

# Numerical Study of Low Rank Approximation Methods for Multidimensional Physics and its Analysis.

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**Abstract** This paper proposes a comparison of the numerical aspect and efficiency of several low rank approximation techniques for multidimensional data, namely CPD, HOSVD, TT-SVD and RPOD. This approach is different from the numerous papers that compare the theoretical aspects of these methods or propose efficient implementation of a single technique. Here, after a brief presentation of the studied methods, they are tested in practical conditions in order to draw hindsight at which one should be preferred. Synthetic data provides sufficient evidence for dismissing CPD, T-HOSVD and RPOD. Then, three examples from mechanics provide data for realistic application of TT-SVD and ST-HOSVD. The obtained low rank approximation provide different levels of compression and accuracy depending on how separable the data is. In all cases, the data layout has significant influence on the analysis of modes and computing time while remaining similarly efficient at compressing information. Both methods provide satisfactory compression, from 0.1% to 20% of the original size within a few percent error in  $L^2$  norm. ST-HOSVD provides an orthonormal basis while TT-SVD doesn't. However it is better suited for higher order  $d$ . Finally, these numerical tests have been performed with `pydecomp`, an open source python library developed by the author.

**Keywords** HOSVD · ST-HOSVD · Tensor Train · Canonical Decomposition · RPOD · POD · SVD.

**Mathematics Subject Classification (2010)** 35Q35 · 15A69 · 15A21 · 78M34

## 1 Introduction and problem setting

In the past 50 years scientific computing has gained tremendous traction and is now ubiquitous to many fields of research and engineering especially in mechanics. It has been accompanied by the explosion of CPU power and the introduction of supercomputers and their massively parallel architectures since the 1990s. Still, the advent of exascale computing has only pushed forward the boundaries of computable problems slightly while raising a series of technical issues. Indeed, supercomputers are expensive infrastructures that require extensive amounts of energy. They produce data so large that storing and transferring data itself has become an issue. A famous simulation of the observable universe [1] performed in 2012, exemplifies the dizzying proportions taken by numerical simulation. Approximately 5000 computing nodes used 300 TB of memory producing 50 PB of raw data in 10 million hours of computing time of which “only” 500 TB of useful data was finally kept. This kind of data is hard to manipulate and storage is usually performed on magnetic bands making it fairly slow to access. Also, any intent at handling such data, even in small slices, is vain on a personal computer, thus impairing the efficiency of analysis.

The above mentioned figures are typical examples of the famous curse of dimensionality which remains the main obstacle to scientific computing development. Current programs are able to manipulate, with proven and often satisfying levels of accuracy, many direct space-time (3+1D) simulations. It is, however, not the case when one wants to perform parametric studies or optimization and control tasks such as shape optimization or active flow control. For these problems, the curse of dimensionality plays a major role and both the computing time and storage cost become out of reach. Extreme cases of the curse of dimensionality are offered by computational chemistry. A toy model may take the following form, let a small  $n = 2$ , be the number of discrete point per dimension, with  $d = 50$  dimensions, then the storage cost  $n^d = 2^{50}$  for a single state amounts to 9PB if all entries are stored. A tensor is a well suited object for such data representation, it is the discrete representation of multidimensional fields, i.e. an order  $d$  tensor of size  $n_1 \times \dots \times n_d$  is filled by sampling a field on a tensor product space  $\Omega = [0, 1]^d$  at discrete grid points. The necessity of storing low rank approximate tensors instead of keeping all the entries becomes essential for large  $d$  as shown above.

Another case for which current techniques offer limited help is real-time simulation, because high precision simulations require CPU times orders of magnitude larger than real time. These issues can be tackled in many ways but a prominent approach since the turn of the century lies in reduced order modeling (ROM) and the various techniques employed such as proper generalized decomposition (PGD) [2], POD-Galerkin ROM [3] or Petrov-Galerkin ROM [4, 5]. The various methods presented in this paper aim primarily at enabling analysis and cheap storage of extensive datasets but can very well constitute the first layer of multidimensional solvers [6] or enable real-time [7] simulation or digital twin approaches.

Most of the methods studied in this paper rely on bidimensional separation methods such as singular value decomposition (SVD) and proper orthogonal decomposition (POD) that are essentially equivalent (see [8, Chapter 1]). They have been rediscovered many times in various fields e.g. as principal component analysis (PCA) in statistics [9, 10], Karhunen-Loëve expansion (KLE) in probability theory [11] or POD in fluid dynamics [12, 13]. These methods provide a decomposition that can be truncated optimally [14] and reflect the physics of the problem studied. In fluid mechanics, POD bases have spurned the first wave of ROM. Indeed, this decomposition provides, among the many possible bases [15], an orthogonal basis of the functional space in which the solution lives. Consequently, many attempted at building Galerkin projection ROM on these reduced bases from the 1980s onward [13, 16–19] but have registered modest success due to instability. Modern approaches are more successful [4, 3].

