

IHPC Seminar, 04/02/2020

Breaking the curse of dimensionality from large data to Reduced Order Models

Dr. Lucas Lestandi

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This work was conducted with

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Agency for
Science, Technology
and Research
SINGAPORE

Context

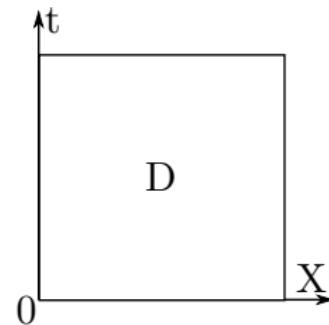
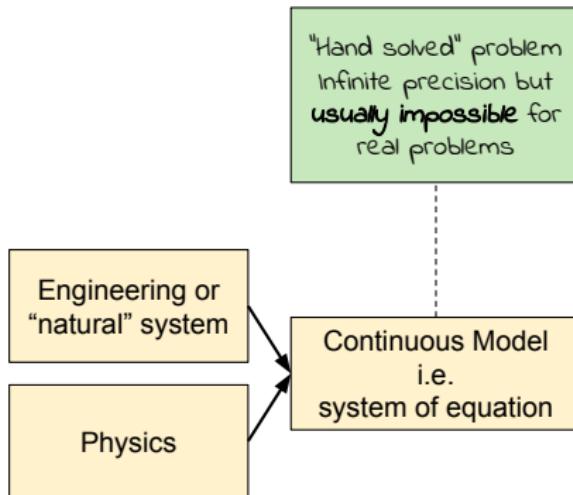
Why do we need Reduced Order Modeling and Low Rank Approximation?

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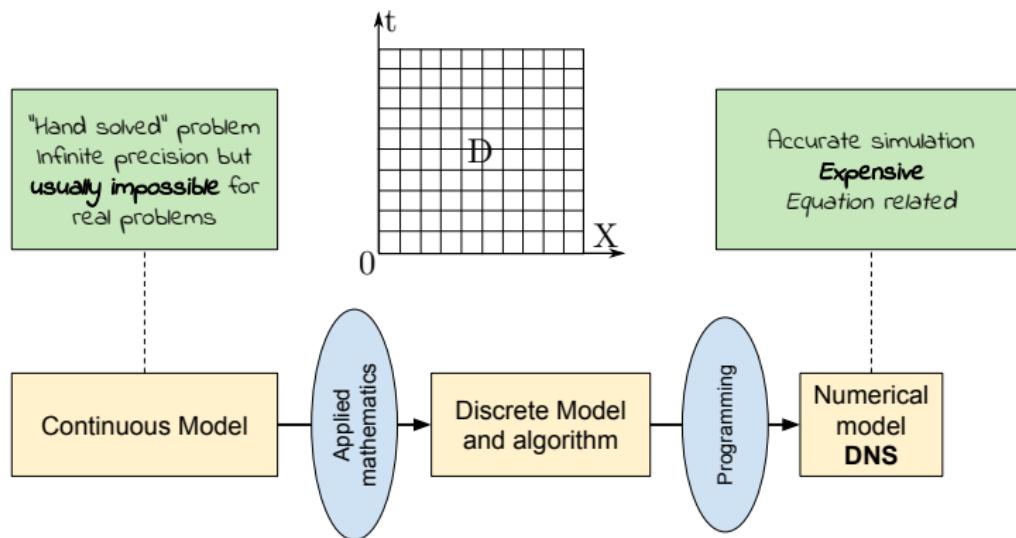
- the curse of dimensionality
- reduce data
- reduce model

Numerical simulation in fluids



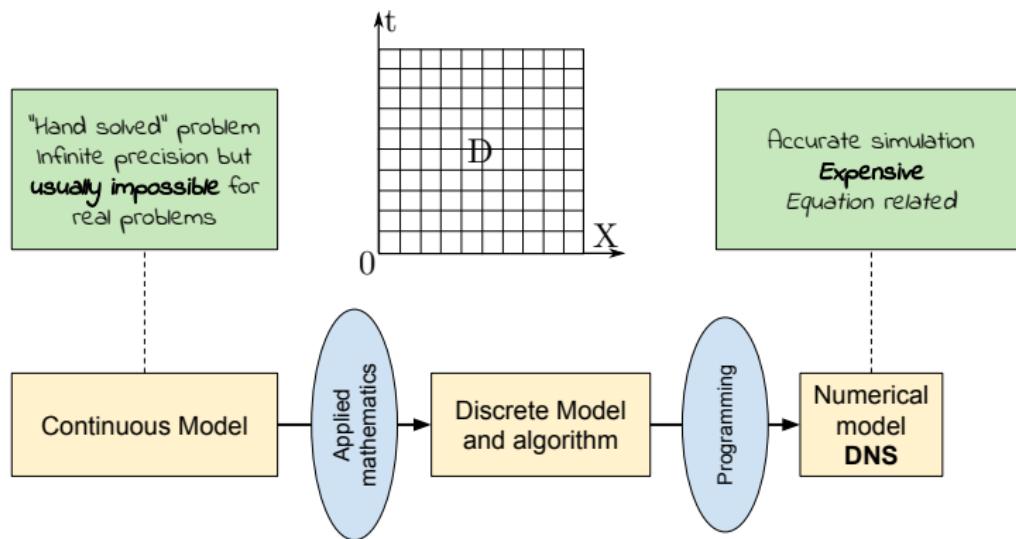
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Numerical simulation in fluids



$$\frac{\partial v}{\partial t} + c \frac{\partial v}{\partial x} = 0 \implies \frac{v_i^{n+1} - v_i^n}{\delta t} + c \frac{v_{i+1}^n - v_{i-1}^n}{\delta x} = 0$$

Numerical simulation in fluids



$$\frac{\partial \mathbf{v}}{\partial t} + c \frac{\partial \mathbf{v}}{\partial x} = 0 \implies \frac{v_i^{n+1} - v_i^n}{\delta t} + c \frac{v_{i+1}^{n+1} - v_{i-1}^{n+1}}{\delta x} = 0 \implies \mathbf{v}^{n+1} = A^{-1} \mathbf{v}^n \quad \text{with } A \in \mathbb{R}^{N \times N}$$

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Solve n_t times linear system of size N :

$$Ax = b, \quad x \in \mathbb{R}^N$$

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The curse of dimensionality

Let $N = 1000$,

d	shape	DoF	Mem
1	1000	10^3	7.8 kB
2	1000^2	10^6	7.6 MB
3	1000^3	10^9	7.4 GB
3D+time	1000^4	10^{12}	7.3 TB

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- Other parameters : viscosity, stiffness, shape,... \Rightarrow many dimensions
- Control, optimization \Rightarrow many queries

Big Data ?

Modern Super Computers

Scale	Name	Loc.	Country	Cores	Pflops	Power (kW)
Local	Condor	TREFLE,I2M	FR	400	NA	NA
National	ASPIRE 1	NSCC	SG	30,912	1	NA
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World	Summit	Oak Ridge	USA	2,414,592	148	10,096

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Large Numerical Simulations

Water drop simulation (2017, F. Desmons)

- 70M points
- time step 10^{-5} , 200 snapshots
- OCCIGEN : 1500 CPU, 6 days
- 2 TB of data

Full Universe (2012, CEA, Curie)

- 550 billion particles, 2 trillion points
- 300TB MEM, 80 000 CPU
- 10M CPU hours
- 50 PB of data

Reduced order modeling and data reduction

Reduced order modeling and data reduction

Change of paradigm

- Break the curse of dimensionality to open new areas

Reduced order modeling and data reduction

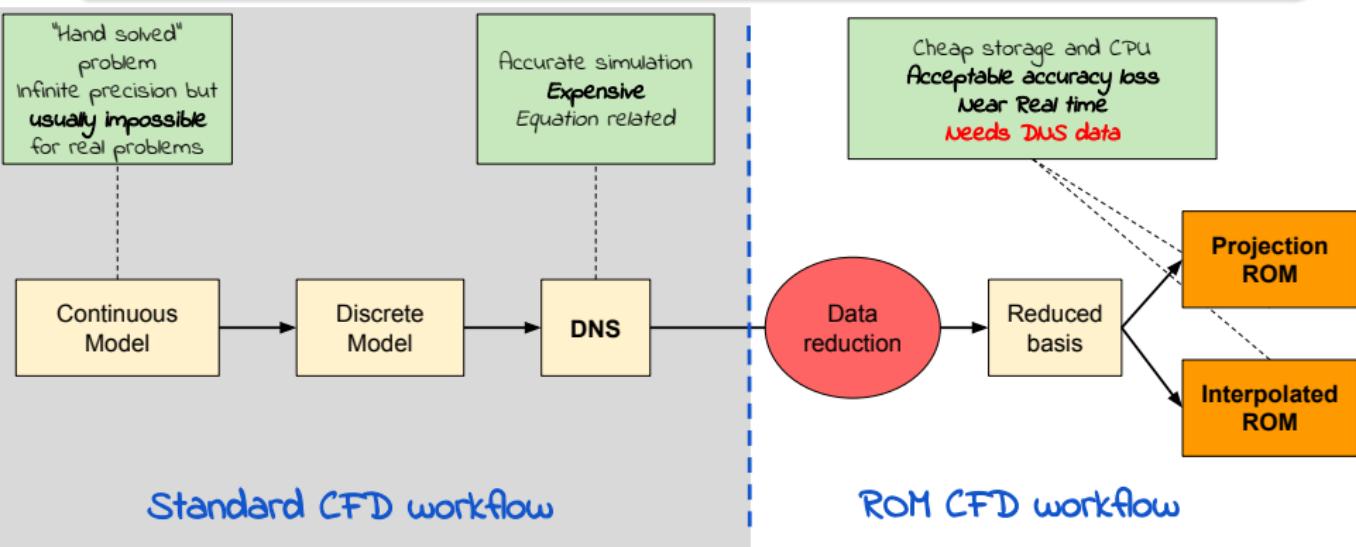
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- Cost from N^d to rNd with $r \ll N$

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Outline

Data decomposition

- Bivariate decomposition

- Tensor formats and approximation

- Numerics

Reduced order models for complex flows

Research Project: Deep Reduced Order Model

Conclusion and perspectives

Data decomposition

Bivariate decomposition

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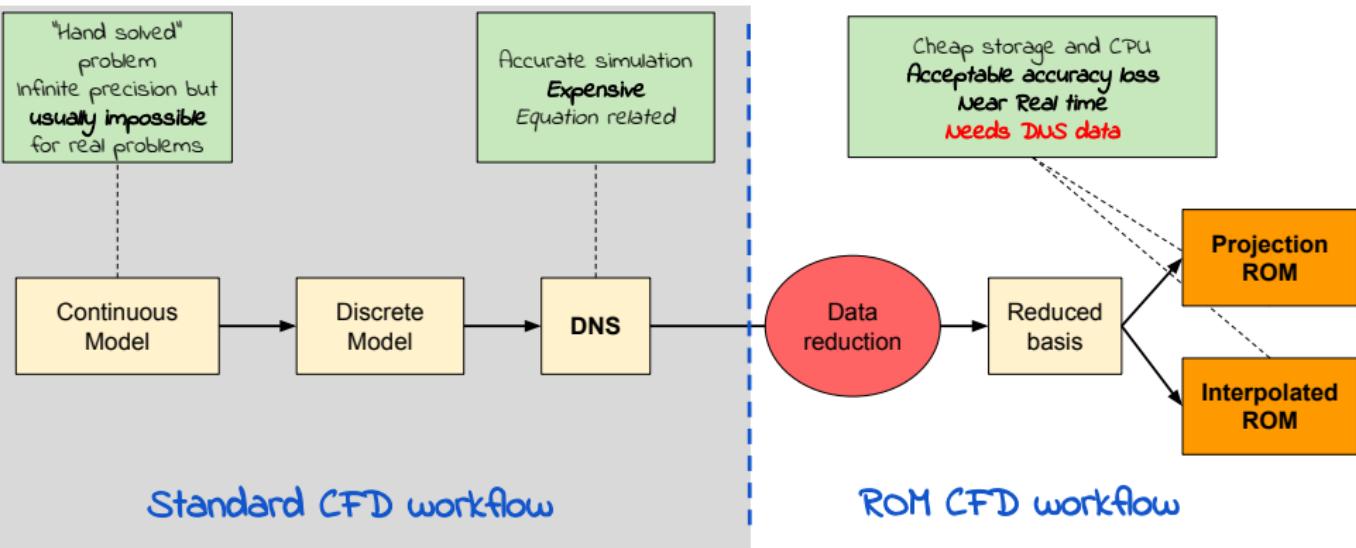
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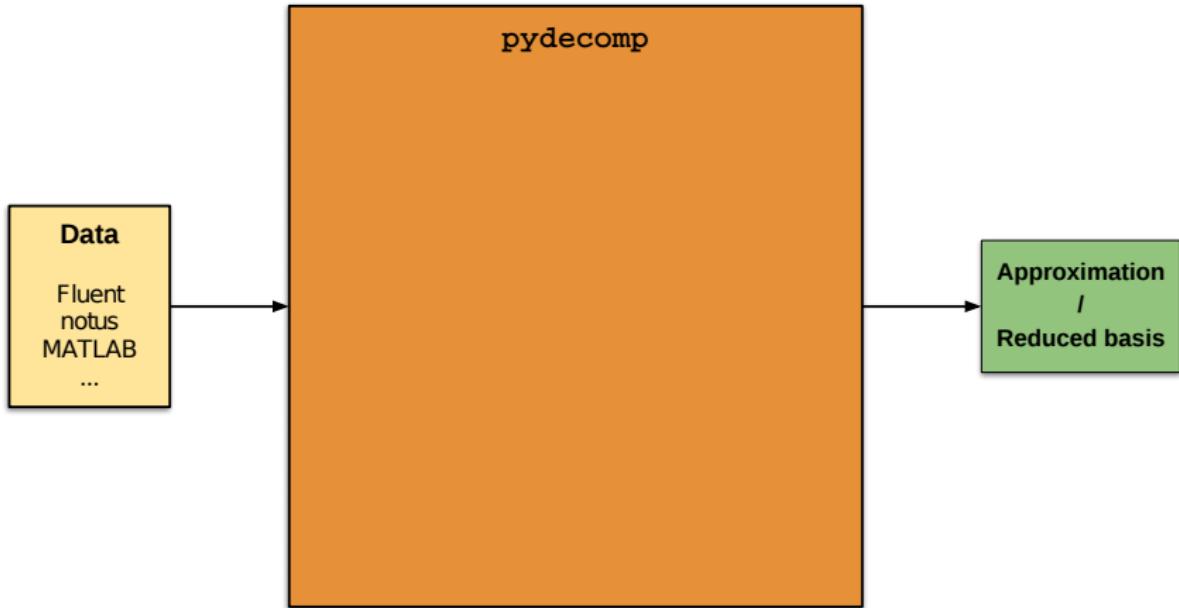
Conclusion and perspectives

Data decomposition



Data decomposition

Build a library that computes data decomposition:



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Conclusion and perspectives

SVD, a General Matrix Decomposition

Theorem (Singular Value Decomposition)

For any matrix $A \in \mathbb{R}^{n \times m}$, there are orthogonal matrices $U \in \mathbb{R}^{m \times m}$ and $V \in \mathbb{R}^{n \times n}$ so that

$$A = U\Sigma V^\top$$

where Σ is a diagonal matrix of size $n \times m$ with diagonal elements $\sigma_{ii} \geq 0$ called singular values.

