Tensor Reduction for Reduced Order Modelling

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Modern day modelisation problem

Increasing complexity of computer modelled problems :

- Multiphysics simulation
- Optimisation and control
- Big data analysis

Example : *Optimizing a flow in a multiparametric framework*

$$\begin{cases} \frac{D\mathbf{v}}{Dt} = \frac{1}{Re}\nabla^2\mathbf{v} - \nabla p \\ \mathbf{v}(x, t=0) = \mathbf{v}_0(x) \quad on\ \Omega \\ \mathbf{v} = \mathbf{f} \quad on\ \partial\Omega \end{cases}$$

Possible parameters : x, t, Re, $\mathbf{v}_0$, $\mathbf{f}$
Example : 5D optimization $\longrightarrow$ reduced order modelling.

One possible way : **Tensor Reduction**

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Tensor reduction ?

Definition : tensor (d-way array)

$A \in \mathbb{R}^{\mathcal{I}}$ where $\mathcal{I} = I_1 \times ... \times I_d$, $d \in \mathbb{N}$ is a (algebraic) tensor.

Tensor Reduction : *find an efficient way to reduce the storage cost of A.*

For K "small" find a good approximation A_K of A with

$$A_K = \sum_{k=1}^{K} \sigma_k \bigotimes_{i=1}^{d} u_i^k \quad \{u_i^k\}_{i,k} \in \mathbb{R}^{I_i} \tag{1}$$

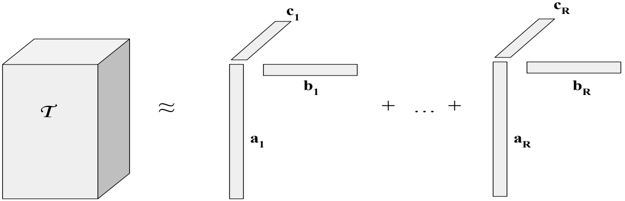

FIGURE 1 – 3D example of tensor decomposition (CP format)

Equivalent functional formulation

Let $f : \Omega \in \mathbb{R}^d \longrightarrow \mathbb{R}^p$ find a (finite) separated expression of f.

$d = 2$ case :

$$f(x_1, x_2) = \sum_k \varphi_1^k(x_1)\varphi_2^k(x_2)$$

Multiparameter case $d > 2$

$$f(x_1, x_2, \ldots, x_d) = \sum_k \varphi_1^k(x_1)\varphi_2^k(x_2)\ldots\varphi_d^k(x_d)$$

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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.*

Theorem (Eckart-Young)

Let $k < r$ *and* $A_k = \sum_{i=1}^{k} \sigma_i U_i V_i^\top$ *where the singular values are ordered decreasingly then*

$$\min_{rank(B)=k} \|A - B\|_2 = \|A - A_k\|_2 = \sigma_{k+1}$$

Remark :

- The SVD can be seen as a particular case of the POD for the l^2-norm.
- The SVD can be used to obtain the eigen vectors of the POD.

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Proper Orthogonal Decompositions

- Developed by several people among the first was Kosambi, J. (1943)
- a.k.a. PCA, KLE, SVD.
- Powerful *a posteriori* data analysis tool
- Functional space approach
- Low-dimensional approximate of high-dimensional process
- Many applications

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

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

.

$\Rightarrow$ For (ϕ_k) an orthogonal basis, the optimization problem reads

$$\min \sum_{i=1}^{n_t} \|u(x,t_i) - \sum_{k=1}^{K} \langle u(x,t_i), \phi_k(x)\rangle \phi_k(x)\|_2^2$$

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Optimisation Problem (OP)

Maximise the least-square projection of $u(x,t)$ on $\phi(x)$

$$\max_{\psi \in L^2(D)} \frac{\langle |(u,\psi)|^2 \rangle}{\|\psi\|^2} = \frac{\langle |(u,\phi)|^2 \rangle}{\|\phi\|^2}$$
$$\text{with} \quad (\phi,\phi) = 1$$

