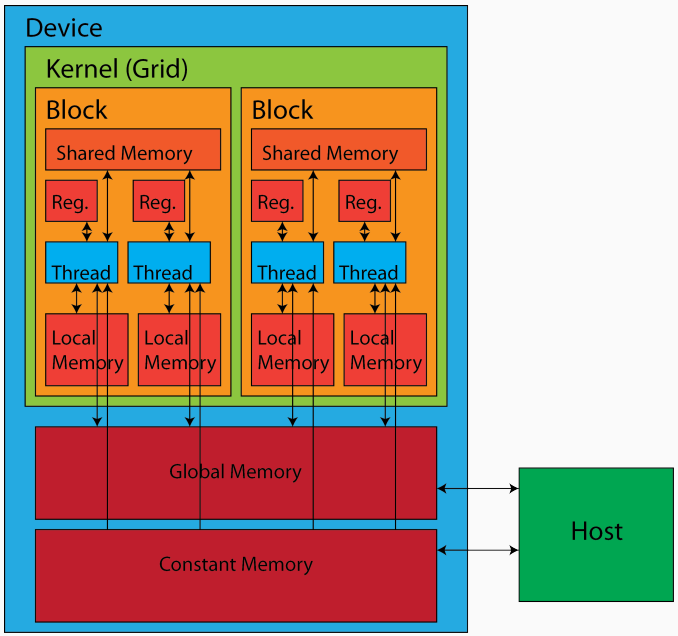


Assign a block of rows i to a thread

- share the memory access to each $\mathbf{b}_{\cdot j}$ to compute all rows i in the block

$\rightarrow$ each thread still requires to access the full matrix $\mathbf{B}$ to finish the computations for a row i

Memory management on GPU



- Data initially stored on the host (in RAM)
  - $\rightarrow$ should be transfer to the device (GPU) to be treated (bottleneck)
- Different kinds of memory
  - $\rightarrow$ global vs shared memory

Smart use of the shared memory: key to provide an efficient code in term of computational time

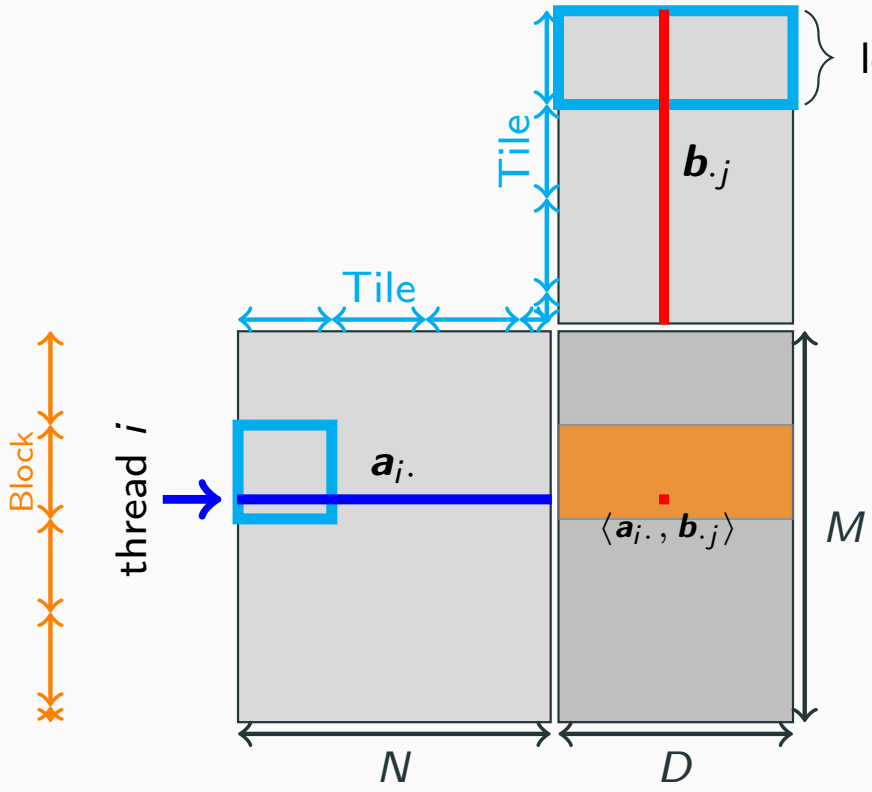
$\rightarrow$ less transfer between global and thread memory (shared mem and/or register)

Code in cuda

Recall: Single Instruction / Multiple Thread model (SIMT)