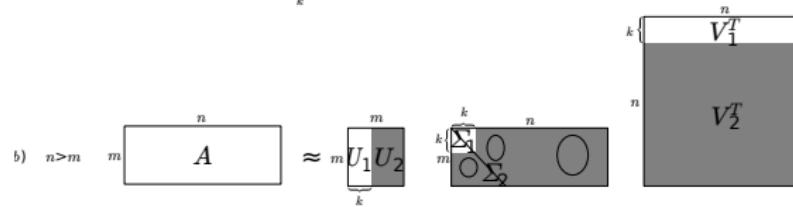
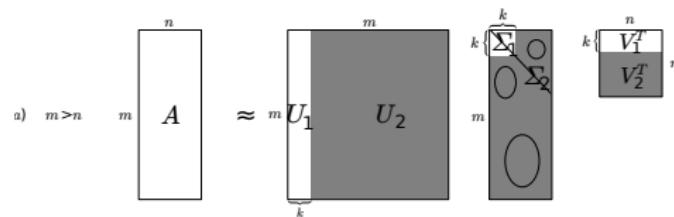
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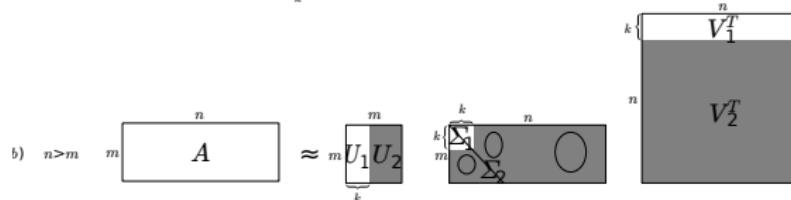
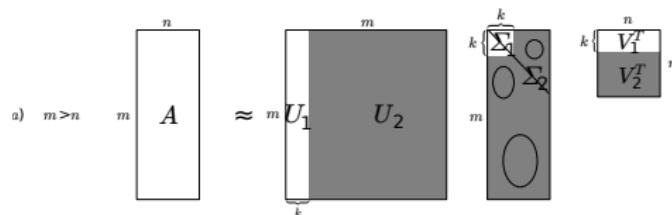
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- **Eckart-Young theorem:** $\min_{\text{rank}(B)=k} \|A - B\|_2 = \|A - A_k\|_2 = \sigma_{k+1}$
- The SVD can be computed by EVD.

SVD for image compression

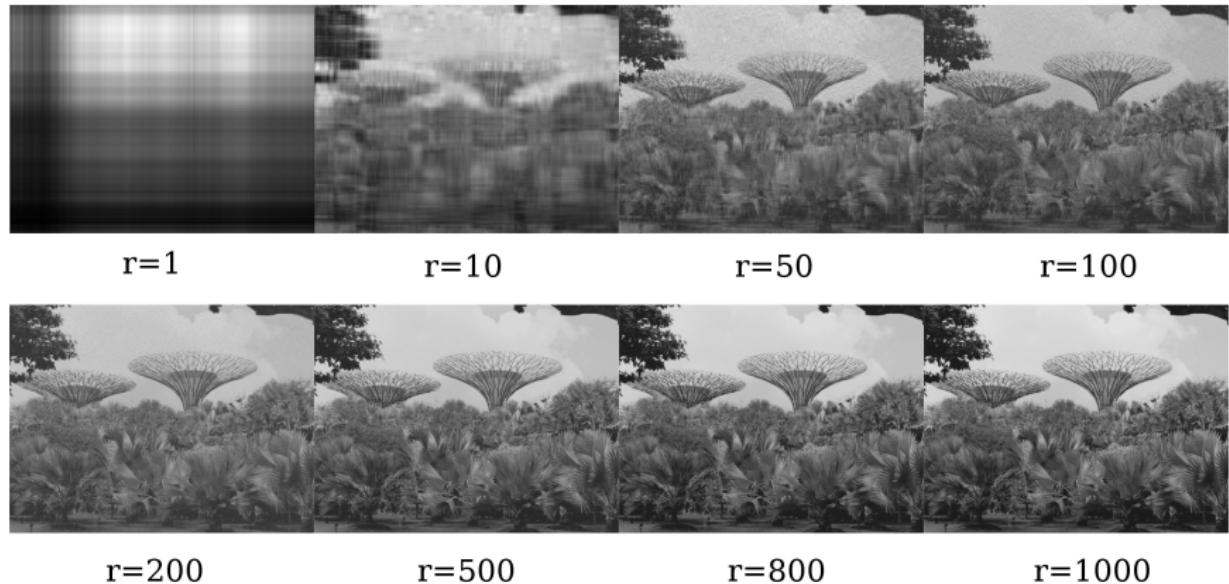
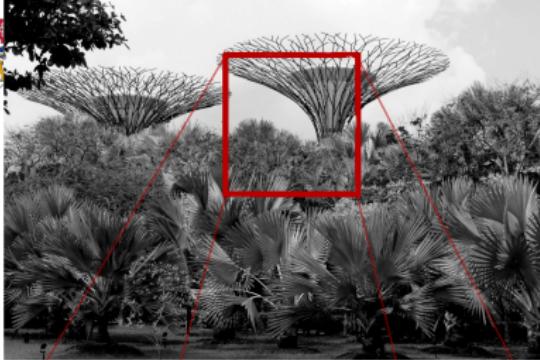


Figure: Singapore garden by the sea SVD reconstruction



jpg(90%), 1.5Mb



SVD ($r=200$), 1.37Mb



Proper Orthogonal Decomposition

POD

- **Goal:** Approximate $u(x, t)$ by a finite sum

$$u(x, t) \simeq u_r(x, t) = \sum_{k=1}^r a_k(t) \phi_k(x)$$

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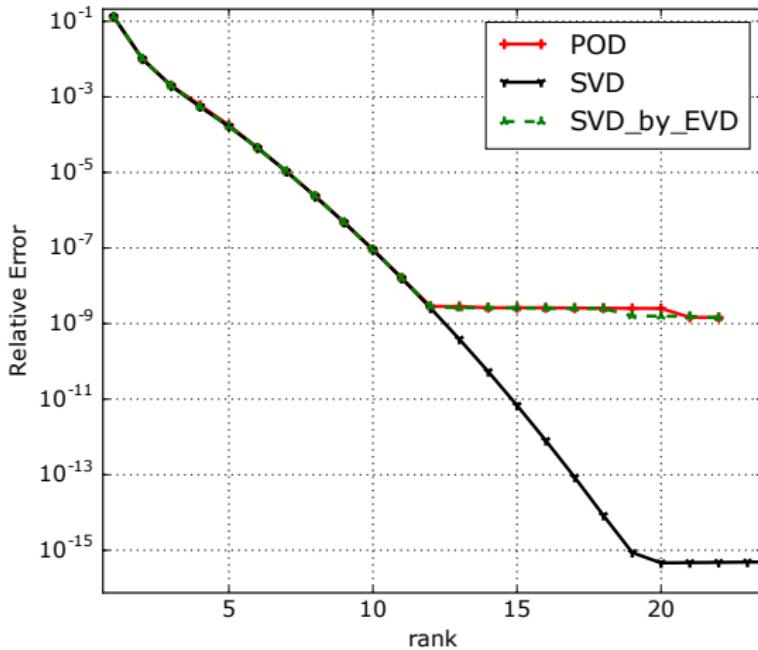
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- Choice of the inner product : l^2, L^2, H^1, \dots

Example: synthetic data

Let f defined on $\Omega = [0, 1] \times [0, 1]$ with $f(x, t) = \sin(\sqrt{x^2 + t^2}) \approx \tilde{f} = \sum_{k=1}^r \phi_k(x) a_k(t)$

$$\mathcal{E} = \frac{\|f - \tilde{f}\|_{L^2}}{\|f\|_{L^2}}$$



High Reynolds number Lid driven cavity

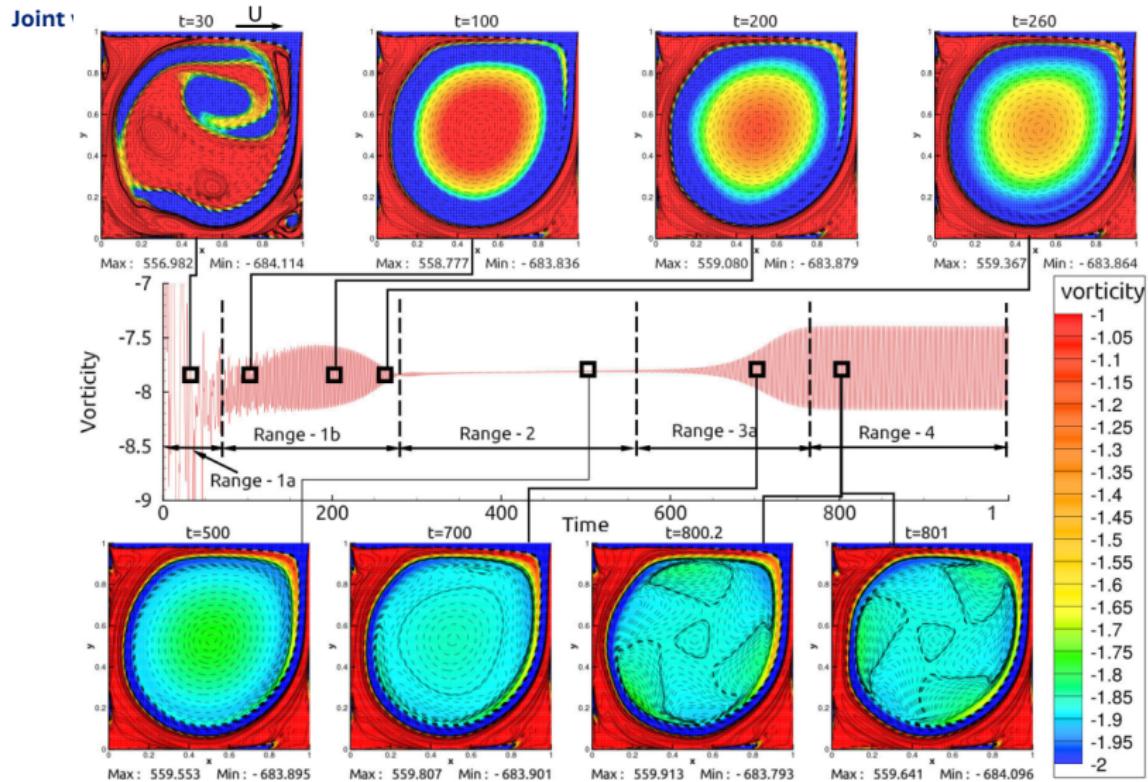


Figure: Vorticity time series at (0.95,0.95) for Re=8800

LDC space modes

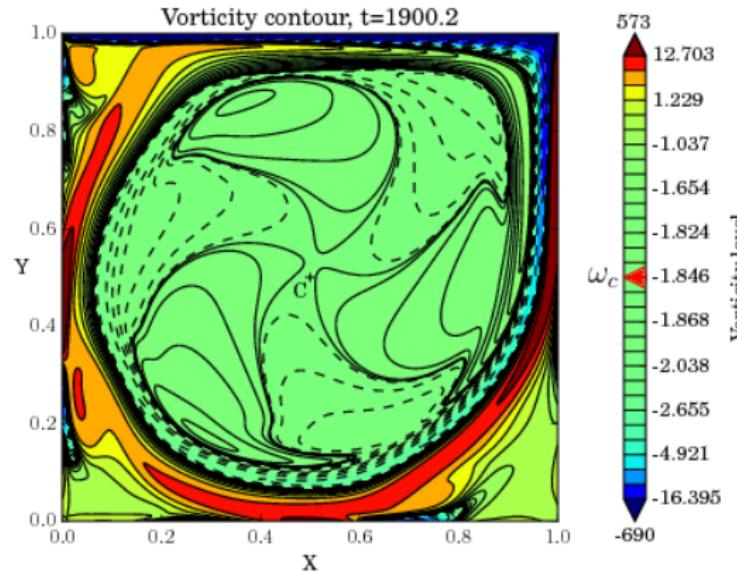


Figure: One snapshot of vorticity contours at $t=1900.2$ for $Re=9800$ in the limit cycle

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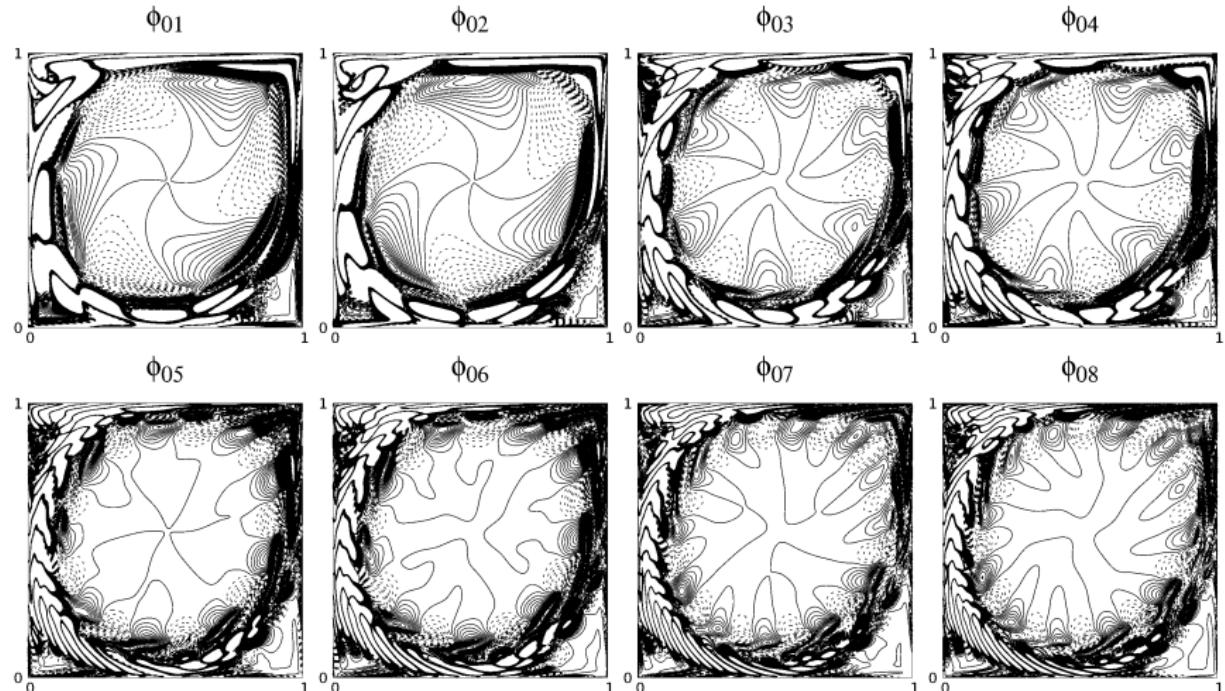