Let $R \in L^2(X \times X)$ be the autocorrelation function defined as :

$$R(x,\xi) = \int_Y u(x,y)\, u(\xi,y)\, dy$$

Prooving the POD existance

- Spectral theory : (OP) $\Leftrightarrow$ first e.v. of $R\phi = \lambda\phi$
- Mercer's theorem : $R(x,\xi) = \sum_{k=1}^{+\infty} \lambda_n \phi_n(x)\phi_n(x)$
- Karhunen-Loève Theorem : There exists a system $(\phi_m, \upsilon_m, \sigma_m)_{m\geq 0}$ such that $(\varphi_m)_{m\geq 0}$ is an orthonormal basis in $L^2(X)$, $(\upsilon_m)_{m\geq 0}$ an orthonormal system in $L^2(Y)$ and $(\sigma_m)_{m\geq 0}$ a sequence of nonnegative. The POD reads

$$f_M(x,y) = \sum_{m=0}^{M} \sigma_m\, \varphi_m(x)\upsilon_m(y), \qquad \forall (x,y) \in X \times Y \qquad (2)$$

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$$T_N(x,y) = \sum_{m=0}^{N} \sigma_m\, \phi_m(x)\psi_m(y), \qquad \forall (x,y) \in X \times Y \qquad (1)$$

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Concept of PGD

Let V a Hilbert space, $\mathcal{A}$ a bilinear form on V and $\mathcal{L}$ a linear form on V. Let

$$\forall u, v \in V, \quad \mathcal{A}(u, v) = \mathcal{L}(v) \tag{3}$$

Let $\mathcal{S}_1 = \{z(x_1, ..., x_n) = \prod_{i=1}^{n} X_i(x_i)\}$ and $\mathcal{S}_m = \{v = \sum_{j=1}^{m} z_j, z_i \in \mathcal{S}_1\}$.

Problem

$\Rightarrow$ Find the best approximation $u_m \in \mathcal{S}_m$ of u solution of eq. (3).

- Additional constraint : orthogonality (otherwise ill-posed for $d \geq 3$).
- Normalise all modes w_i^j but one.

Post-processing

Let $\mathcal{L}(v) = \int fv$ and $\mathcal{A}(u, v) = \int uv$. Then the problem reads :

$$u_n = \arg\min_{u \in V_n} \|f - u\|_{L^2} \tag{4}$$

Progressive Separated Representation Algorithm and Convergence

- Assuming that z_n is known, compute s the best rank-1 approximation of $f - z_n$, $z_{n+1} = z_n + s$.
- This algorithm converges toward f (Falcó and Nouy).

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A 2D PGD Algorithm for data Reduction

Goal : Approximate $u(x,y)$ by its PGD approximation : $u_m(x,y) = \sum_{j=1}^{m} X_j(x)Y_j(y)$.

Idea : Assume u_{m-1} is known and compute iteratively the separated representation $X^m(x)Y^m(y) \simeq \mathcal{R}_{m-1}(x,y) = f(x,y) - u_{m-1}(x,y)$.

Progressive separated representation

$u_0 = 0,\ m = 0.$

Enrich u_m until stopped :

- Compute X^m, Y^m using ***fixed point algorithm*** :
  - $p = 0$, guess X_0, Y_0.
  - Until Convergence (p loop) :

    solve (on X_p)

$$\forall X*,\ \int_\Omega X^* Y_{p-1}\left(\left(\sum_{i=1}^{m-1} X^i Y^i + X_p Y_{p-1}\right) - f\right) = 0, \quad \text{imposing } \|X_p\| = 1$$

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$$\forall Y*,\ \int_\Omega X_p Y^*\left(\left(\sum_{i=1}^{m-1} X^i Y^i + X_p Y_p\right) - f\right) = 0$$

    Check Convergence
- $u_m = u_{m-1} + X^m Y^m$
- Stopping criterion : $\varepsilon = \|X^m Y^m\| / \|X^1 Y^1\| \leq \varepsilon_{enrich}$.