One extension of these work lies in the decomposition of multidimensional problems. Hitchcock is usually considered to have introduced tensor decomposition [20] in 1927. But, it is Tucker [21] that popularized the subject in the 1960s with the eponymous format, followed by Carroll and Chang [22] and Harshmann [23] in 1970 who introduced the canonical/parafac format and decomposition (CPD). The detailed review by Kolda and Bader [24] in 2009 is the basis of many of the modern developments in the field but it is devoid numerical study. CPD has received dwindling interest due to poor numerical performance except in the context of ROM in which the PGD [2] has been extensively studied. For data analysis, the PGD can be interpreted a continuous form of CPD (see [8, Chapter 1] and [25]). Tucker format was at the center of attention since DeLathauwer paper in 2000 [26] which proposed an efficient approximation strategy, the Higher Order SVD (HOSVD) followed by HOOI [27]. More recently, he coauthored Vannieuwenhoven ST-HOSVD [28] that improved significantly the computing time. The early 2010s have seen the introduction of formats that overcome the exponential growth of the core tensor in Tucker format. Oseledets and co-authors proposed the tensor train (TT) format [29–31], also known as matrix product state (MPS), together with its decomposition algorithm. The storage cost of this format is linear in  $d$  allowing tensorization of data, i.e. the method is so efficient at handling large  $d$  that a new strategy consists in increasing artificially the number of dimensions. To do so, one may need to rely on partial evaluations of the interest data as performed TT-DMRG-cross [32, 33]. This approach is also known as blackbox algorithms [34] in the context of hierarchical tensors (HT) developed by Grasedyck, Kressner and Tobler [35, 36]. HT actually incorporates all previously mentioned formats and approximations into a general  $d$ -linear format. These recent developments have been reviewed in [37] while an extensive mathematical analysis of tensors and their approximation is given in Hackbusch's book [25].

Finally, these formats have been extended to the continuous framework as they are often used to separate data representing functions. A functional TT was proposed by Bigoni and Gorodetsky [38, 39] while many approaches now consider  $n$ -way array tensors and multivariate function as a single object [25, 40, 41]. Additionally, a Recursive-POD (RPOD) was proposed in [42]. Finally, in [43], the authors propose a practical presentation of these methods for actual decomposition. The present paper proposes to apply the methods detailed in [43] to actual data and devise a context dependent hierarchy of methods for compression. The goal is to complement method specific numerical studies and high performance parallel implementations such as [44]. Also this study tackles phenomena analysis, in the same spirit as that POD has been used for decades to analyze modal behaviors in mechanics. This paper supports, with examples, that the same is possible for multidimensional decomposition.

In this paper, we focus on the practical aspect of using decomposition methods in the context of multidimensional data compression and analysis. For this reason, we do not enter in the theory behind each of these methods, this work has already been performed in [43]. But, a short reminder of the methods is given in the next sections.

The paper is organized as follows. The next subsection presents the problem formulation. Section 2 briefly reviews bivariate decomposition methods. Higher dimension formats and methods are presented in section 3. Finally, section 4 focuses on numerical experimentation on various examples from the mechanics background. These results are analyzed and compared in this last section in order to provide relevant insight to the reader for practical use of these methods.

## 1.1 Problem formulation

The goal of this paper is to *present and compare low rank approximation techniques on actual numerical data with a dual objective of compression rate and accuracy for further use and analysis*. The general formulation of this problem is presented here.

It is assumed that the following field is known, at least in a discrete representation e.g. as a result of a finite elements method,

$$\begin{aligned} f : \Omega &\subset \mathbb{R}^d \rightarrow E \subset \mathbb{R} \\ \mathbf{x} &\mapsto f(\mathbf{x}) \end{aligned}$$

where  $\Omega = \prod_{i=1}^d [a_i, b_i]$ .

We are seeking  $\tilde{f}$  the “best” separated approximation of  $f$ . A separated representation of a function consists in a combination (sum and product) of univariate functions. In this paper, for practical reasons, these functions are normalized and orthogonal (when possible) to the others so that it constitutes a basis. The definition of the “best” separated approximation of  $f$  depends strongly on the chosen norm to measure approximation error which is defined as

$$\mathcal{E}(f, \tilde{f}, N) = \frac{\|f - \tilde{f}\|_N}{\|f\|_N} \quad (1)$$

where  $N$  is commonly  $L^2(\Omega)$  for functions or  $l^2$  for discrete representations of fields (tensors) but any appropriate norm can be used.

The other constraint on this optimization problem is the (reduced) space  $\mathcal{V}$  to which  $\tilde{f}$  belongs. We can then define the general optimization problem for multidimensional problem optimization.

*Approximation problem* Find  $\tilde{f} \in \mathcal{V}$ , such that

$$\tilde{f} = \underset{v \in \mathcal{V}}{\operatorname{argmin}} \mathcal{E}(f, v, N_{\mathcal{V}}) \quad (2)$$

where  $N_{\mathcal{V}}$  is the chosen norm on  $\mathcal{V}$ . Some additional constraints may be needed to ensure existence and unicity of the solution as detailed in later sections.

One should note that this process is highly compatible with discrete representation. In this context, the multivariate function is replaced by an order  $d$  tensor  $\mathcal{F} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ . If a few modes containing the most relevant information is conserved, then a reduced approximation is obtained.

Each numerical implementation of the formats, is provided with meaningful comparison of complexity and compression rate for a given approximation error. The compression rate (CR) is defined by this formula

$$\text{CR} = \frac{\text{Mem\_cost}(\tilde{f})}{\text{Mem\_cost}(f)}. \quad (3)$$

It enables, with a single indicator, to compare methods with different output formats. It can be interpreted as a “practical” CR, that compares the output memory cost versus the initial full tensor memory requirement.