Figure: $Re=9800$, first 8 POD space modes

LDC time modes

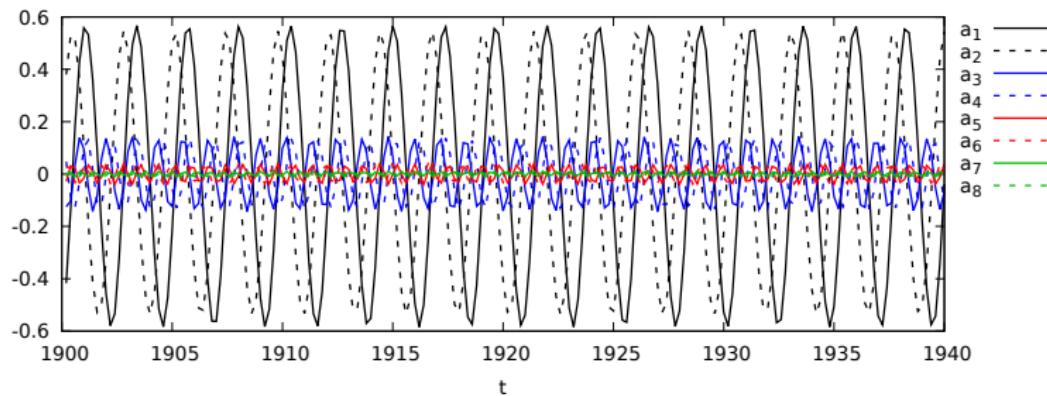
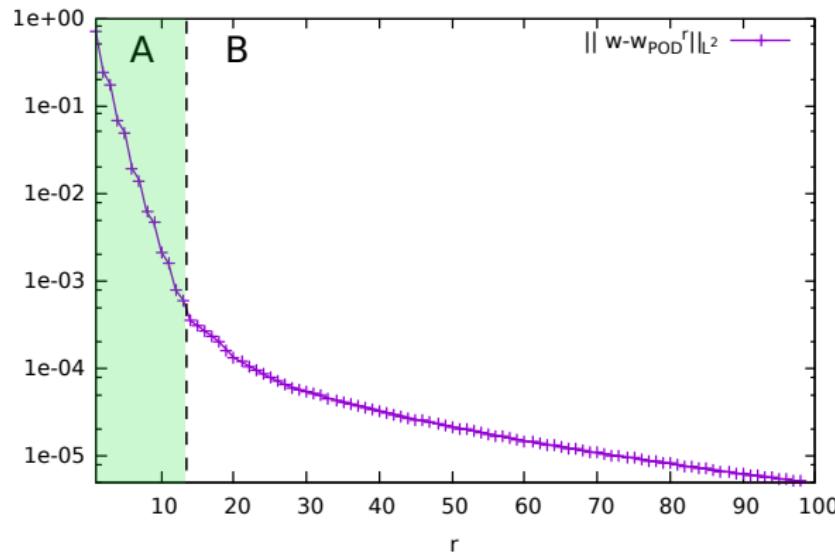


Figure: Re=9800, first 8 POD time modes

Error decay



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Tensors

A generalisation of matrices to higher dimensions. i.e. $A \in \mathbb{R}^{n_1 \times \dots \times n_d}$.

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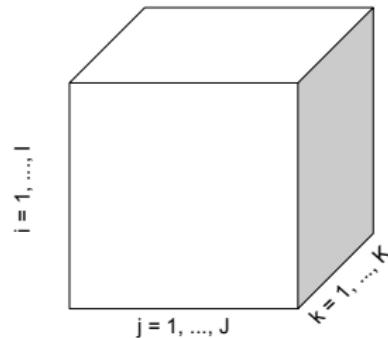


Figure: Order 3 tensor

Tensor related Key Properties

- **Tensor product, \otimes :**

$$\begin{aligned}\otimes : \quad \mathbb{R}^{\mathcal{I}} \times \mathbb{R}^{\mathcal{J}} &\rightarrow \quad \mathbb{R}^{\mathcal{I} \times \mathcal{J}} \\ (\mathcal{X}, \mathcal{Y}) &\mapsto \quad \mathcal{X} \otimes \mathcal{Y}\end{aligned}$$

Entry-wise $\mathcal{T} = \mathcal{X} \otimes \mathcal{Y}$ reads

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- **Matricisation:** Ordering the elements of a tensor into a matrix **allows SVD**.

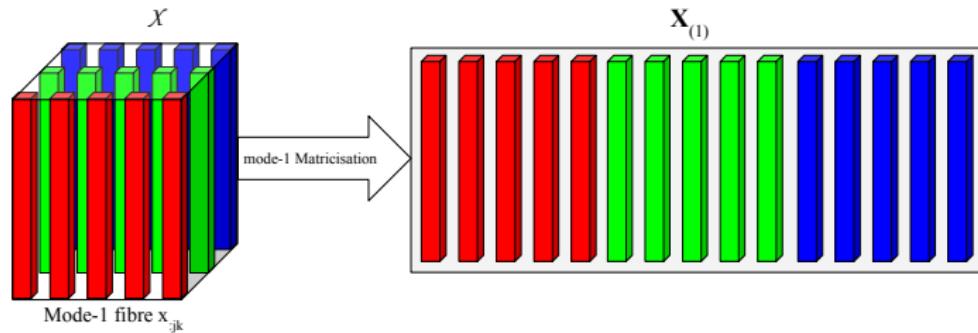


Figure: Mode one matricisation of third order tensor with $\mathbf{X} \in \mathbb{R}^{I \times J \times K}$.

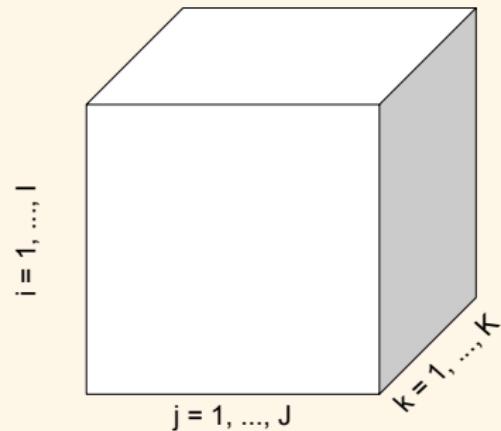
Full Tensor Format

A d -way array.

- High storage cost : $\mathcal{O}(n^d)$
- No evaluation cost

Can be used if n^d remains small

$$\mathcal{X} = \sum_{i \in \mathcal{I}} x_i e_{1,i_1} \otimes \cdots \otimes e_{d,i_d}$$



Canonical Tensor Format and CP Decomposition

$\mathcal{T} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ is a finite sum of rank-1 tensors.

$$\mathcal{T} = \sum_{i=1}^r \bigotimes_{\mu=1}^d \mathbf{t}_{\mu,i} \quad \text{where } \mathbf{t}_{\mu,i} \in V_\mu = \mathbb{R}^{n_\mu} \quad (1)$$

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■ Storage cost : $\mathcal{O}(drn)$

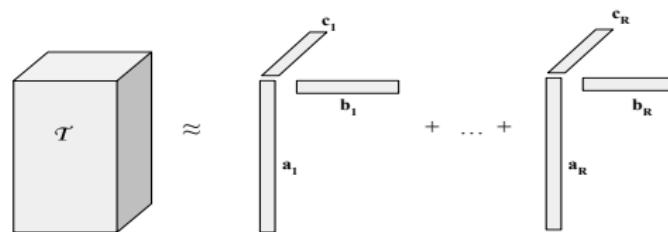


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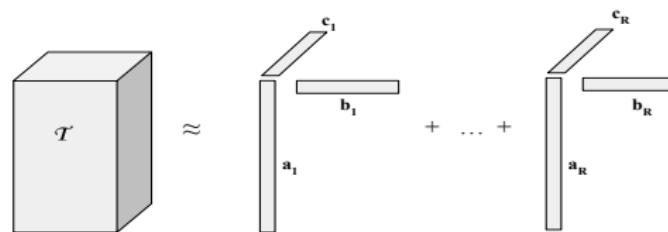


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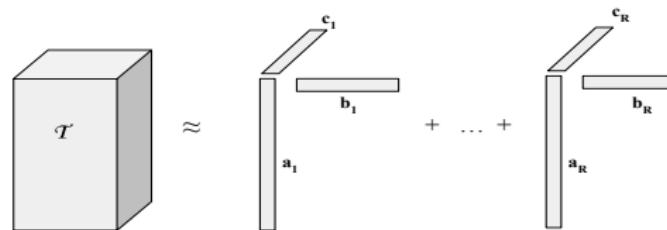


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- **Find the best canonical decomposition: ill-posed problem.**

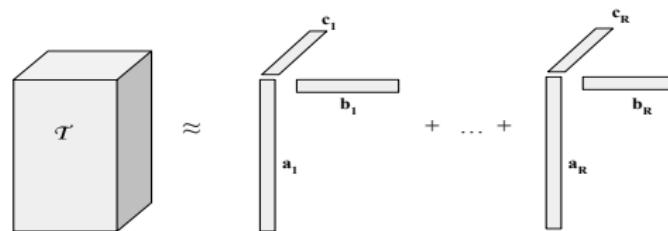


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- Discrete PGD \approx CP decomposition

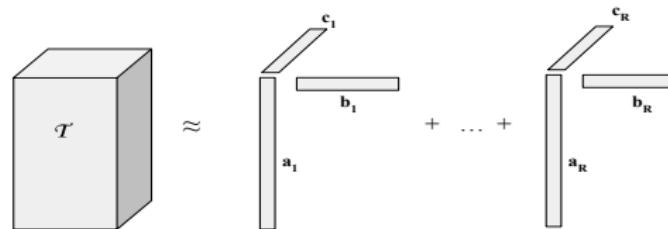


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Tucker Tensor Format

$\mathcal{T} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ in Tucker format.

$$\mathcal{T} = \sum_{i_1=1}^{k_1} \cdots \sum_{i_d=1}^{k_d} w_{i_1, \dots, i_d} u_{1, i_1} \otimes \cdots \otimes u_{d, i_d} \quad (2)$$

with the core tensor $\mathcal{W} \in \mathbb{R}^{k_1 \times \dots \times k_d}$.

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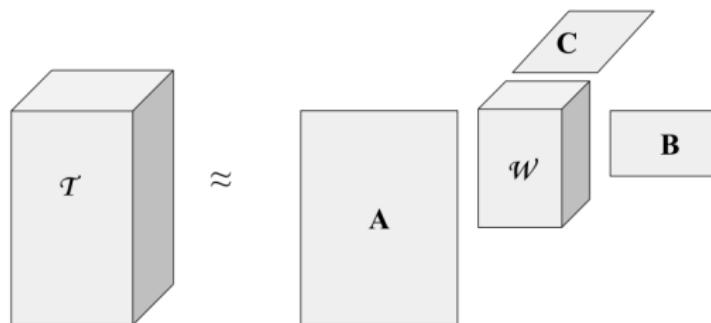
with the core tensor $\mathcal{W} \in \mathbb{R}^{k_1 \times \dots \times k_d}$.

k is the tucker rank of \mathcal{T} .

Storage cost : $\mathcal{O}(k^d + dkn) \Rightarrow$ intractable if d is large.

Algorithms: ST-HOSVD, T-HOSVD with almost best approx.

Heavily relies on matricization.

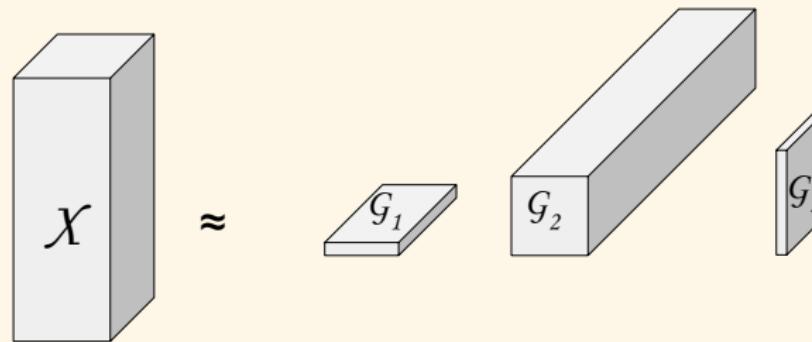


Tensor train

$\mathcal{T} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ in TT format.

$x_{i_1, \dots, i_d} = \mathbf{G}_1(i_1)\mathbf{G}_2(i_2) \cdots \mathbf{G}_d(i_d)$, with $\mathbf{G}_\mu \in \mathbb{R}^{k_{\mu-1} \times k_\mu}$

Storage cost (TT) : $\mathcal{O}(k^2 dn)$



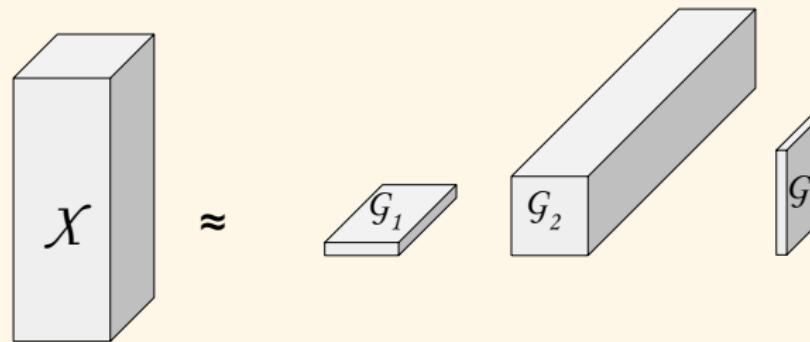
Goal Get rid of the core tensor.

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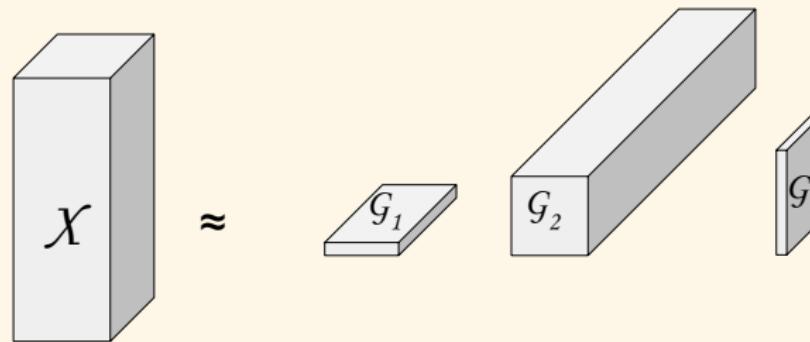
Idea Encode the modes and their relations into matrix products (MPS) for each element.