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PGD vs POD

PGD separation

$$u_M^{pgd}(x,y) = \sum_{j=1}^{M} X_j(x)Y_j(y)$$
$$= \sum_{j=1}^{M} \sigma_j^{pgd} X_j^*(x)Y_j^*(y)$$

with $X_j^* = X_j/||X_j||$ and $Y_j^* = Y_j/||Y_j||$

POD separation

$$u_M^{pod}(x,y) = \sum_{j=1}^{M} \sigma_j^{pod} \varphi_j(x) v_j(y)$$

We proove that $\sigma_j^{pod} = \sigma_j^{pgd}, \quad \forall j = 1, \ldots, M$
The same holds for the eigen function (wich are solution of the same problem).

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Transient temperature

Continuous problem

We consider the case of having a heat source term The heat model to handle is the following : *find a temperature field T satisfying*

$$\begin{aligned} \partial_t T - \text{div}\,(\gamma \nabla T) + \beta T = S, &\qquad \text{in } \Omega \times J, \\ T = 0, &\qquad \text{in } \partial\Omega \times J, \\ T(\cdot, 0) = a_0(x), &\qquad \text{in } \Omega. \end{aligned}$$

- $t \in J =]0, b[$ and $x \in \Omega$
- γ is the conduction parameter
- β is the heat transfer coefficient
- a_0 is an initial conduction
- The source can be $S(x,t) = a(x) \otimes \theta(t)$ or not.

Numerics : Separeted source term

- $I = (0,1)$ and $J = (0,1)$.
- We consider

$$S_1(t,x) = (\theta \otimes a)(x,t) = e^t(x - 0.4),$$
$$S_2(t,x) = (\theta \otimes a)(x,t) = e^t|x - 0.4|.$$

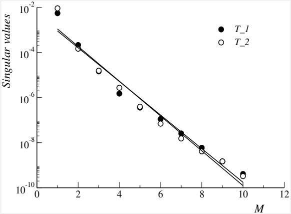
- The corresponding solutions are denoted by T_1 and T_2, respectively.
- The heat problem is discretized by an Euler scheme/Gauss-Lobatto-Legendre spectral method (the time step is $\delta t = 10^{-2}$ and the polynomial degree is $N = 64$.
- Quadrature formulas are used to evaluate the matrix representation of the operators B and A.

Remarks

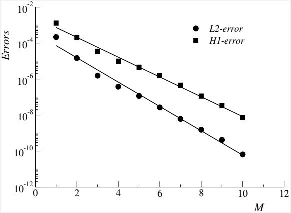
- S_1 indefinitely smooth ans S_2 enjoys moderate spacial regularity ($a \in H^\tau(I)$ with τ no bigger than $3/2$)
- Our aim is to show that the regularity has not much importance in the separation aptitude of both temperature fields T_1 and T_2

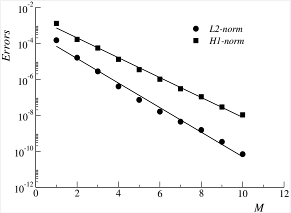
Numerics : Separeted source term

Singular values for T_1 and T_2



Truncation errors versus the cut-off M, for T_1 and T_2





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Definitions

1. A vector space special case.
   Let E a tensor space, then $\exists U, V | E = U \otimes V$ where U and V are vector spaces.
2. A generalisation of matrices to higher dimensions. i.e. $A \in \mathbb{R}^{\mathcal{I}}$ where $\mathcal{I} = I_1 \times ... \times I_d$. A is an order d tensor i.e. a d-way array.