## 2 Bivariate separation

A separated sum approximation for bivariate function reads as follow

$$f(\mathbf{x}, t) \approx \tilde{f}_r(\mathbf{x}, t) = \sum_{k=1}^r a_k(t) \phi_k(\mathbf{x}) \quad (4)$$

where we can impose a number of conditions on  $\{a_k\}$  and  $\{\phi_k\}$ . Such approximation can be obtained through POD or PGD. A similar formulation can be written for algebraic spaces i.e. vectors and matrices in the 2D case. For any  $A \in \mathbb{R}^{m \times n}$ ,

$$A \approx A_r = \sum_{i=1}^r \sigma_i \mathbf{u}_i \otimes \mathbf{v}_i \quad (5)$$

where  $\otimes$  is the tensor product of  $\mathbf{u}_i \in \mathbb{R}^m$  and  $\mathbf{v}_i \in \mathbb{R}^n$  and  $\sigma_i \in \mathbb{R}_+^*$ . This decomposition can be obtained via SVD and is equivalent to the PCA.

## 2.1 Singular Value Decomposition (SVD)

This method can be viewed as a generalization of the eigenvalues decomposition (EVD) for rectangular matrices [45].

**Theorem 1** *For any matrix  $A \in \mathbb{R}^{m \times n}$ , there are orthogonal matrices  $U \in \mathbb{R}^{m \times m}$  and  $V \in \mathbb{R}^{n \times n}$  so that*

$$A = U \Sigma V^\top \quad (6)$$

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

Hereafter, it is assumed that the singular values are ordered decreasingly i.e. if  $i < j$  then  $\sigma_{ii} \geq \sigma_{jj}$ .

The Eckart-Young theorem [14] ensures that the  $r$ -truncated SVD is the best rank  $r$  approximation in the form of eq. 5 of a matrix in  $l^2$  norm.

This is why SVD is the main tool for low rank approximation even when applied to higher dimensional problems. Many algorithms and computing libraries are available to compute SVD on full (e.g. `dgesvd` from Lapack,...) and sparse matrices relying on Lanczos algorithms.

*EVD solver to compute full matrix SVD* In this paper, the link between SVD and EVD is exploited and the actual implementation uses `dsyevd` from Lapack as it ensures higher quality of the modes (mainly orthogonality) while significantly lowering the size of the singular value problem, see [43] section on bivariate decomposition for more details. As shown in Tab. 1 for any  $A \in \mathbb{R}^{m \times n}$  with standard SVD decomposition  $A = U \Sigma V^\top$  it is possible to solve a EVD problem of size  $\min(m, n)$  to obtain the SVD at a lower computational cost, in particular for “tall” or “wide” matrices. However this method main drawback is that the eigen values are computed to machine precision ( $\epsilon = 10^{-16}$ ) which limits the approximation error to  $10^{-8}$ .

$m \geq n$	$A^\top A = V \Sigma^\top \Sigma V^\top = V \Sigma^2 V^\top$	is a $n \times n$	eigen value problem and $U = AV \Sigma^{-1}$
$n \geq m$	$AA^\top = U \Sigma \Sigma^\top U^\top = U \Sigma^2 U^\top$	is a $m \times m$	eigen value problem and $V = \Sigma^{-1} U^\top A$

Table 1: Solving an equivalent EVD to SVD can lead to substantial complexity gains for  $n \gg m$  or  $m \gg n$ .

## 2.2 Proper Orthogonal Decomposition (POD)

It was discovered many times in many different fields, however it is often attributed to Kosambi [46] who introduced it in 1943. It is a linear procedure that computes a basis of orthogonal proper modes. They are obtained by solving Fredholm’s equation for data. Additionally, the POD offers an optimal approximation of the energy in term of  $L^2$  norm.

*POD Problem formulation (scalar case)* Find the best approximation, in the sense of a given inner product  $(\cdot, \cdot)$  and average operator  $\langle \cdot, \cdot \rangle$ , of  $f : \mathcal{D} = \Omega_x \times \Omega_t \rightarrow \mathbb{R}$  as a finite sum in the form

$$\tilde{f}_r(\mathbf{x}, t) = \sum_{k=1}^r a_k(t) \phi_k(\mathbf{x}) \quad (7)$$

where  $(\phi_k)_k$  are orthogonal for the chosen inner product.  $a_k$  is given by  $a_k(t) = (f(\cdot, t), \phi_k(\cdot))$  then  $a_k$  only depends on  $\phi_k$ .

Discrete POD problem is often found in the literature as follows. Let  $\{f_1, \dots, f_{n_t}\}$  the snapshots of  $f$  i.e. the representation of  $f$  at discrete time  $\{t_j\}_{j=1}^{n_t}$ . The snapshot space is  $\mathcal{F} = \text{span}\{f_1, f_2, \dots, f_{n_t}\}$ .

POD generates an orthonormal basis of dimension  $r \leq n_t$ , which minimizes the error from approximating the snapshots space  $\mathcal{F}$ . The POD basis verifies the optimum of the following:

$$\min_{\{\phi\}_{k=1}^r} \sum_{j=1}^{n_t} \|f_j - \tilde{f}_{r,j}\|^2, \text{ s.t. } (\phi_k, \phi_j) = \delta_{kj} \quad (8)$$

where  $\tilde{f}_{r,j} = \sum_{k=1}^r (f_j, \phi_k) \phi_k$  and  $\delta_{kj}$  is the Kronecker symbol. One may observe that  $\sum_{k=1}^r \cdot$  is the first order approximation of the time mean operator  $\langle \cdot \rangle$ . This problem can be solved with discrete EVD. Although it is the most common formulation of discrete POD in mechanics literature, it can be misleading regarding the construction and properties of the POD.