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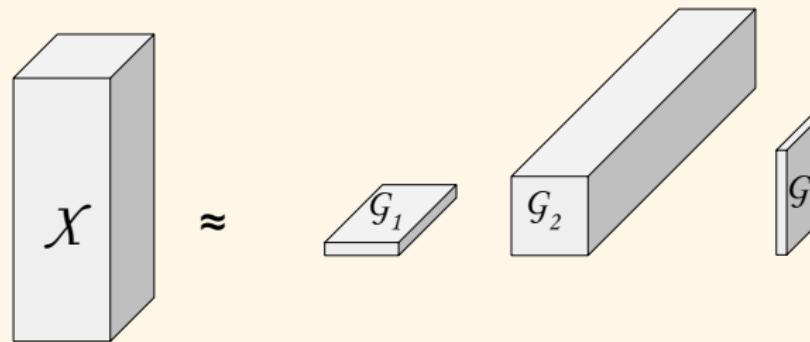
Pros Efficient for high d . Easy implementation. Continuous version

Tensor train

$\mathcal{T} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ in TT format.

$x_{i_1, \dots, i_d} = \mathbf{G}_1(i_1)\mathbf{G}_2(i_2) \cdots \mathbf{G}_d(i_d)$, with $\mathbf{G}_\mu \in \mathbb{R}^{k_{\mu-1} \times k_\mu}$

Storage cost (TT) : $\mathcal{O}(k^2 dn)$



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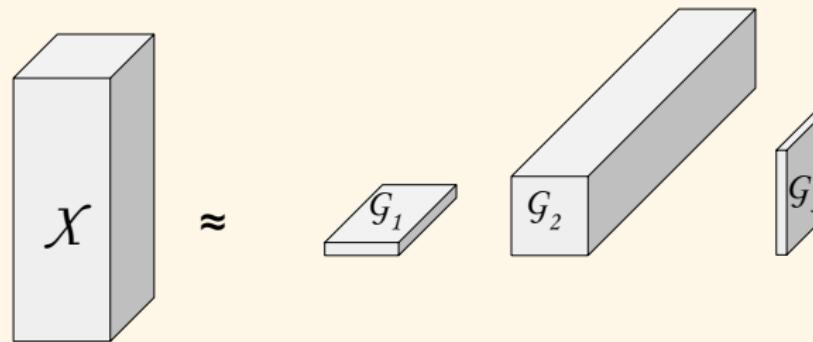
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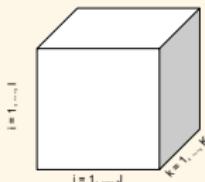
Cons Basis is not orthonormal.

Algo TT-SVD, same idea as ST-HOSVD but different format.

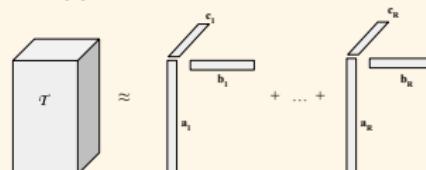
Tensor decomposition recap

Full

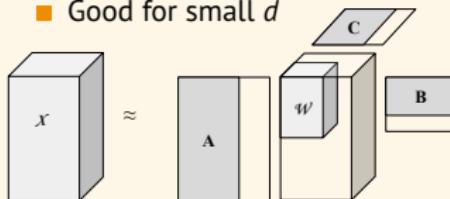
- Original data format.
- Exponential storage cost : $\mathcal{O}(n^d)$

**Canonical**

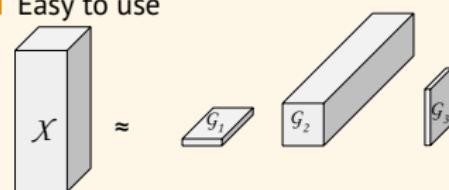
- Linear storage cost : $\mathcal{O}(rnd)$
- Easy programming and No limit on d
- Approximation issues !

**Tucker**

- Exponential storage cost on rank : $\mathcal{O}(k^d + dkn)$
- Easy approximation with (ST-)HOSVD.
- Good for small d

**Tensor Train**

- d linear storage cost $\mathcal{O}(dk^2n)$, Great for large d
- TT-SVD + sampling algorithms.
- Easy to use



Lestandi 2018

Azaiez, Lestandi, and Rebollo 2019

Data decomposition

Bivariate decomposition

Tensor formats and approximation

Numerics

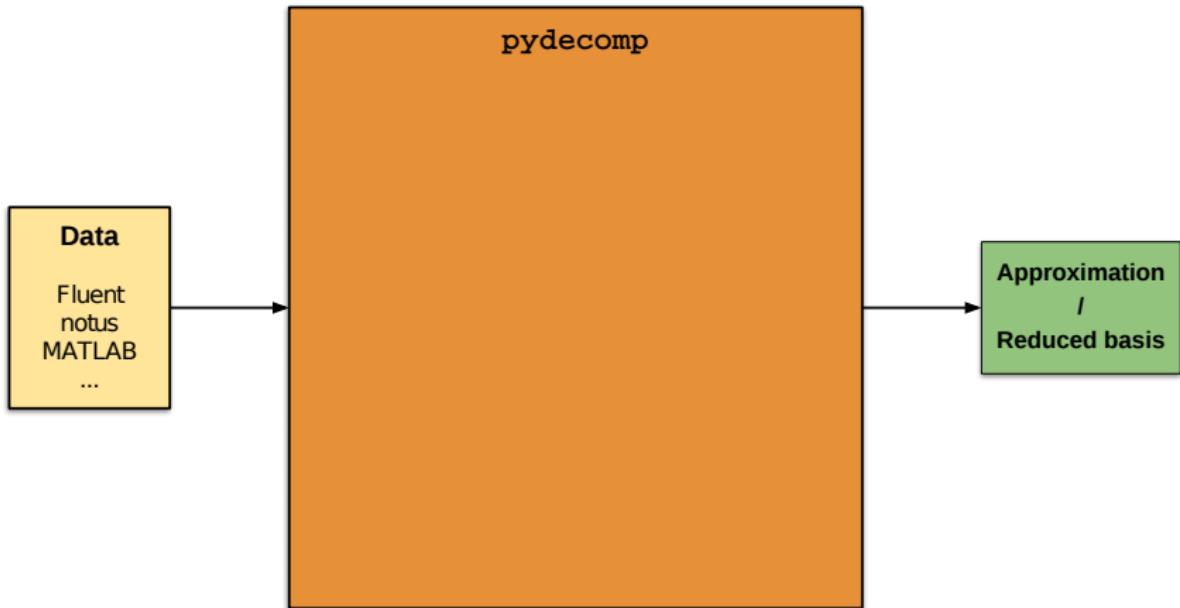
Reduced order models for complex flows

Research Project: Deep Reduced Order Model

Conclusion and perspectives

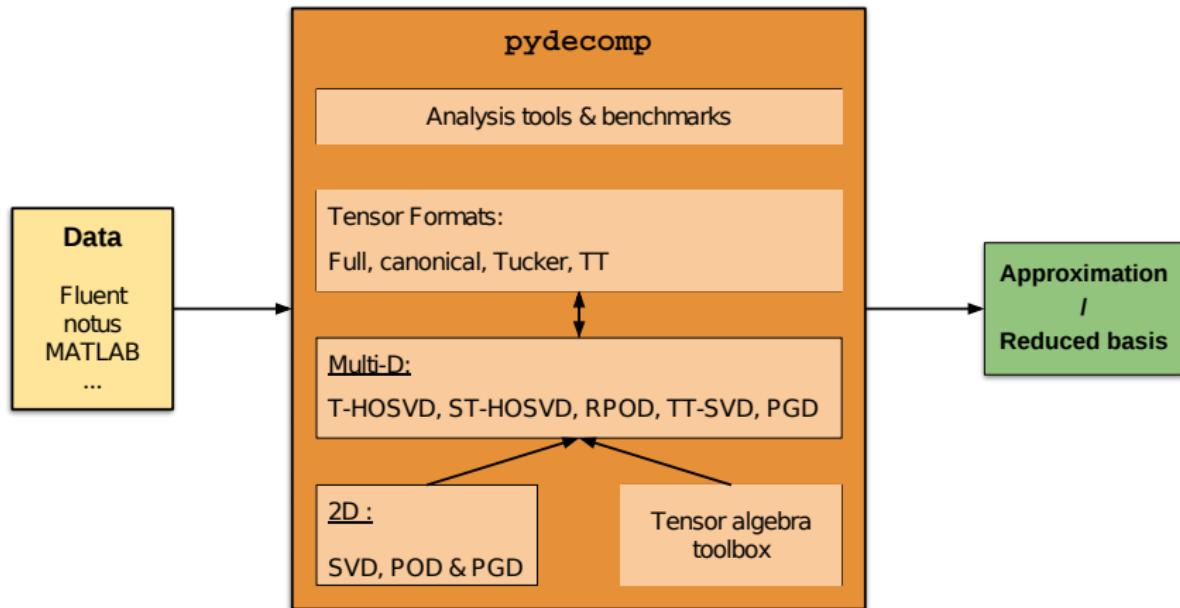
[pydecomp: a data decomposition library](#)

https://git.notus-cfd.org/llestandi/python_decomposition_library



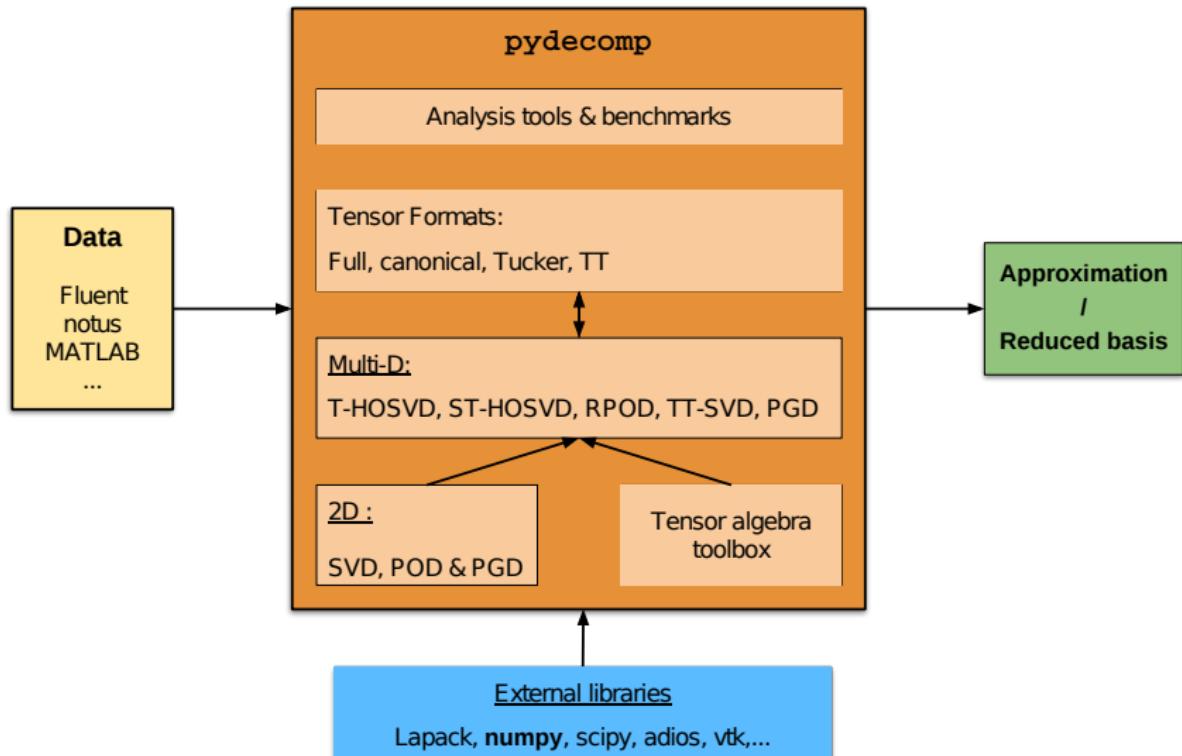
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Synthetic data 3D

$$\mathcal{E} = \frac{||\mathcal{T}_{\text{exact}} - \mathcal{T}_{\text{approx}}||}{||\mathcal{T}_{\text{exact}}||}$$

$$CR = \frac{\text{Mem_cost}(\mathcal{T}_{\text{decomp}})}{\text{Mem_cost}(\mathcal{T}_{\text{exact}})} (\times 100 \text{ for \%}).$$

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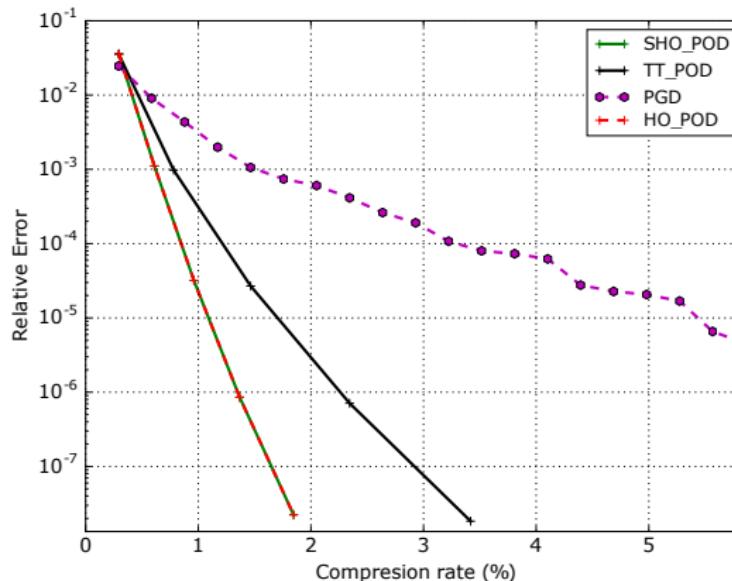


Figure: Approximation error of $f(x, y, z) = \frac{1}{1+x+y+z}$ with 32 grid points per dimension.