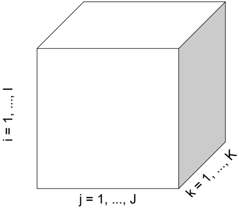


FIGURE 2 – Order 3 tensor

Tensor related Key Properties

- **Tensor product,** $\otimes$:

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

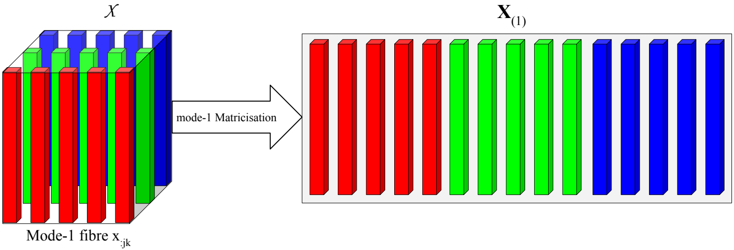
  Enrty-wise $\mathscr{T} = \mathscr{X} \otimes \mathscr{Y}$ reads

$$T_{\boldsymbol{ij}} = x_{\boldsymbol{i}} y_{\boldsymbol{j}}$$

  where $\boldsymbol{i} = \{i_1, ..., i_p\}$ and $\boldsymbol{j} = \{j_1, ..., j_q\}$.

- **Tensor rank** : $rank(A)$ is the minimum number of rank one tensor that generates A. A rank one tensor can be written as the outer product of d vectors.

- **Matricisation** : is the process of ordering the elements of a tensor into a matrix.



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Full Tensor Format

A d-way array that stores all the coefficient in the canonical basis.

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

Can be used if n^d remains small

Canonical Tensor Format and the CP Decomposition

$\mathcal{T} \in \mathbb{R}^{\mathcal{I}}$ where $\mathcal{I} = I_1 \times ... \times I_d$ is represented as a finite sum of rank-1 tensors.

$$\mathcal{T} = \sum_{i=1}^{r} \bigotimes_{\mu=1}^{d} \mathbf{t}_{\mu,i} \quad where\, \mathbf{t}_{\mu,i} \in V_\mu = \mathbb{R}^{\mathcal{I}_\mu} \tag{5}$$

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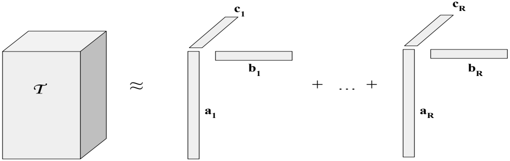

FIGURE 4 – CP decomposition of third order tensor $\mathcal{T} \in \mathbb{R}^{I \times J \times K}$.

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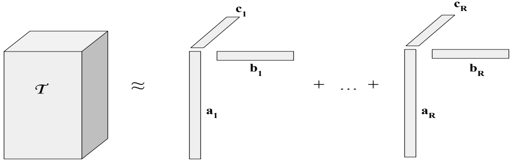

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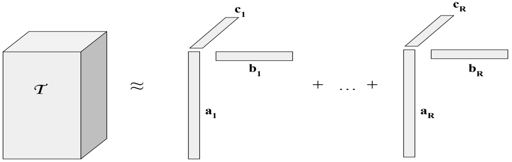

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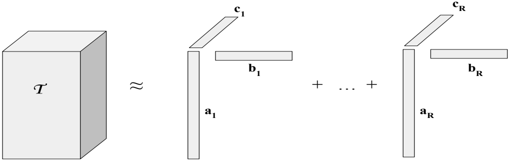

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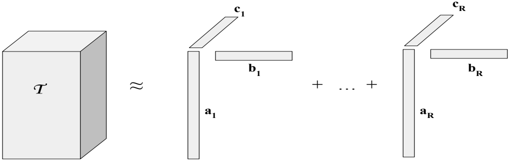

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with the weights $w_{i_1,\ldots,i_d} \in \mathbb{R}$. They form the core tensor $\mathcal{W} \in \mathbb{R}^{k_1 \times \cdots \times k_d}$.
$\boldsymbol{k}$ is the representation rank of $\mathcal{T}$ in the tucker format $\mathcal{T}_{\boldsymbol{k}}$.