*Optimality of the POD basis* The POD basis generated by the POD algorithms is optimal with respect to the chosen scalar product (usually  $L^2$ ) i.e. the truncated approximation of  $f$  has the lowest error for a fixed rank  $r$ .

Subsequently, we admit that this problem can be solved numerically by an EVD method (see [43] and [8, Sec 1.2] for details and discussion on POD discrete implementation). POD can be seen as a continuous version of the SVD for bivariate functions  $f(x, t)$ , for this reason, in the next section, we only present the one version of the methods while the continuous and discrete approach can be switched freely.

### 2.3 Proper Generalized Decomposition (PGD)

This method has been developed in the last 15 years or so for solving and computing separated representation of solutions of PDEs. This linear enrichment process has been shown to be very efficient for parabolic problems (see [2]). PGD can be degraded to the specific case of function approximation, *a posteriori* PGD, i.e. the linear system reads  $f = u$  (see [8, sec 1.3 and sec 3.1] for details). It is essentially equivalent to POD for the 2D case and leads to the same numerical approximation and basis but the algorithm is different. For higher dimensions, *a posteriori* PGD can be interpreted as equivalent to CP decomposition and the algorithm is a direct extension of the 2D version.

*Enrichment algorithm* For the sake of concision, this presentation relies on the strong form of the problem which is sufficient for *a posteriori* PGD. The main idea is to enrich progressively  $u_r = \sum_{i=1}^r X_i(x)Y_i(y)$ , the approximation of  $f$ , until the approximation error is small enough with  $u_r \xrightarrow[r \rightarrow \infty]{} u = f$ . At step  $r$ , the *enrichment* process adds  $X_r(x)Y_r(y)$  the best rank-1 approximation of  $f - u_{r-1}$ , it reads

$$X_r Y_r = \underset{X^* \in L^2(\Omega_x), Y^* \in L^2(\Omega_y)}{\operatorname{argmin}} \|X^* Y^* - (f - u_{r-1})\|_{L^2} \quad (9)$$

$X_r$  and  $Y_r$  are searched under the constrain of orthogonality to  $\{X_i\}_{i=1}^{r-1}$  and  $\{X_i\}_{i=1}^{r-1}$  respectively and  $\|X_r\| = 1$  for practical reasons. This best rank-1 approximation is obtained by a *fixed point algorithm* that computes alternatively the best  $X_r^k$  given  $Y_r^{k-1}$  and the best  $Y_r^k$  given  $X_r^k$  until convergence is reached. The specificities and extenstion to multi-dimension algorithm are discussed in [2,8] while many improvement and variations are available in the literature[47, 40].

## 3 Multi-dimensional decomposition formats and methods

We are interested in the approximation of  $d$  dimensional data whether it is a tensor  $\mathcal{F} \in \mathbb{R}^{n_1 \times \dots \times n_d}$  or a function of  $d$  variables  $f(x_1, \dots, x_d)$ . Four decomposition formats and their methods are compared in this article: *canonical*, *Tucker*, *tensor train decompositions* and *recursive POD*. They have been presented in details in [43,8] which is why they are briefly exposed in this section and only the most natural framework i.e. either function or tensor approach is presented. In this paper, the focus is set on tensors for which all the data is already available and is supposed to originate from mechanics and in particular fluid dynamics. This implies that the approximation must account for all the data available since it is expensive to obtain and excludes of the study subsampling techniques such as cross approximation or greedy sampling.

First, a few definitions are introduced in order to describe accurately tensor decompositions and the associated algorithms. Let  $\mathcal{F} \in \mathbb{R}^{n_1 \times \dots \times n_d}$  be an *order d* tensor with the multi-index  $\mathcal{N} = n_1 \times \dots \times n_d$ .

*Products on tensors.* The tensor product  $\otimes$  is the generalization of outer product to tensors.

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

Entry-wise  $\mathcal{T} = \mathcal{X} \otimes \mathcal{Y}$  reads  $T_{ij} = x_i y_j$ . It will mostly be used for vector to vector product to generate higher dimension objects. The **Kronecker** product (of matrices) is noted with the same sign  $\otimes$  when no confusion is possible. The **Hadamar** (entrywise) product is noted  $*$  while the **Kathri-Rao** product is noted  $\odot$ . Detailed definitions and discussion can be found in [43,24].