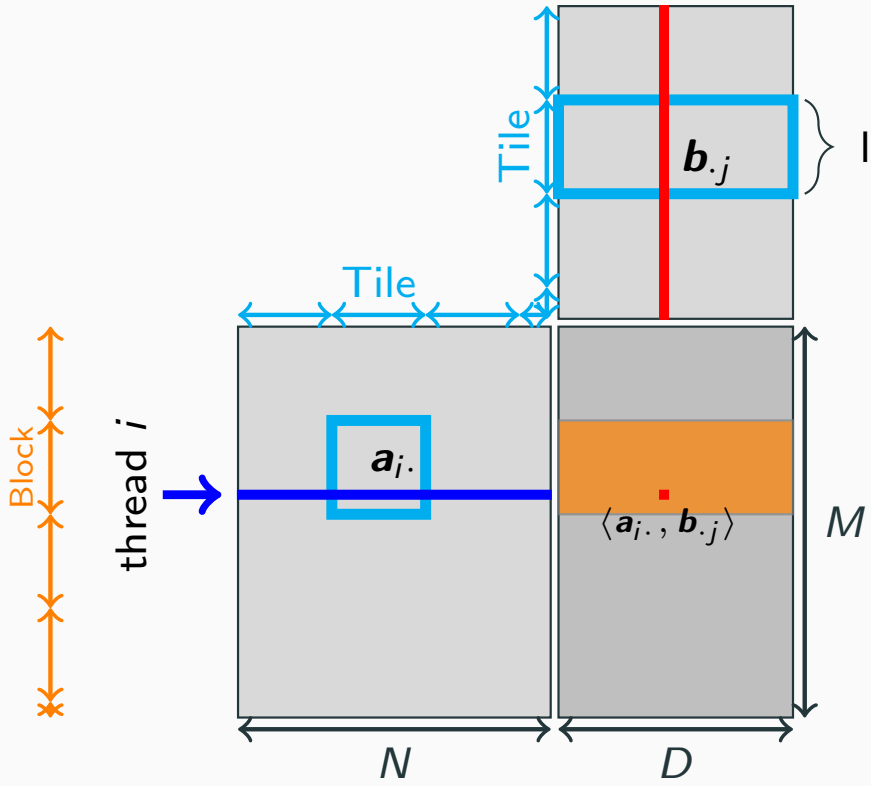
```
__global__ void simpleMultiply(float* a,
                               float* b,
                               float* c,
                               int N)
{
  int row = threadIdx.x + blockIdx.x*blockDim.x;
  int col  = threadIdx.y + blockIdx.y*blockDim.y;
  float sum = 0.0f;
  for (int i = 0; i < N; i++) {
    sum += a[row*N+i] * b[i*N+col];
  }
  c[row*N+col] = sum;
}
```

MatMult: Tiled implementation (block sub-matrix product)



- Tasks (scanning rows $\mathbf{a}_i$) divided into tiles
- All thread use the shared memory within a block
  - $\rightarrow$ a single memory transfered of each tile in $\mathbf{B}$ for all threads

MatMult: Tiled implementation (block sub-matrix product)



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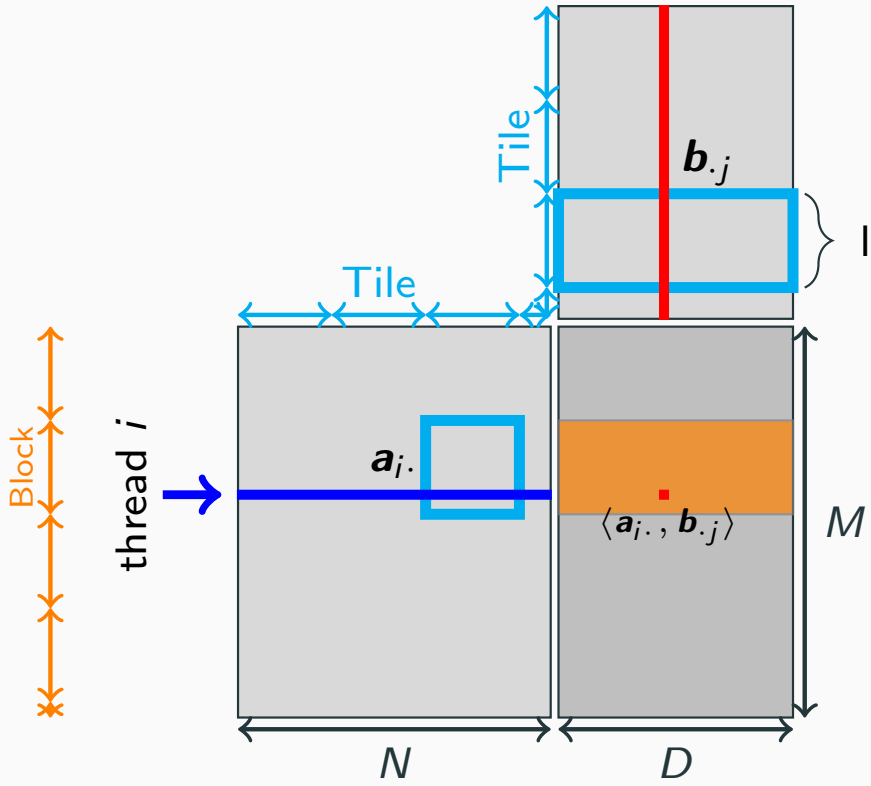