Higher dimensions

$$f(\mathbf{x}) = \sin(||\mathbf{x}||_2)$$

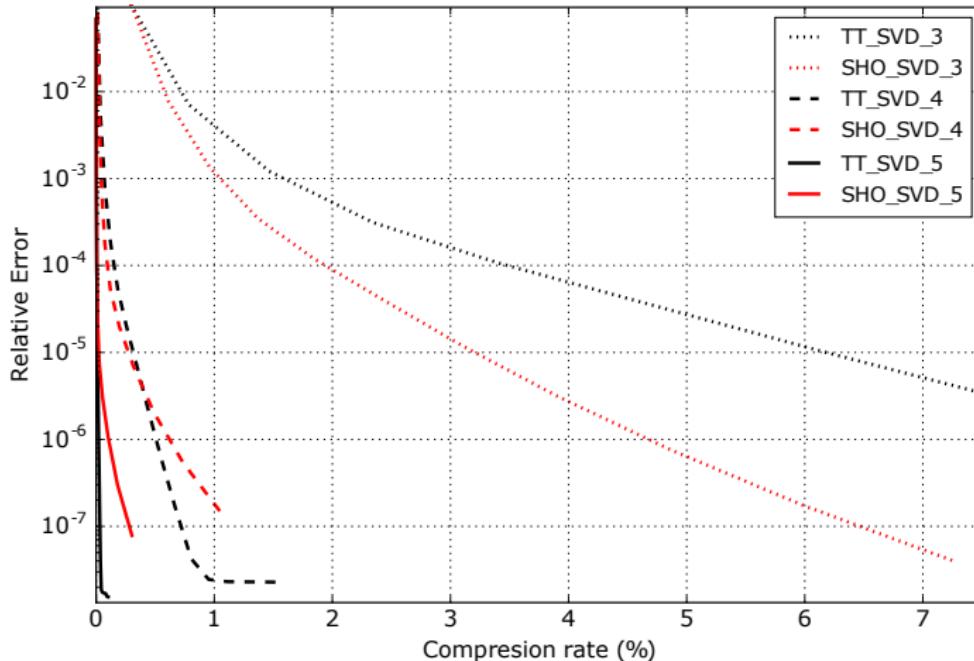


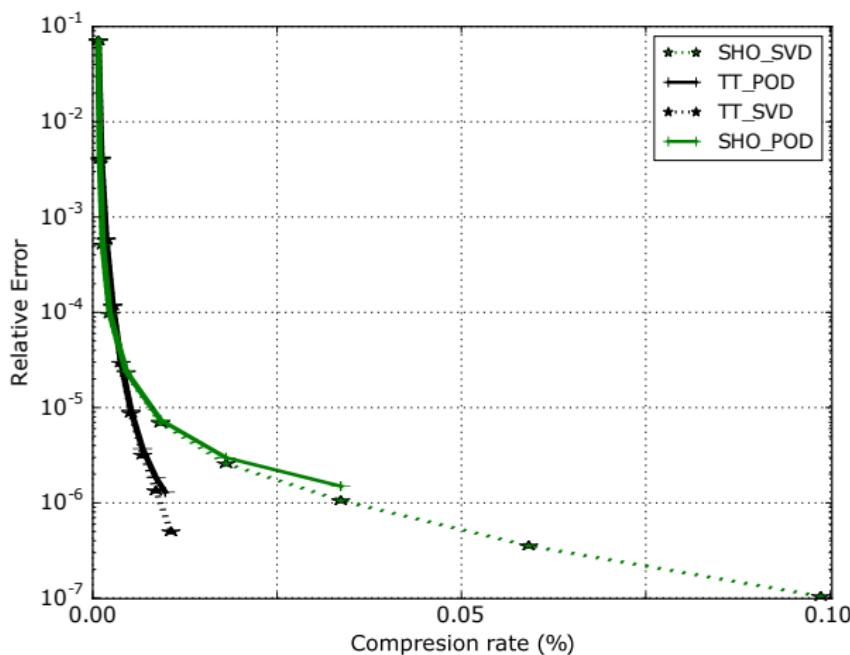
Figure: f_2 decomposition with $d = 3$ to 5 on a 32^d grid with 3 methods, L^2 scalar product.

Scalar product influence

$$\begin{aligned}f_s(x_1, x_2, x_3, x_4, x_5) &= x_1^2 \{\sin[5x_2\pi + 3\log(x_1^3 + x_2^2 + x_4^3 + x_3 + \pi^2)] - 1\}^2 \\&\quad + (x_1 + x_3 - 1)(2x_2 - x_3)(4x_5 - x_4) \cos[30(x_1 + x_3 + x_4 + x_5)] \\&\quad \log(6 + x_1^2 x_2^2 + x_3^3) - 4x_1^2 x_2 x_5^3 (-x_3 + 1)^{3/2}\end{aligned}$$

$\Omega = [0, 1]^5$, cartesian grid, $n = 40$

Scalar product influence



method	comp.	eval.
ST-HOSVD	1.096	1.23
ST-HOPOD	2.378	0.98
TT-SVD	1.205	1.19
TT-POD	2.206	1.13

Table: CPU times (s) on f_v for $n = 40, d = 5, \epsilon = 10^{-12}$

Experimental data: Droplet evaporation

Lestandi 2020

Input data

- 320 × 356 camera spatial resolution
- 51 wavelength
- 29 snapshots

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⇒ Tensor of size $29 \times 51 \times 320 \times 356$ in a 800MB MATLAB file.

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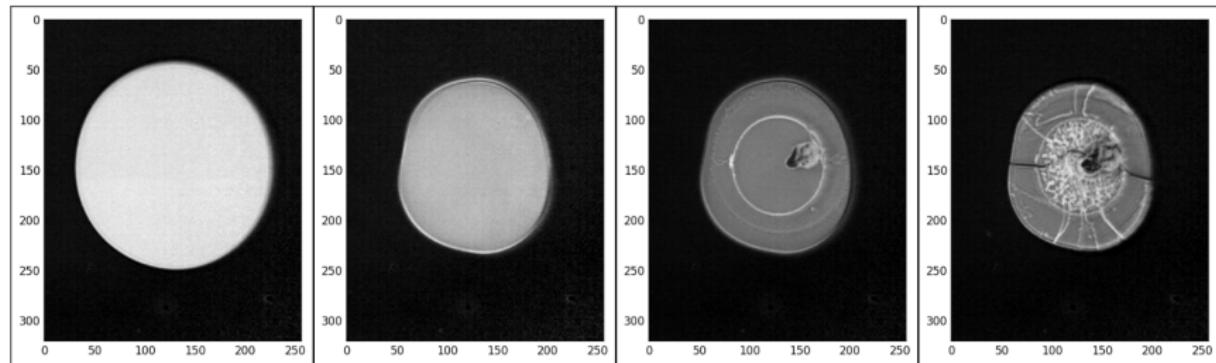
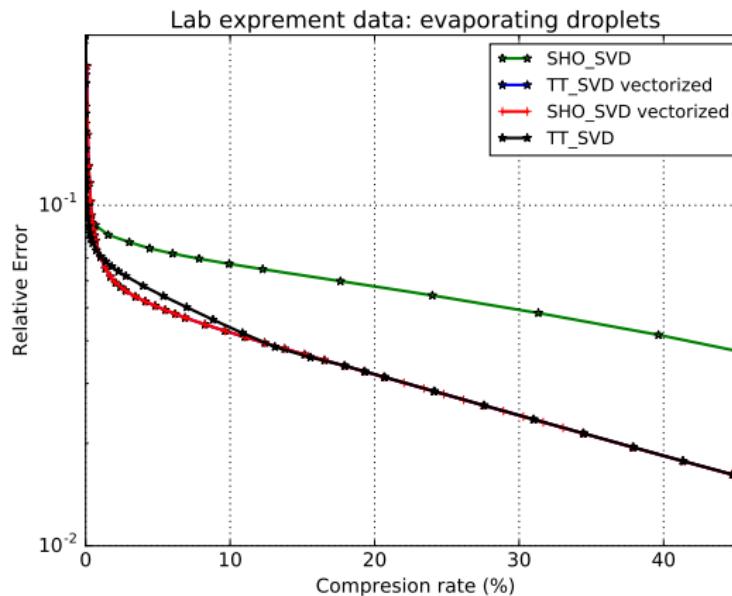
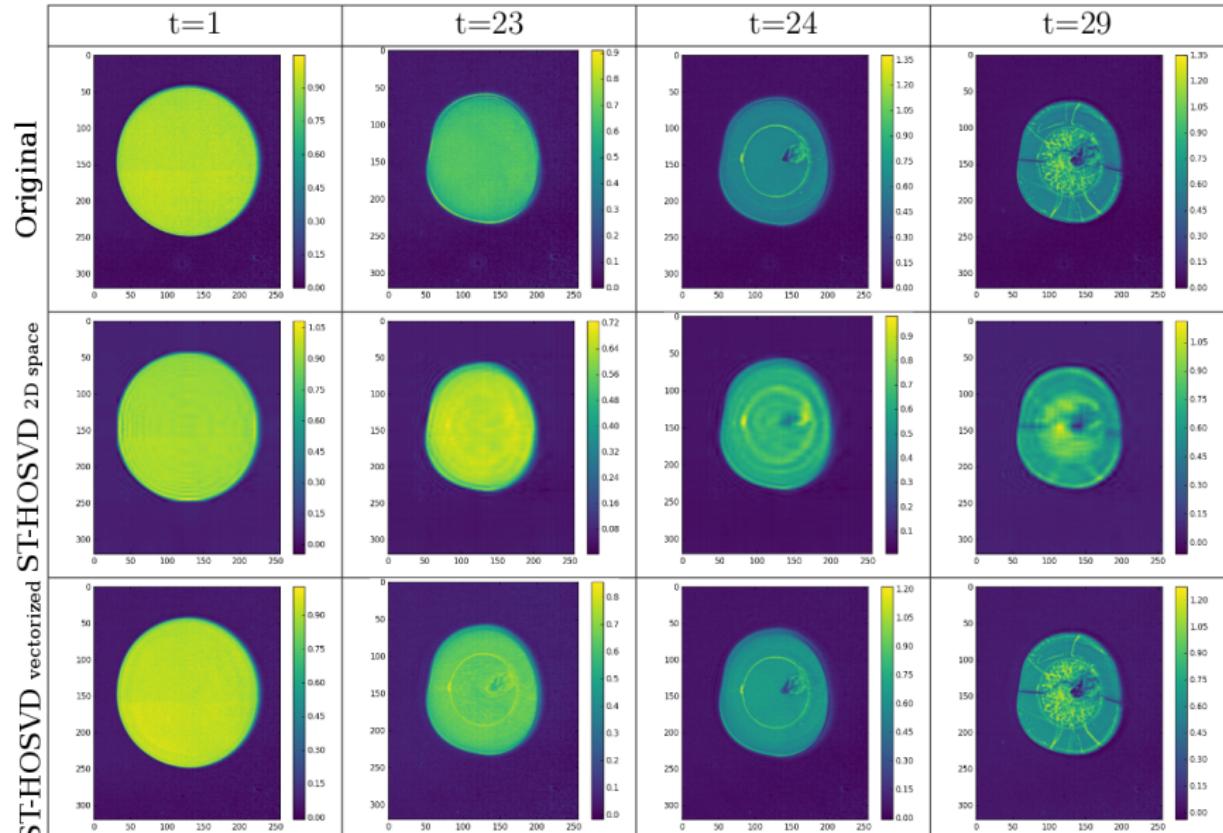


Figure: Evaporating droplets. Data provided by C. Pradère

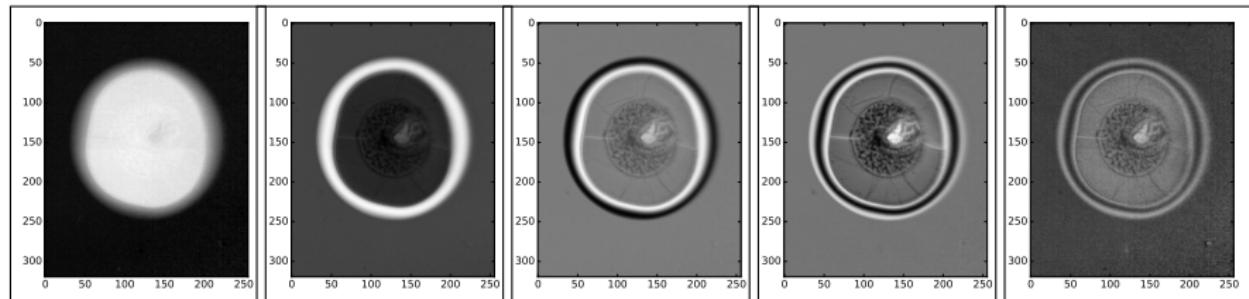
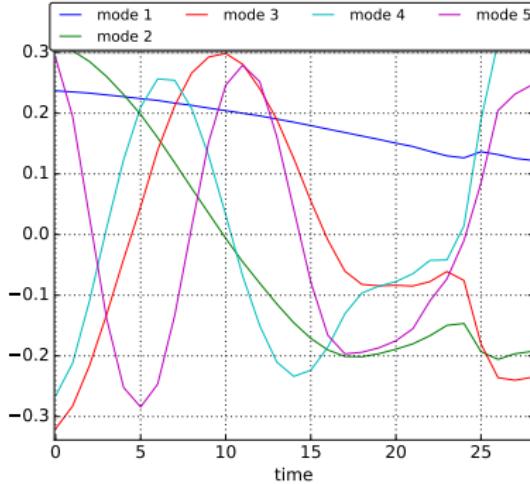
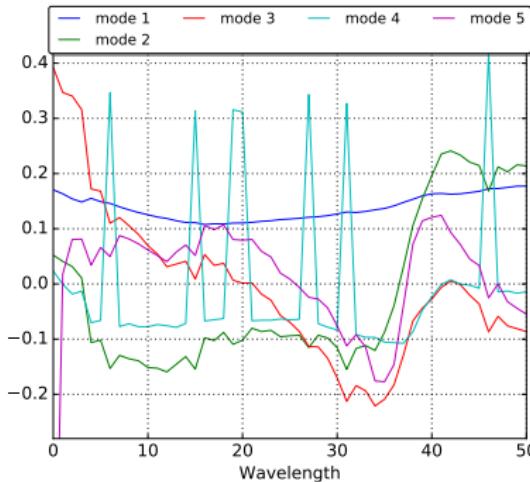
Droplet evaporation data approximation



Droplet evaporation data approximation



Droplet evaporation data modes



Spatial modes from vectorized data layout (1 to 5, left to right).