*Matricization.* is the process of ordering the elements of a tensor into a matrix. The mode- $\mu$  matricization of a tensor  $\mathcal{X} \in \mathbb{R}^{\mathcal{N}}$  is denoted by  $\mathbf{X}_{(\mu)}$  and arranges the mode- $\mu$  fibres to be the columns of the resulting matrix. The map from tensor entries to matrix entries is uniquely defined and corresponds to `reshape` operation when implementing

$\mu$ -mode product. The  $\mu$ -mode (matrix) product, for  $1 \leq \mu \leq d$  of tensor  $\mathcal{X} \in \mathbb{R}^{n_1 \times \dots \times n_d}$  with matrix  $\mathbf{A} \in \mathbb{R}^{m \times n_\mu}$  is denoted by  $\mathcal{X} \times_d \mathbf{A}$  and is of size  $n_1 \times \dots \times n_{\mu-1} \times m \times n_{\mu+1} \times \dots \times n_d$ . Element-wise, we have

$$(\mathcal{X} \times_\mu \mathbf{A})_{i_1 \dots i_{\mu-1} j i_{\mu+1} \dots i_d} = \sum_{i_\mu=1}^{n_\mu} x_{i_1 i_2 \dots i_d} a_{j i_\mu}$$

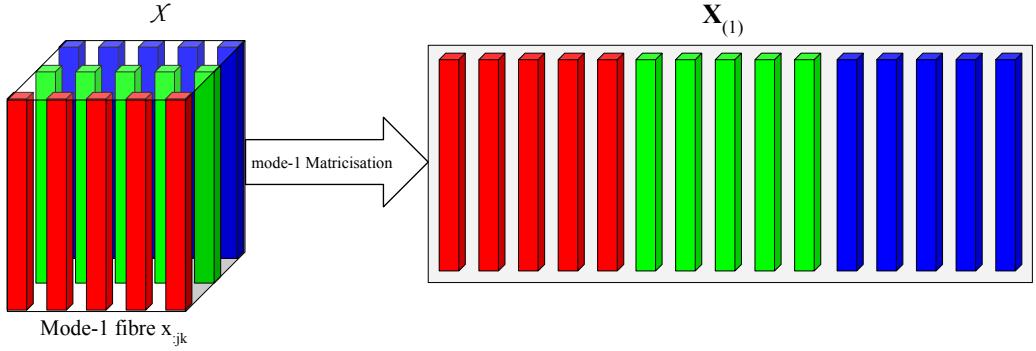


Fig. 1: Mode one matricization of third order tensor with  $\mathbf{X} \in \mathbb{R}^{I \times J \times K}$ .

It is equivalent to say that each mode- $\mu$  fiber is multiplied by the matrix  $A$ , i.e.

$\mathbf{Y} = \mathbf{X} \times_{\mu} \mathbf{A} \Leftrightarrow \mathbf{Y}_{(\mu)} = \mathbf{A} \mathbf{X}_{(\mu)}$ . This operation can be extended to **multilinear multiplication** (see [28]) for processing multiple  $\mu$ -mode products in a single operation.

$$[(\mathbf{I}, \dots, \mathbf{I}, \mathbf{M}, \mathbf{I}, \dots, \mathbf{I}) \cdot \mathbf{X}]^{(n)} = \mathbf{M} \mathbf{X}^{(n)}$$

Then in general, the unfolding of a multilinear multiplication is given by

$$[(\mathbf{M}_1, \dots, \mathbf{M}_d) \cdot \mathbf{X}]^{(n)} = M_n \mathbf{X}^{(n)} (\mathbf{M}_1 \otimes \dots \otimes \mathbf{M}_{n-1} \otimes \mathbf{M}_{n+1} \otimes \dots \otimes \mathbf{M}_d)^T$$

In the following subsections, a brief presentation of each format and most suitable decomposition is provided. Again, more details can be found in [43, 8]. The hierarchical format is not presented as it does not improve, in itself the compression algorithm but merely enable the handling of larger numbers of dimension with other algorithms such as TT or HOSVD. The reader is referred to [25] for theoretical developments and [48] for `htucker` toolbox and multiple references.

### 3.1 Canonical decomposition

The canonical or PARAFAC decomposition (CPD) consists in sum of rank-1 tensors. A rank-1 tensor of order  $d$  can be written by a single tensor product of  $d$  vectors. The algebraic CPD reads

$$\mathcal{F} \approx \mathcal{F}_r = \sum_{k=1}^r \bigotimes_{i=1}^d \tilde{\mathbf{x}}_i^k \quad (10)$$

where  $r$  is the rank of the approximation and  $\{\{\tilde{\mathbf{x}}_i^k\}_{k=1}^r\}_{i=1}^d$  are  $r$  sets of vectors associated with each dimension,  $\forall, i \leq d, k \leq n_i, \tilde{\mathbf{x}}_i^k \in \mathbb{R}_i^n$ . A schematic view of such a decomposition is given in Fig. 2.

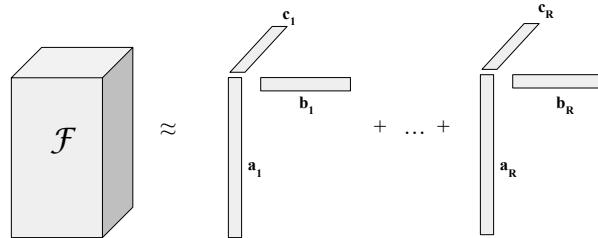


Fig. 2: CP decomposition of third order tensor  $\mathbf{X} \in \mathbb{R}^{I \times J \times K}$ .

The continuous formulation of the canonical decomposition reads

$$f(x_1, \dots, x_d) \approx f_r(x_1, \dots, x_d) = \sum_{k=1}^r \prod_{i=1}^d X_i^k(x_i) \quad (11)$$

where  $\{\{X_i^k\}_{k=1}^r\}_{i=1}^d$  can be viewed as basis functions in the functional space of  $f$ . This kind of function decomposition is typically obtained through PGD (see [2, 49, 47]).