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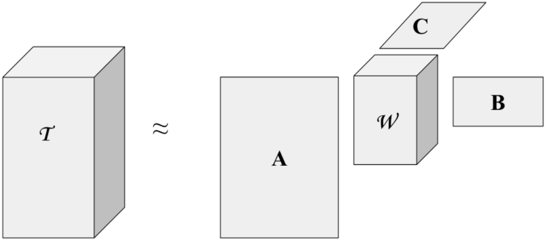

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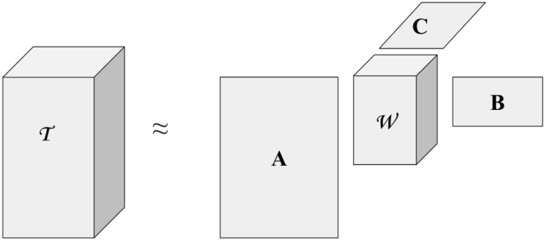

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T-HOSVD

Goal Find an approximate representation of $\mathcal{T}$,
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Idea Compute the singular vectors of each dimension separately.

- Compute SVD on each mode matricization of $\mathcal{T}$: U_μ is given by $SVD(\mathcal{M}_\mu(\mathcal{T}))$.
- Modes are orthonormal $\Rightarrow$ core tensor given by projection on the basis

$$w_{i_1,\dots,i_d} = \langle \mathcal{T}, \otimes_{\mu=1}^{d} u_{\mu,i_\mu} \rangle$$

Pros Easy to implement, *almost* best approximation i.e. $\varepsilon \leq \sum_{\mu=1}^{d} \|\tilde{\Sigma}_\mu\|_F^2$

Cons $\mathcal{W}$ may become big. Same as SVD.

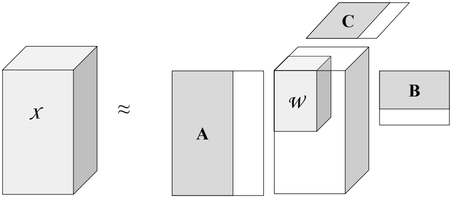

FIGURE 6 – Truncated HOSVD / Tucker Decomposition of a third order array $\boldsymbol{\mathcal{X}}$

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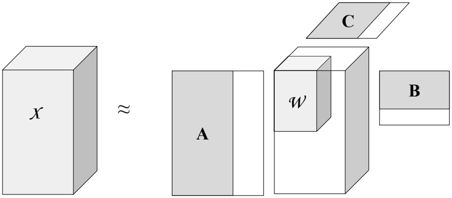

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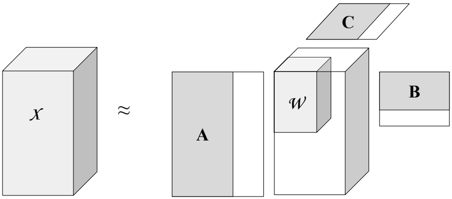

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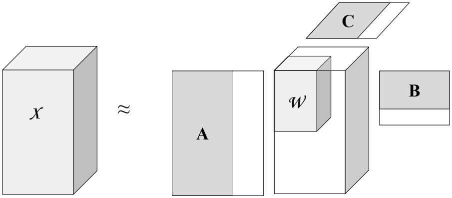

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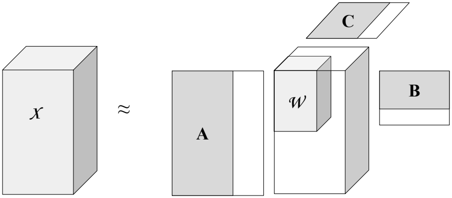

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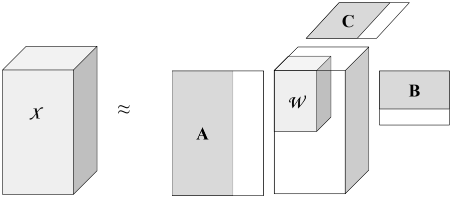