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Bivariate decomposition

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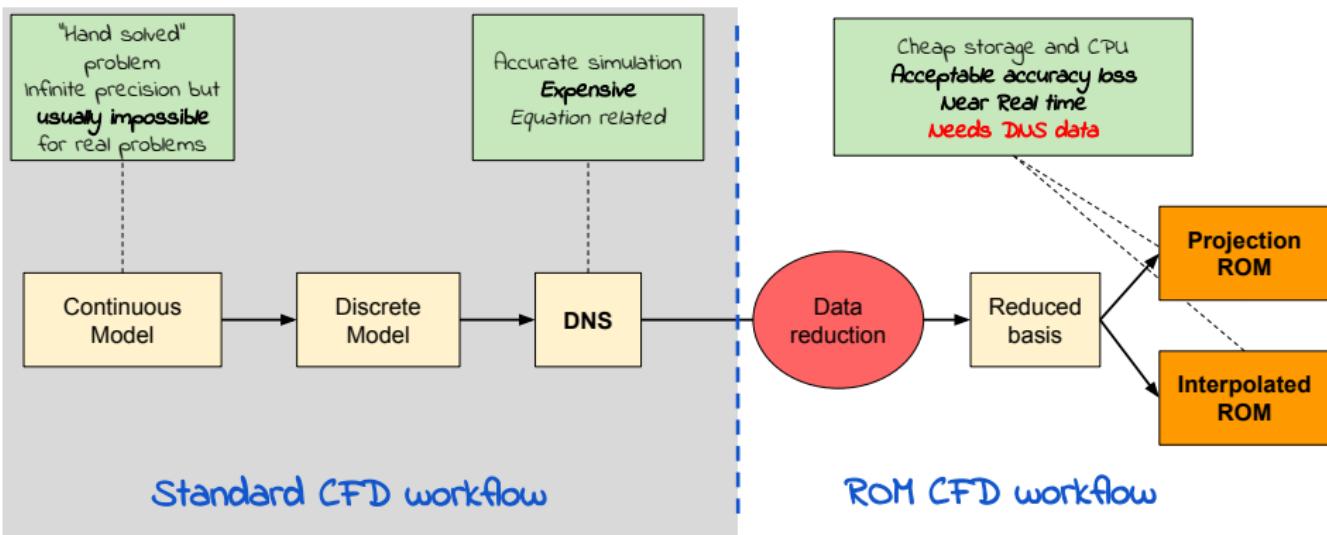
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Reduced order models for complex flows

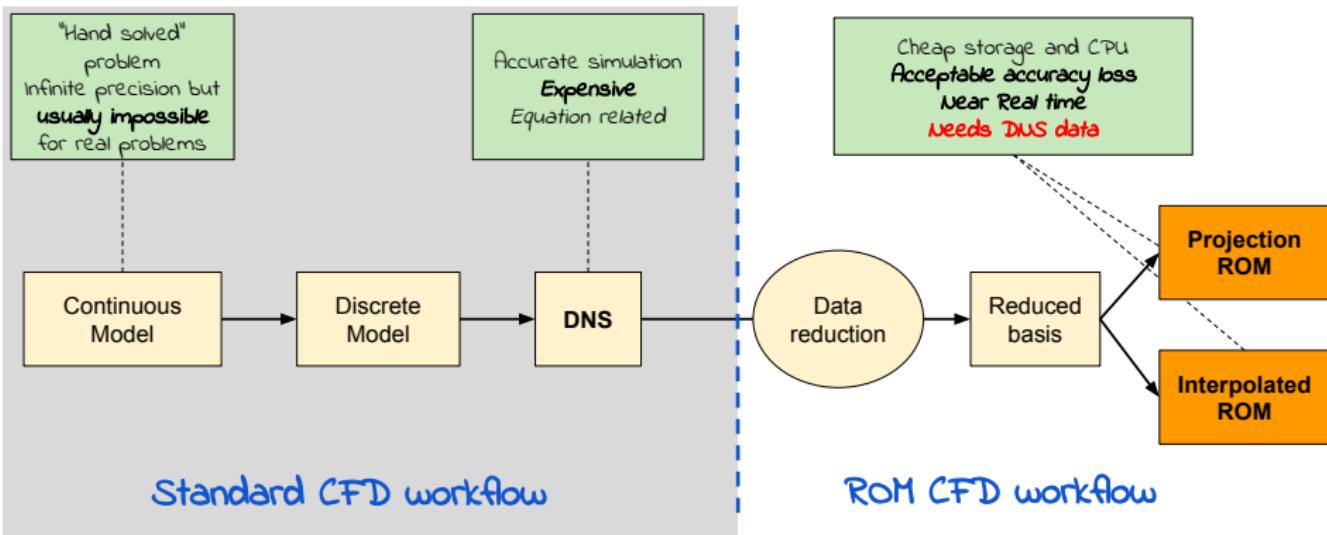
Research Project: Deep Reduced Order Model

Conclusion and perspectives

Reduced Order Modeling (ROM)



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The goal of ROM

Reduce the computing time by orders of magnitude.

Typical applications

- Parametric study
- Shape optimization
- Control (flow, heat transfer...)

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Example

ROM of standard flow for several Re

- Compute DNS for Several $\{Re_i\} \in [Re_l, Re_u]$ (and know the physics)
- Train ROM
- Compute ROM solutions for any $Re \in [Re_l, Re_u]$

Interpolated ROM

Why not interpolate directly?

Goal: Create a ROM for $Re \in [55 - 130]$, precompute a dozen of Re_i

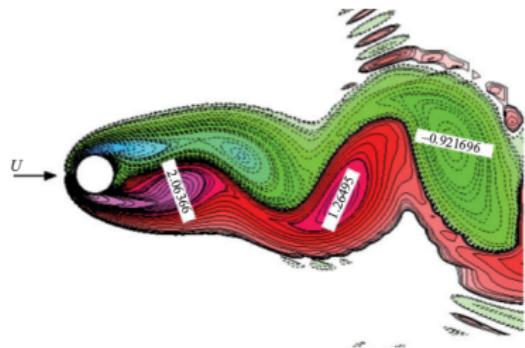


Figure: Flow past a circular cylinder, $Re=75$

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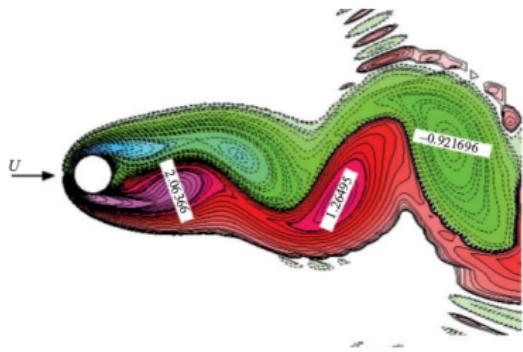


Figure: Flow past a circular cylinder, $Re=75$

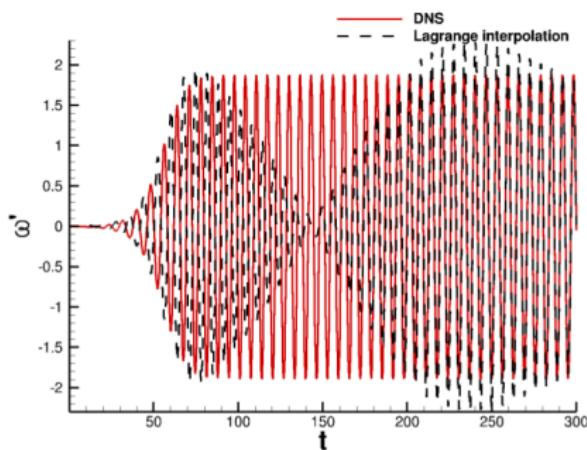
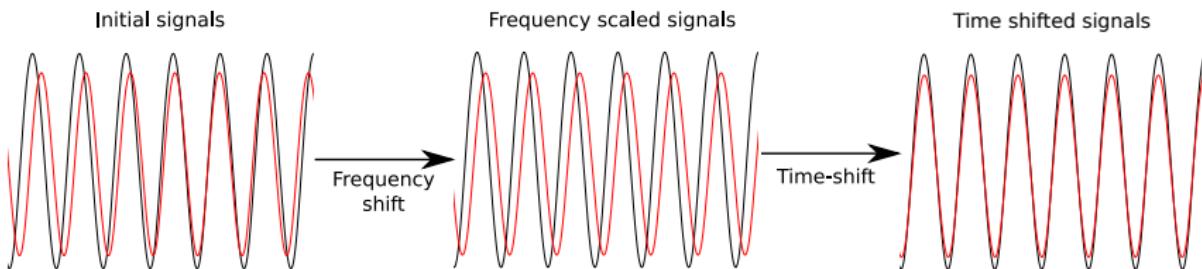


Figure: Direct Lagrange interpolation of the local time series in the cylinder wake

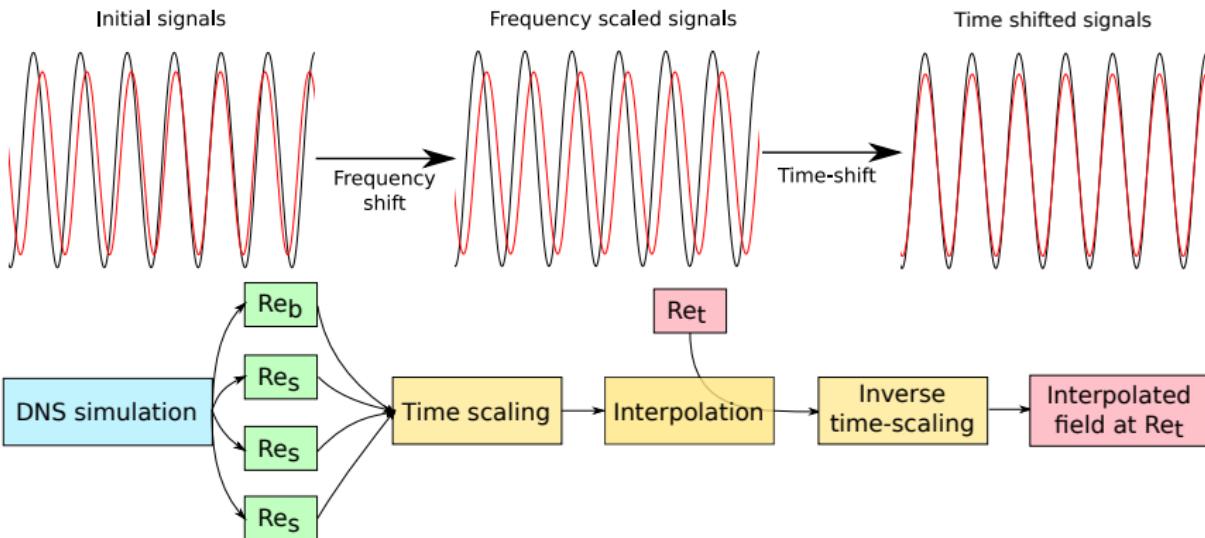
Using the physics : time-scaling interpolation

We take advantage of a relationship between St and Re .



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Time scaling interpolation in action

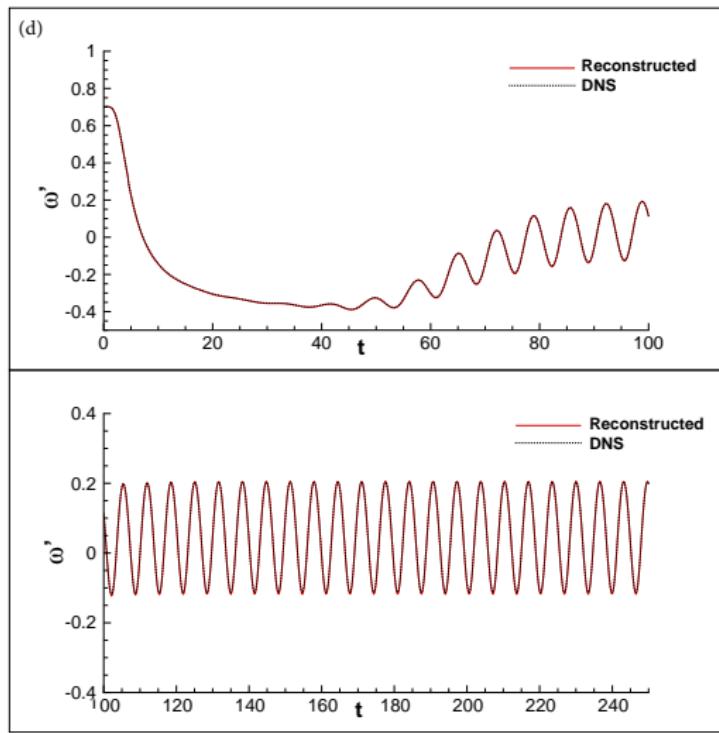
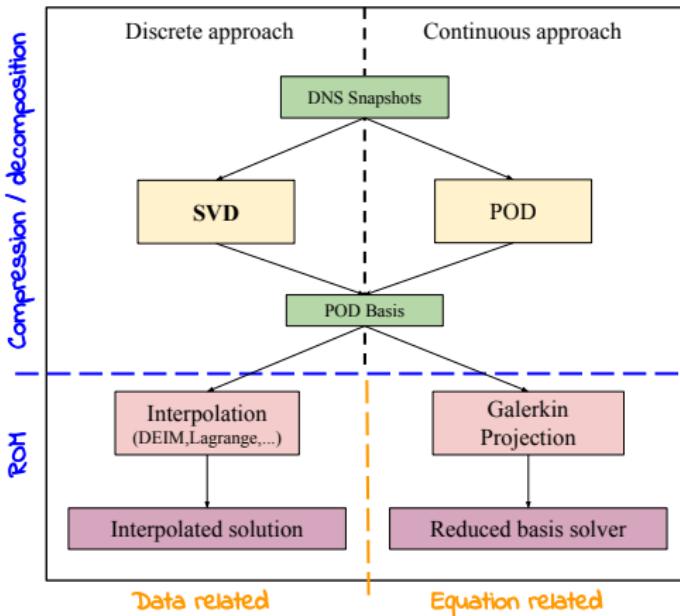


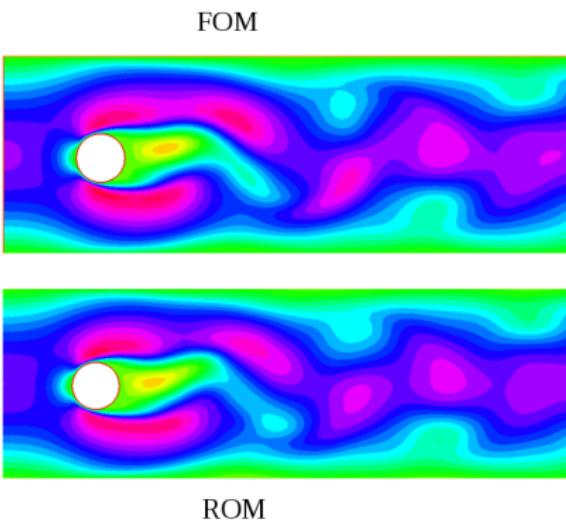
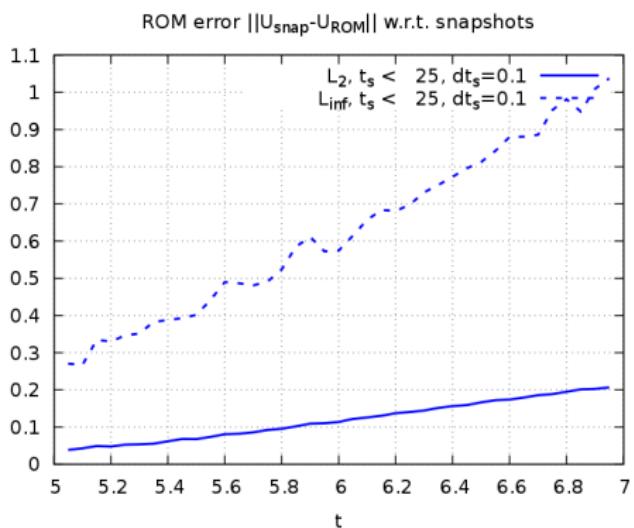
Figure: Reconstructed disturbance at $(1.104, 0)$ for $Re=83$, with donor $Re = \{78, 80, 86, 90\}$

POD-Galerkin

1. PDE in weak form
2. Full Order Model,
 $n_{dof} = O(10^6)$
3. Compute a reduced basis (RB) from snapshots e.g. with POD
4. Project PDE onto RB : typical POD-Galerkin ROM
 $n_{dof} = O(10)$
5. Stabilization term?, Tuning....