In practice, this decomposition is obtained through a successively enriching algorithm such as PGD or alternating least squares (ALS). The storage cost is linear in  $d$  ( $\mathcal{O}(drn)$ ), but the convergence of these methods is not certain. The idea of the algorithm is to compute progressively the basis in all dimensions by enriching it of a new vector at each iteration so as to ensure closedness of the optimization problem. This process does not produce an optimal basis but it improves after each iteration although the improvement might become negligible for poorly separable functions, the tensor version of the algorithm is given in Algorithm 1.

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**Algorithm 1:** Alternating Least Square (ALS)

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input :  $\mathcal{F} \in \mathbb{R}^{I_1 \times \dots \times I_d}$ 
output:  $\mathcal{X} = w \otimes_{i=1}^d \mathbf{x}_i$ 
Initialize  $\forall 1 \leq i \leq d, \quad \mathbf{x}_i$  ;
while  $Error \geq \varepsilon$  do
    for  $i = 1, d$  do
        1    $V = \mathbf{X}_1^\top \mathbf{X}_1 * \dots * \mathbf{X}_{i-1}^\top \mathbf{X}_{i-1} * \mathbf{X}_{i+1}^\top \mathbf{X}_{i+1} * \dots * \mathbf{X}_d^\top \mathbf{X}_d$ ;          /*  $V \in \mathbb{R}^{R \times R}$  */
        2    $\mathbf{X}_i = \mathcal{F} \cdot (\mathbf{X}_d \odot \dots \odot \mathbf{X}_{i+1} \odot \mathbf{X}_{i-1} \odot \dots \odot \mathbf{X}_1) V^\dagger$ ;      /*  $\dagger$  denotes the Monroe-Penrose pseudo-inverse */
        3    $w_i = \|\mathbf{X}_i\|_2$ ;
        4    $\mathbf{X}_i = \frac{\mathbf{X}_i}{w_i}$ 
return  $\mathcal{X} = [w; \mathbf{X}_1, \dots, \mathbf{X}_d]$ 

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### 3.2 Tucker decomposition

Tucker decomposition uses a similar format as to Canonical but takes advantage of all the combinations of modes of different dimensions storing the associated weight in a *core tensor*  $\mathcal{W}$  whose entries are  $w_k$  with  $k = k_1, \dots, k_d$ . A 3D visual is given in Fig. 3. The tucker format approximation reads

$$\mathcal{F} \approx \mathcal{F}_k = \sum_{k_1=1}^{r_1} \dots \sum_{k_d=1}^{r_d} w_k \otimes_{i=1}^d \hat{\mathbf{x}}_i^{k_i} \quad (12)$$

where the rank  $\mathbf{r} = (r_1, \dots, r_d)$  of the core tensor is the Tucker rank of the decomposition. Each basis  $\{\hat{\mathbf{x}}_i^k\}_{k=1}^{r_i}$  is orthogonal and contains  $r_i$  vectors of size  $n_i$ . For each dimension  $i$ , the overall basis can be concatenated into a matrix  $\hat{\mathbf{X}}_i$  of size  $r_i \times n_i$ . The functional Tucker decomposition reads

$$f(x_1, \dots, x_d) \approx f_k(x_1, \dots, x_d) = \sum_{k_1=1}^{r_1} \dots \sum_{k_d=1}^{r_d} w_k \prod_{i=1}^d X_i^k(x_i) \quad (13)$$

Any tensor can be represented exactly in Tucker format, however, we are interested in approximated with minimal

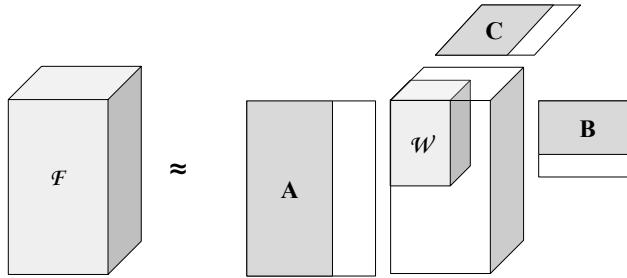


Fig. 3: *Truncated* Tucker Decomposition of a third order tensor  $\mathcal{F} \approx (\mathbf{A}, \mathbf{B}, \mathbf{C}) \cdot \mathcal{W}$  with  $r_i \leq n_i$  for  $i = 1, 2, 3$ .

( $l^2$  or  $L^2$ ) error and minimal rank i.e. size of  $\mathcal{W}$ , thus minimum storage cost. Many algorithms are available to compute Tucker decomposition (HOOI, T-HOSVD, ST-HOSVD,...). In this paper we focus on ST-HOSVD (sequentially truncated) proposed by [28] that has superseded the commonly used T-HOSVD [26] (truncated). Indeed, it provides a similar accuracy (as shown in the numerics section) to T-HOSVD while significantly reducing the number of operations.

The storage cost of Tucker format is quasi-linear in  $d$  for small  $r$  ( $\mathcal{O}(r^d + drn)$ ) but this cost grows exponentially with  $d$  which limits the use for  $d \geq 5$ . The convergence is certain with a quasi-optimal error estimate.

The idea of the ST-HOSVD is to perform successively SVDs on each dimension against all the others after flattening the tensor and truncate the decomposition to a prescribed level. The core tensor containing the associated weight is corresponds to multiplying the singular values or by projecting of  $\mathcal{F}$  onto the basis. This process is detailed in algorithm 2.