- Accumulation (addition of the intermediate results) when scanning tiles across **A**

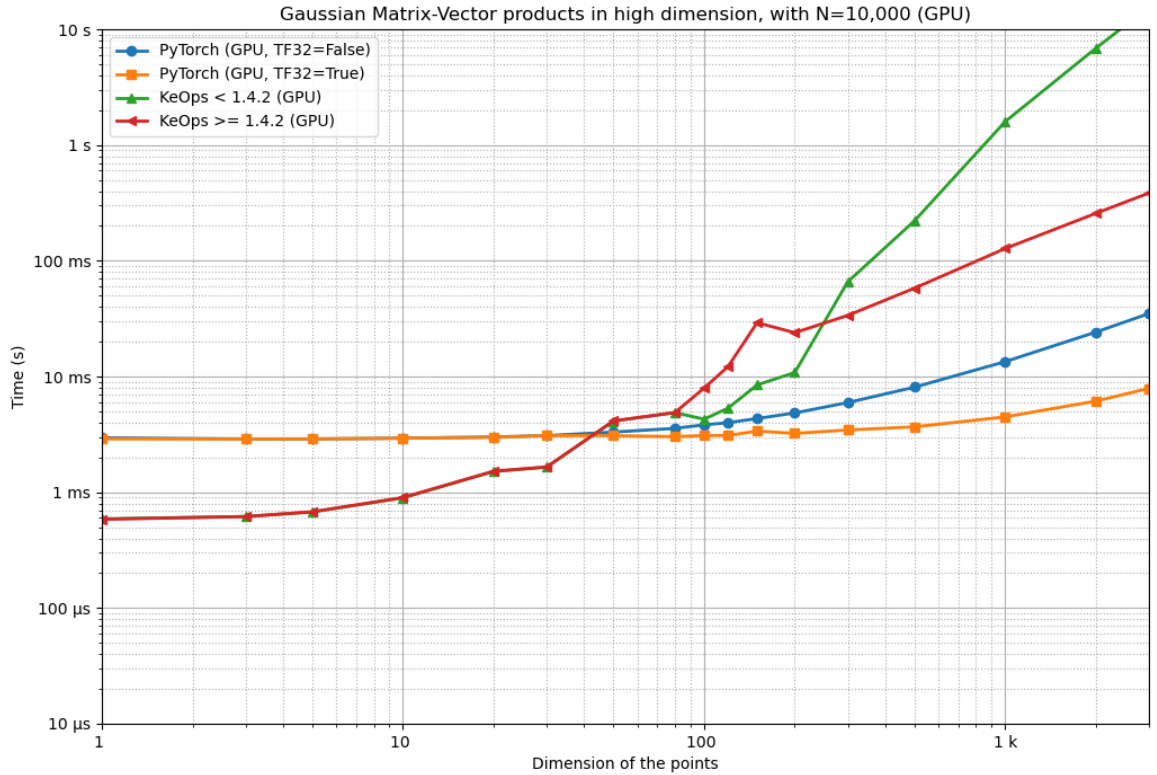
Code

```
__global__ void coalescedMultiply(double*a,
                                  double* b,
                                  double*c,
                                  int N)
{
  __shared__ float aTile[TILE_DIM][TILE_DIM];
  __shared__ double bTile[TILE_DIM][TILE_DIM];

  int row = blockIdx.y * blockDim.y + threadIdx.y;
  int col = blockIdx.x * blockDim.x + threadIdx.x;
  float sum = 0.0f;
  for (int k = 0; k < N; k += TILE_DIM) {
    aTile[threadIdx.y][threadIdx.x] = a[row*TILE_DIM+threadIdx.x];
    bTile[threadIdx.y][threadIdx.x] = b[threadIdx.y*N+col];
    __syncthreads();
    for (int i = k; i < k+TILE_DIM; i++)
      sum += aTile[threadIdx.y][i]* bTile[i][threadIdx.x];
  }
  c[row*N+col] = sum;
}
```

Shared Memory limitation

Using the shared memory is critical (10× faster). But is very limited...



Benchmark

- Optimization needs an understanding of GPU architecture
- Memory optimization: coalescing, shared memory
- Execution configuration: latency hiding
- Instruction throughput: use high throughput inst, reduce wasted cycles
- Do measurements!
  - Use the Profiler, simple code modifications
  - Compare to theoretical peaks

Computation on GPU

JIT with cuda: nvrtc

Meta programming