Navier Stokes-PODG is unstable

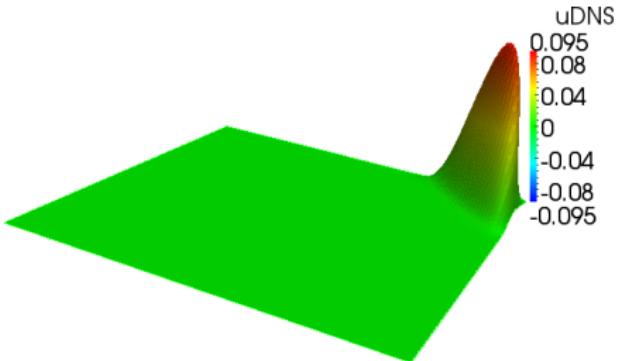


Stabilized PODG in action

Joint work with S. Rubino and T. Chacon

A convection-dominated
convection-diffusion-reaction
problem

$$\begin{cases} \partial_t u - \nu \Delta u + \mathbf{b} \cdot \nabla u + g u = f & \text{in } [0, T] \times \Omega \\ u(x, 0) = u_0(x) & \text{in } \Omega \\ u(x, t) = 0 & \text{on } [0, T] \times \partial\Omega \end{cases}$$



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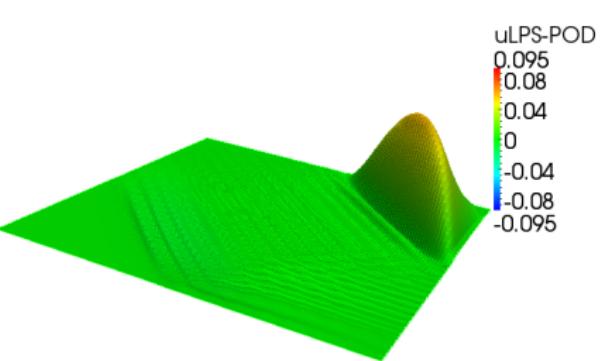
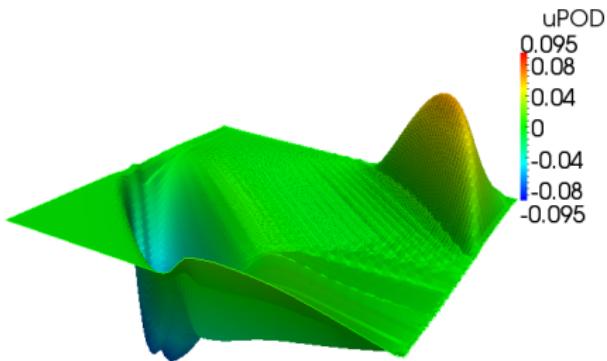
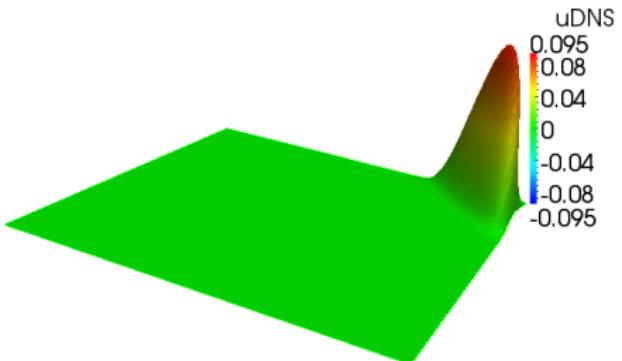


Figure: Numerical solution at $T = 1.25$:

L. Lestandi · From large data to reduced order models .

Data decomposition

Bivariate decomposition

Tensor formats and approximation

Numerics

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Conclusion and perspectives

Opening new horizons to ROM with Deep Learning

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Opening new horizons to ROM with Deep Learning

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Breaking the curse of dimensionality

- **low dimensional** representation of non-linear features, including function approximation, blackbox approximation.
- Uncovering non linear features through DNN encoding
- Mixing the two previous items into a solver and applying ROM ideas i.e. building DeepROM.

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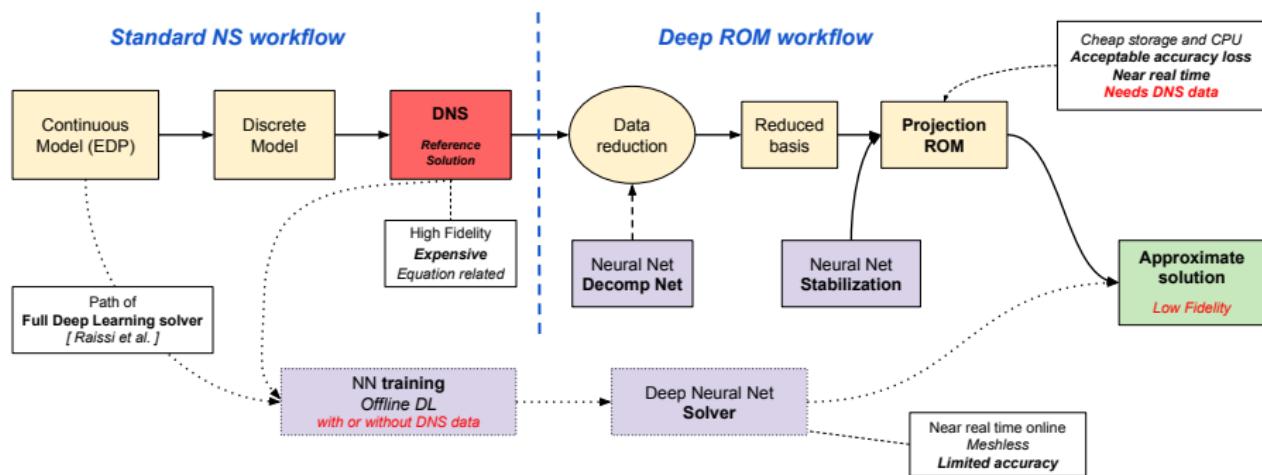
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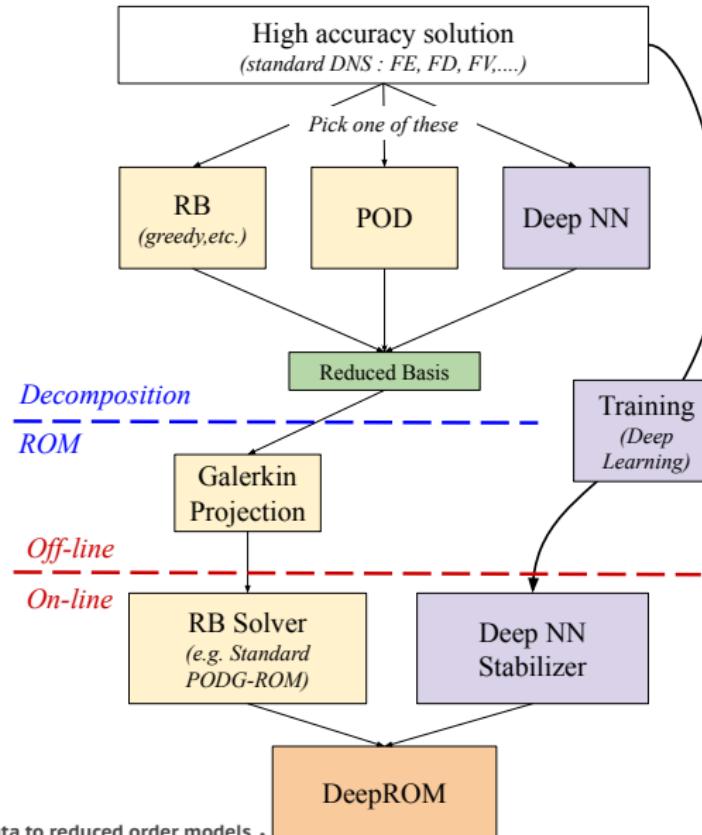
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2. Construct a fluid dynamics analysis/compressor system. Generating (very) low rank representations and feature map.
3. PDE solving using Deep learning and make appropriate use of ROM knowledge.

Making up for ROM shortcomings



A DeepROM diagram



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Conclusion

Data reduction

Features implemented in **pydecomp**:

- Tensor formats and decomposition
- Functional decomposition
- Numerical insight and rule of thumb

ROM for fluid dynamics

- Study of complex LDC flow
- Time-scaling interpolation
- State of the art of DNN with PDEs and DeepROM plan

Future work

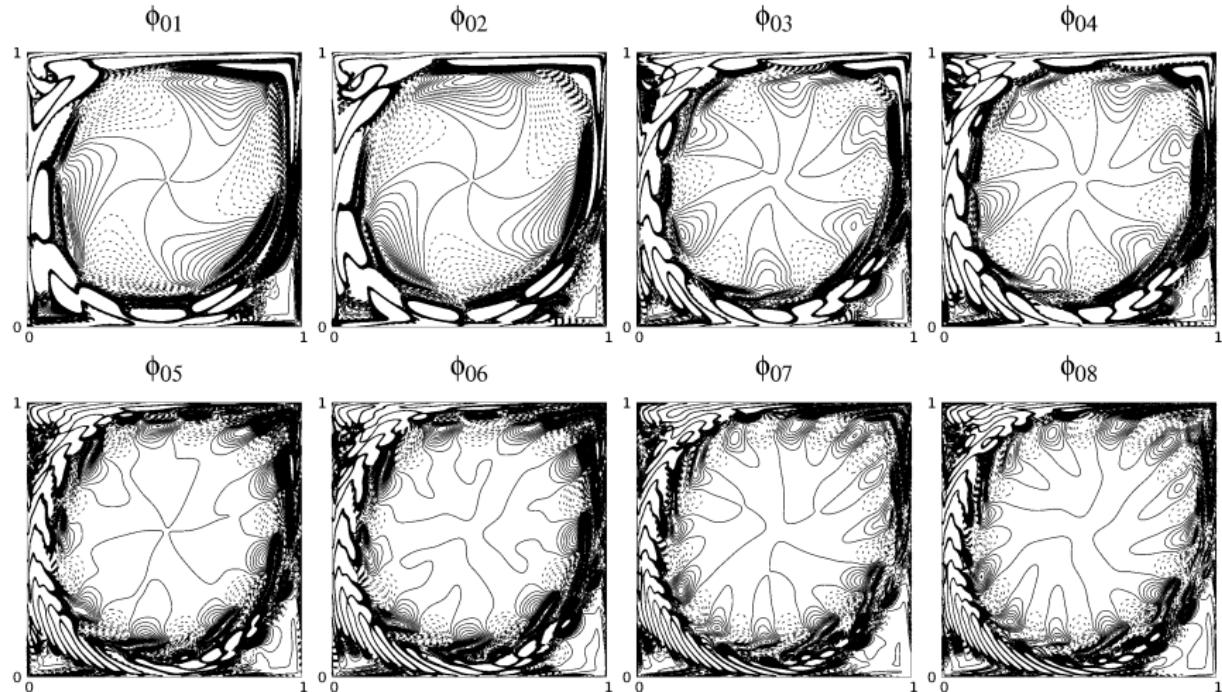
DeepROM

- DNN non-linear interpolation
- Projected ROM (Stabilized POD-G)
- DNN basis generation (GAN,LSTM...)
- Explore DNN architectures

Explore DNN and PDE synergies

- Meshless solving of PDE
- PDE + data hyper reduction
- PDE aided interpolation

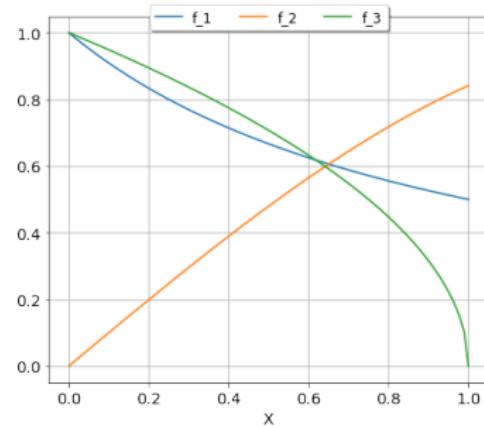
Thank you for your attention!



MLP approximator

In order to be able to increase the dimension, we introduce the following functions defined on $\Omega = [0, 1]^d$:

$$\begin{aligned}f_1(\mathbf{x}) &= \frac{1}{1 + \sum_i x_i} \\f_2(\mathbf{x}) &= \sin(||\mathbf{x}||_2) \\f_3(\mathbf{x}) &= \sqrt{1 - \prod_i x_i}\end{aligned}$$



As usual the error is measured relative to the exact function f in L^2 or l^2 norm. As the difference is usually negligible for regular grid, we will simply use l^2 :

$$\mathcal{E} = \frac{\|f - f_{NN}\|_2}{\|f\|_2}$$

MLP example

Following *Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow, 2nd Edition* by **Aurélien Géron** (Chap 10 for now) , we will use the sequential `keras` API on our simple "interpolation" problem.

```
Entrée [158]: model = keras.models.Sequential()
model.add(keras.layers.Flatten(input_shape=[d,]))
N=10
L=2
for i in range(L):
    model.add(keras.layers.Dense(N, activation="relu")) # L deep layers
model.add(keras.layers.Dense(1, activation="linear")) # output layer
# See Book for more elegant writing
model.summary()

Model: "sequential_9"
```

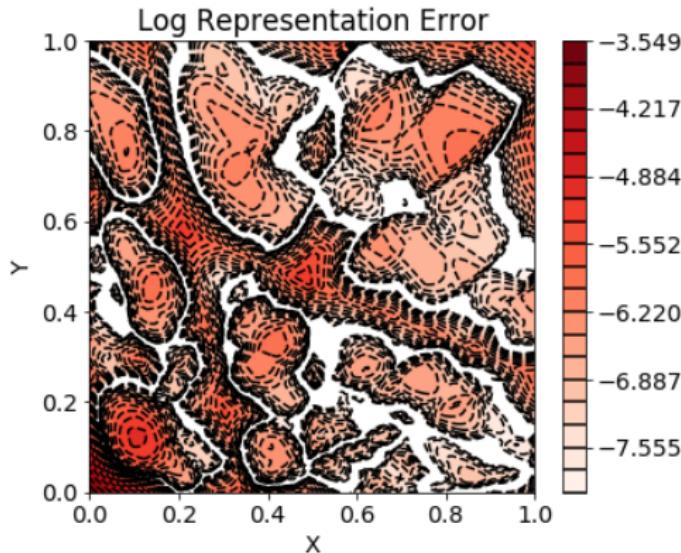
Layer (type)	Output Shape	Param #
<hr/>		
flatten_9 (Flatten)	(None, 2)	0
dense_19 (Dense)	(None, 100)	300
dense_20 (Dense)	(None, 100)	10100
dense_21 (Dense)	(None, 1)	101
<hr/>		
Total params:	10,501	
Trainable params:	10,501	
Non-trainable params:	0	

MLP example

```
L2err= 0.0031758773723378868
Linf_error= 0.028756439685821533
f= <function f1 at 0x0000001D5EE136E18>
```

Parameters:

N_train	501
N_test	172
N_valid	33
loss	MSE
batch size	1
epoch	10



Optimized search on hyperparameters

We can also do an optimized search on parameters using Keras. Then we use less training data (N_train=101,N_valid=44,N_test=32).

```
Entrée [213]: from scipy.stats import reciprocal
from sklearn.model_selection import RandomizedSearchCV

param_distrib = {
    "n_hidden": [0, 1, 2, 3],
    "n_neurons": np.arange(1, 100),
    "learning_rate": reciprocal(3e-4, 3e-2),
}

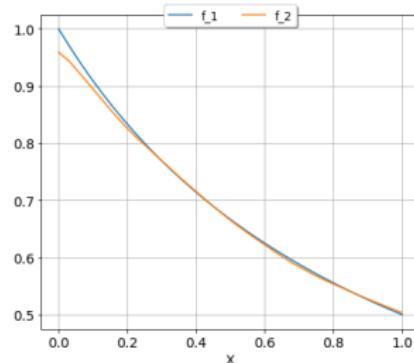
rnd_search_cv = RandomizedSearchCV(keras_reg, param_distrib, n_iter=10, cv=5,
rnd_search_cv.fit(X_train, f_train, epochs=100,
                    validation_data=(X_valid, f_valid),
                    callbacks=[keras.callbacks.EarlyStopping(patience=10)])
```

```
Entrée [214]: rnd_search_cv.best_params_
```

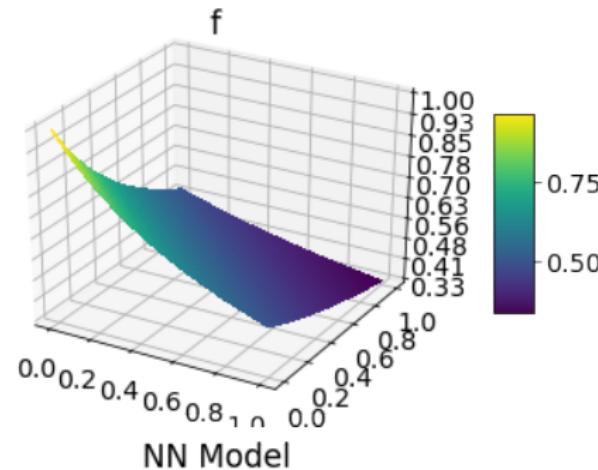
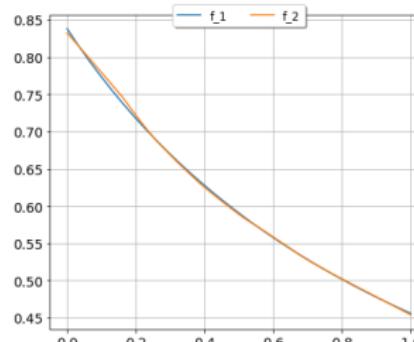
```
Out[214]: {'learning_rate': 0.024827442804036565, 'n_hidden': 3, 'n_neurons': 74}
```

Optimized MLP approximation

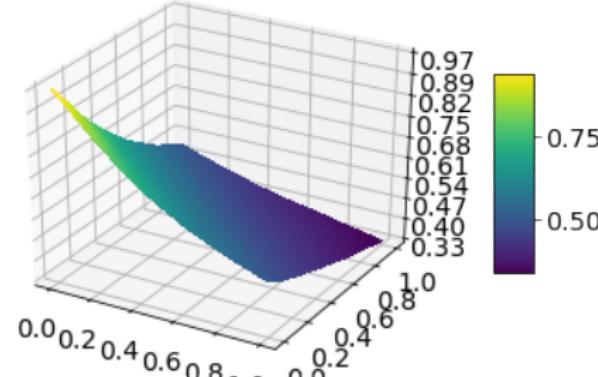
$y = 0.0$
grid size: 32



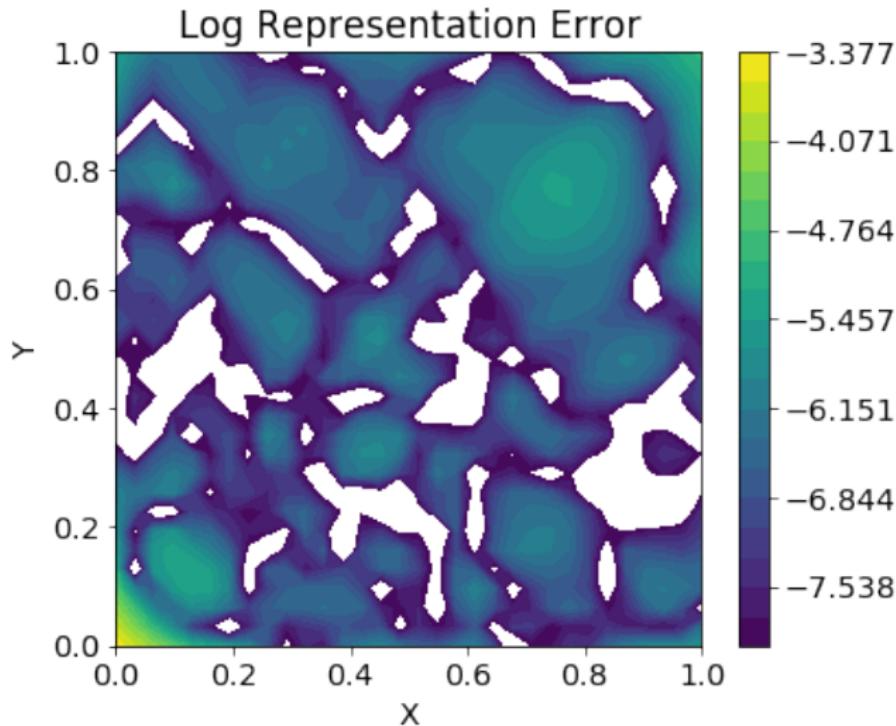
$y = 0.1935483870967742$
grid size: 32



NN Model



Optimized MLP approximation



Short term roadmap to improve approximation

- Improve understanding of tensor flow and MLP engineering
 - loss function
 - training algorithm
 - batch size
 - architecture
 - ...
- training points (from Cartesian to greedy/random sampling of space)
- number of dimensions influence
- preprocessing : centering, spread, etc.
- literature examples and existing solutions

Stabilized POD-Galerkin

Navier-Stokes weak form

$$\left\{ \begin{array}{lcl} \frac{d}{dt}(\mathbf{u}, \mathbf{v}) + b(\mathbf{u}, \mathbf{u}, \mathbf{v}) + \nu(\nabla \mathbf{u}, \nabla \mathbf{v}) - (p, \nabla \cdot \mathbf{v}) & = & \langle \mathbf{f}, \mathbf{v} \rangle \quad \forall \mathbf{v} \in \mathbf{x}, \text{ in } \mathcal{D}'(0, T), \\ (\nabla \cdot \mathbf{u}, q) & = & 0 \quad \forall q \in Q, \text{ a.e. in } (0, T), \end{array} \right.$$

We consider the following space for the POD setting:

$$\mathbf{x}^r = \text{span} \{ \varphi_1, \dots, \varphi_r \}.$$

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We introduce the stabilization term

$$(P'_R(\tilde{\mathbf{u}}_r \cdot \nabla \tilde{\mathbf{u}}_r), P'_R(\tilde{\mathbf{u}}_r \cdot \nabla \varphi))_\tau$$

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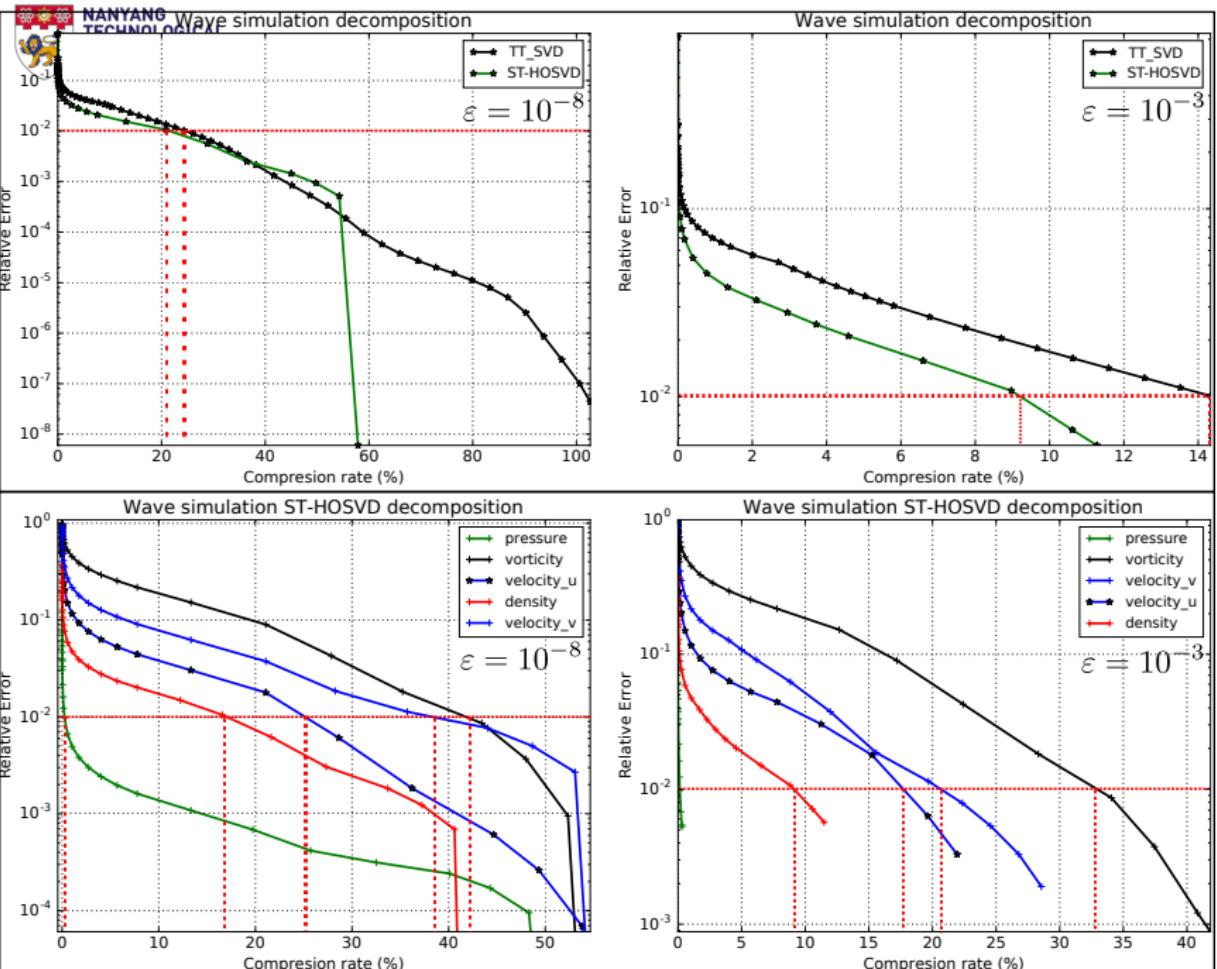
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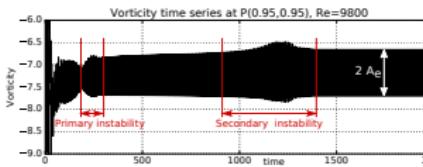
Then the Streamline-Derivative PODG reads:

$$\begin{aligned} & \frac{d}{dt}(\tilde{\mathbf{u}}_r, \varphi) + b(\mathbf{u}_D, \tilde{\mathbf{u}}_r, \varphi) + b(\tilde{\mathbf{u}}_r, \mathbf{u}_D, \varphi) + b(\tilde{\mathbf{u}}_r, \tilde{\mathbf{u}}_r, \varphi) + \nu(\nabla \tilde{\mathbf{u}}_r, \nabla \varphi) \\ & + (P'_R(\tilde{\mathbf{u}}_r \cdot \nabla \tilde{\mathbf{u}}_r), P'_R(\tilde{\mathbf{u}}_r \cdot \nabla \varphi))_\tau = \langle \mathbf{F}, \varphi \rangle, \end{aligned}$$

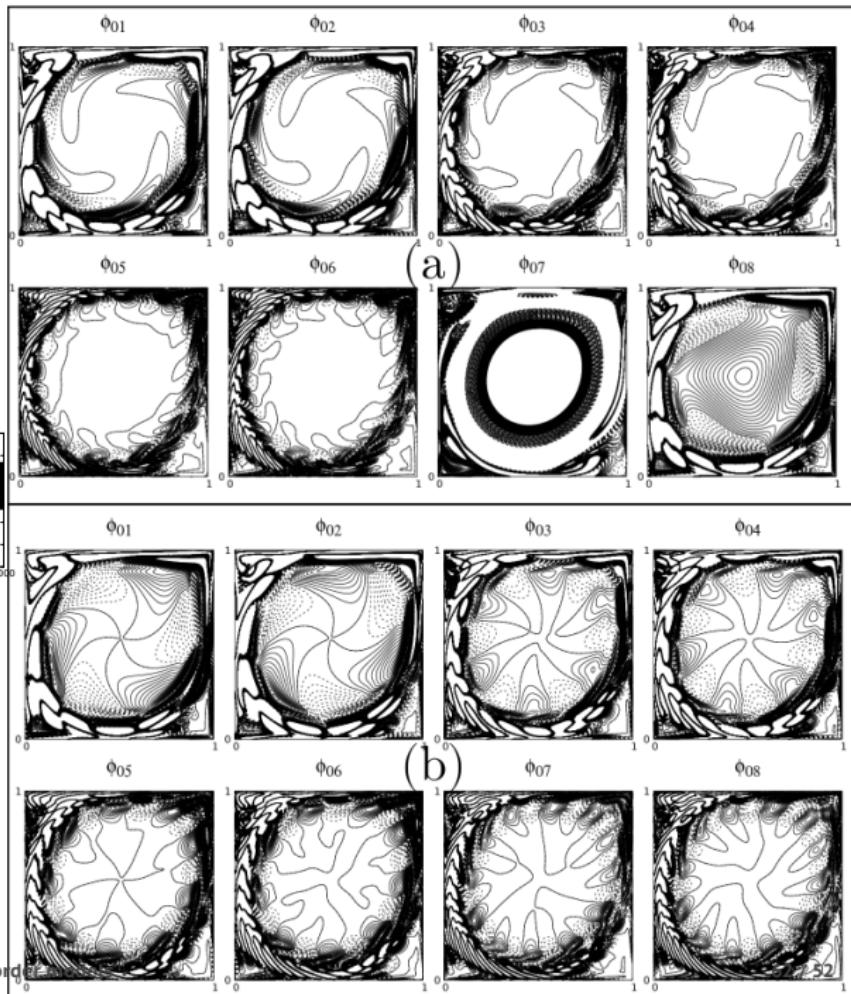


POD, an analysis tool

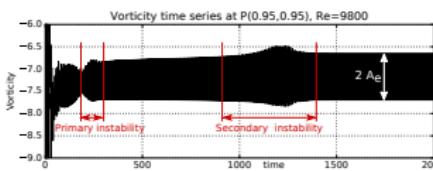
POD, an analysis tool



- (a) $t \in [500, 600]$
 (b) $t \in [1900, 2000]$



POD, an analysis tool



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