---

**Algorithm 2:** ST-HOSVD

---

```

input :  $\mathcal{F} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ , truncation rank  $r$ , processing order  $p = (p_1, \dots, p_d)$ 
output:  $\hat{\mathcal{X}} = (\hat{X}_1, \dots, \hat{X}_d) \cdot \hat{\mathcal{W}}$ 

 $\hat{\mathcal{W}} = \mathcal{F}$  ;
for  $i = p_1, \dots, p_d$  do
    /* Compute SVD of  $\hat{\mathcal{W}}_{(i)}$  then truncate to  $r_i$  */
    1    $(\mathbf{U}, \Sigma, \mathbf{V}^\top) = \text{SVD}(\hat{\mathcal{W}}_{(i)})$  ;
    2    $(\mathbf{U}_{tr}, \Sigma_{tr}, \mathbf{V}_{tr}^\top) = \text{truncate}(\mathbf{U}, \Sigma, \mathbf{V}^\top, r_i)$ ;
    3    $\hat{X}_i = \mathbf{U}_{tr}$  ;
    4    $\hat{\mathcal{W}}_{(i)} = \Sigma_{tr} \mathbf{V}_{tr}^\top$  ;
return  $\mathcal{X} = [\hat{\mathcal{W}}; \hat{X}_1, \dots, \hat{X}_d]$ 

```

---

### 3.3 Recursive decomposition

The Recursive-POD (RPOD) is not properly a format but merely a convenient generalization of POD to higher dimensions. Note that as for the other methods, POD and SVD remain interchangeable. The idea is to perform PODs recursively on the first variable of the function or its partial decomposition until all the parameters have been separated. This creates a tree structure (shown in Fig. 4) that does not allow the bases  $\{X_i^k\}_{k=1}^{r_i}$  to be orthogonal but enables efficient truncation. Because of the tree irregularity for a prescribed accuracy, it is not possible to give meaningful *a priori* storage cost. The general expression of RPOD reads

$$f(x_1, \dots, x_d) \approx \sum_{k_1=1}^{R_1} \cdots \sum_{k_{d-1}=1}^{R_{d-1}(k_1, \dots, k_{d-2})} X_1^{k_1}(x_1) \dots X_d^{(k_1, \dots, k_{d-1})}(x_d) \quad (14)$$

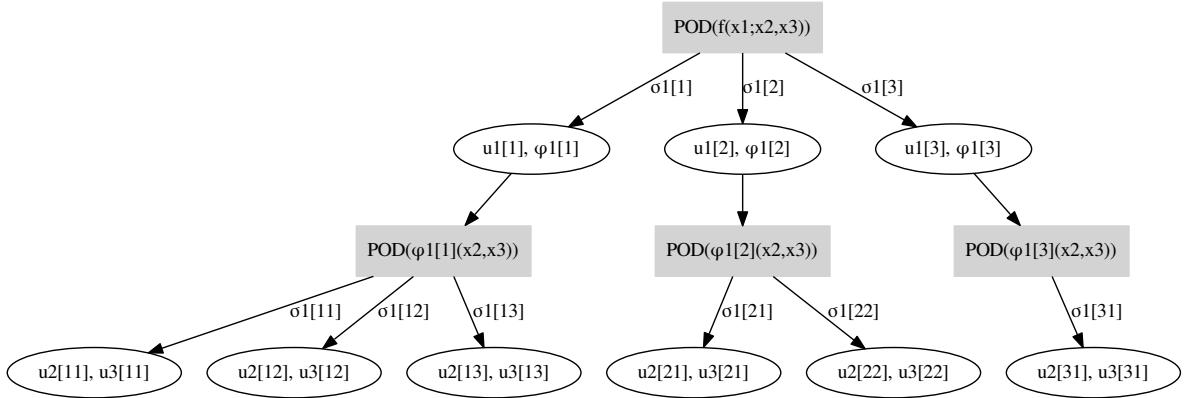


Fig. 4: Example of a Recursive POD graph of  $f(x_1, x_2, x_3)$

To better understand the method, the trivariate function  $f(x_1, x_2, x_3)$  RPOD, shown in Fig. 4, is presented in more details.

1. Separate  $x_1$  from  $(x_2, x_3)$  with standard truncated POD at appropriate rank  $r_1$ :

$$f(x_1, (x_2, x_3)) \approx \sum_{k_1=1}^{R_1} X_1^{k_1}(x_1) \Phi^{k_1}(x_2, x_3)$$

2. Repeat the POD on each  $\Phi^{k_1}(x_2, x_3)$  i.e. for all  $1 \leq k_1 \leq r_1$ :

$$\Phi^{k_1}(x_2, x_3) \approx \sum_{k_2=1}^{R_2(k_1)} X_2^{k_1, k_2}(x_2) X_3^{(k_1, k_2)}(x_3)$$

3. Then the full sum can be easily reconstructed:

$$f(x_1, (x_2, x_3)) \approx \sum_{k_1=1}^{R_1} \sum_{k_2=1}^{R_2(k_1)} X_2^{k_1, k_2}(x_2) X_1^{k_1}(x_1) X_3^{(k_1, k_2)}(x_3)$$

This algorithm can easily be extended to larger dimensions. Then notation can be quite clumsy (see eq. 14) and it has motivated the tree structure and implicit recursion programming in the actual implementation. Also, notice how the last two variables share the same decomposition and rank. Algorithm 3 produces RPOD tree decomposition as shown in Fig. 4. This kind of approach is rare in the scientific computing community and may be a drawback for less experienced scientific computing programmers.