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Recursive-POD tensor representation

- The POD expansion may be recursively adapted to multi- parametric functions.

$$T(x,y,z) = \sum_{m \geq 0} \sigma_m V_m(y,z)\, \varphi_m(x), \tag{7}$$

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$$V_m(y,z) = \sum_{k \geq 0} \sigma_m^{(k)}\, w_m^{(k)}(z)\, v_m^{(k)}(y), \tag{8}$$

$\Longrightarrow$ The function $T \in L^2(X \times Y \times Z)$ admits the expansions

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Comparison of errors for feasible R-POD and PGD

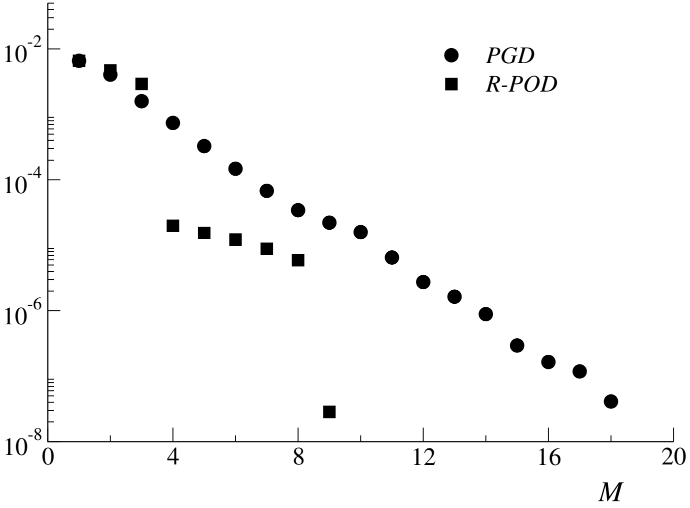

FIGURE 7 – Function $T_2(x, y, z) = \sin(xyz)$.

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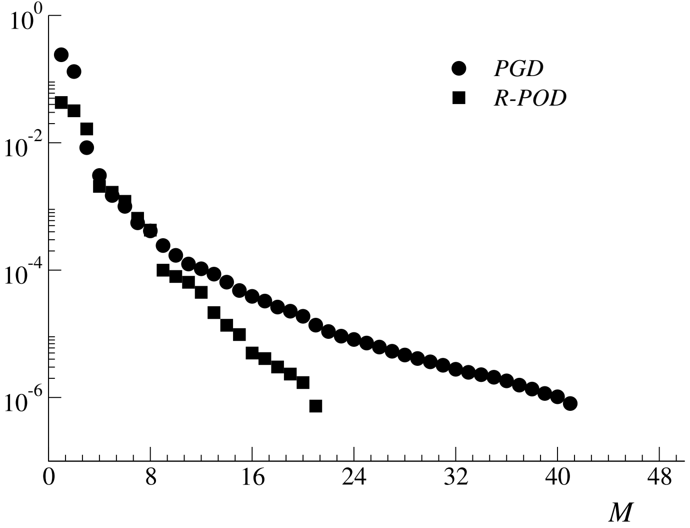

FIGURE 8 – Function $T_4(x, y, z) = \frac{1}{x+2y-z+5}$.

Numerical Experiments

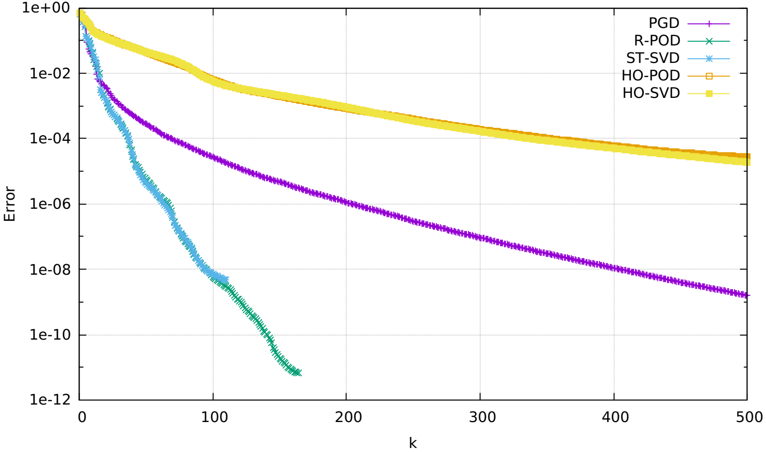

FIGURE 9 – Approximation error of $\mathcal{T}$ singular by $\bar{\mathcal{T}} = \sum_{i=1}^{k} \sigma_i \boldsymbol{x}_i \boldsymbol{y}_i \boldsymbol{z}_i$ where the sum is ordered to that the error is minimum. $f(x, y, z) = x^2(\sin(5y\pi + 3\ln(x^3 + y^2 + \pi^2)) - 1) + (x + z - 1)(2y - z)\cos(30(x - z))\ln(6 + (x^2y^2 + z^3)) - 4(x^2yz^3)(1 - z)^{1.5}$

Numerical Experiments transient Lid Driven Cavity DNS

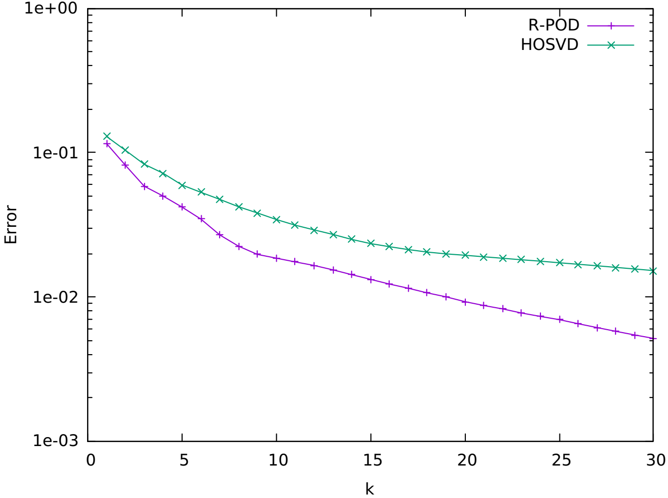

FIGURE 10 – Approximation error of the vorticity field for a series of DNS simulation of LDC for $Re \in [400, 800]$. 3 parameters : space, time, Reynolds. Transient to steady state.

Conclusion and Future Development

Recap 1 2D : SVD, PGD, POD are equivalent

Recap 2 3D : answer is more complex, generally R-POD/ST-HOSVD is better

Future work Build multi-parameter ROM for non-linear problems

- Interpolate accurately on Reduced Bases (DEIM, Grassman manifold interpolation,...)
- Linear and non-linear PDE data
- ...

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A few papers on that matter

- Recursive POD expansion for reaction-diffusion equation. Adv. Model. and Simul. in Eng. Sci. (2016) 3 :3
- Error Bounds for POD expansions of parameterized transient temperatures. Comput. Methods Appl. Mech. Engrg. 305 (2016) 501–515
- Karhunen-Loève's truncation error for bivariate functions Comp. Methods in Applied Mech. and Engineering, V. 290, 15 , Pages 57-72 June (2015)
- Mercer's spectral decomposition for the characterization of thermal parameters. Journal of Computational Physics, V. 294, Pages 1-19, (2015)
- Vannieuwenhoven, N., Vandebril, R., Meerbergen, K. (2012). A New Truncation Strategy for the Higher-Order Singular Value Decomposition. SIAM Journal on Scientific Computing, 34(2), A1027–A1052.
- Kolda, T. G. ,Bader, B. W. (2009). Tensor decompositions and applications. SIAM Review, 51(3), 455–500.
- Hackbush, W.-(Max-P.-I. for M. in the S. (2014). Tensor spaces and numerical Tensor calculus.

THANK YOU FOR YOUR ATTENTION !