---

**Algorithm 3:** RPOD

---

```

input :  $f \in L^2(\mathcal{D})$ , computing domain  $\mathcal{D}$ , target error  $\varepsilon$ 
output:  $\text{rpod\_tree} = [[\mathcal{R}, \mathcal{S}, \mathcal{X}]]$ 

1  $\mathcal{R} = []$ ; /* List containing the exact RPOD rank */
   $\mathcal{S} = []$ ; /* List containing the local singular values */
   $\mathcal{X} = []$ ; /* List containing the local eigen functions */
2  $\phi(x, \mathbf{w}) = f(x_1, (x_2, \dots, x_d))$ ;
3  $[R, \sigma_R, \mathbf{U}_R(x), \mathbf{V}_R(\mathbf{w})] = \text{trunc\_POD}(\phi, \varepsilon)$ ;
4  $\mathcal{R}.\text{append}(R)$ ;
   $\mathcal{S}.\text{append}(\sigma_R)$ ;
   $\mathcal{X}.\text{append}(\mathbf{U}_R)$ ;
  if  $\text{dim}(\mathbf{w}) > 2$  then
    5   for  $m \leq R$  do
      6      $\phi(x, \mathbf{s}) = V_r(\mathbf{w})$ ;
         $(\mathcal{R}_{loc}, \mathcal{S}_{loc}, \mathcal{X}_{loc}).\text{append}(\text{RPOD}(\phi, \mathcal{D}/\Omega_1, \varepsilon))$ ;
    7    $(\mathcal{R}, \mathcal{S}, \mathcal{X}).\text{append}(\mathcal{R}_{loc}, \mathcal{S}_{loc}, \mathcal{X}_{loc})$ ;
  else
    8    $\mathcal{X}.\text{append}(\mathbf{V}_R)$ ; /* Last dimension, then keep  $\mathbf{V}_R$  as RPOD modes */
  return  $f_{\mathcal{R}} = [[\mathcal{R}, \mathcal{S}, \mathcal{X}]]$ 

```

---

### 3.4 Tensor train (TT)

TT is a relatively recent method popularized by Oseledets team around 2010 [29,30] that allows easy implementation and is very efficient for  $d \geq 5$ . This format was first presented as a product of matrices that describe each entry of the studied tensor which is why it is also known as matrix product state (MPS) in the literature. It can be viewed as a specific case of hierarchical formats (see below) and boasts a  $d$ -linear storage cost  $\mathcal{O}(dn r^2)$  which makes it a good candidate for large dimension decomposition.

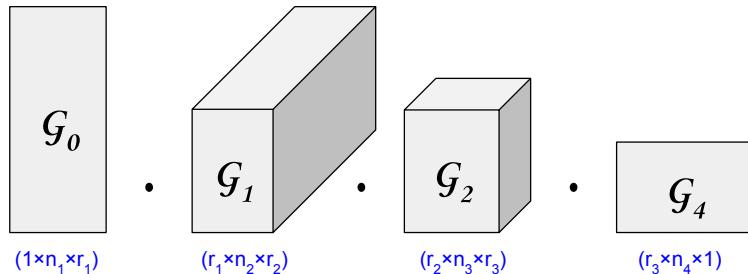


Fig. 5: Visual representation of the TT decomposition of an order 4 tensor of dimension  $n_1 \times n_2 \times n_3 \times n_4$  and TT rank  $(r_1, r_2, r_3)$ .

The functional TT decompostion reads

$$f(x_1, \dots, x_d) \approx \sum_{k_1, \dots, k_{d-1}} G_1(x_1, k_1) G_2(k_1, x_2, k_2) \cdots G_d(k_{d-1}, x_d) \quad (15)$$

where  $G_i(k_{i-1}, x_i, k_i)$  are the entries of a matrix of functions (for all  $i \leq d$ ) and of size  $r_{i-1} \times r_i$  (by convention  $r_0 = r_d = 1$ ).  $(r_1, \dots, r_d)$  is the tensor-train rank of the decomposition. For any  $\mathbf{x} = (x_1, \dots, x_d)$ , one can evaluate the value of  $\mathbf{G}_i$  matrices and then compute the approximation of  $f(\mathbf{x})$  at this specific point by evaluating matrix product  $\mathbf{G}_1(x_1)\mathbf{G}_2(x_2) \cdots \mathbf{G}_d(x_d)$ . Equivalently, the same can be applied to tensor  $\mathcal{F} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ , in which case each  $\{x_j\}_{j=1}^d$  are replaced by and integer index  $\{i_j\}_{j=1}^d$  and the decomposition reads  $\forall 1 \leq i_1 \leq n_1, \dots, 1 \leq i_d \leq n_d$ ,

$$\mathcal{F}(i_1, \dots, i_d) \approx G_1(i_1) G_2(i_2) \cdots G_d(i_d). \quad (16)$$

Fig. 5 shows a visual of the decomposition of a 4th order tensor.

Among the many algorithms (TT-cross, TT-DMRG-cross,...) developed by Oseledets team to compute TT, TT-SVD has been chosen for this article. It is easy to implement and efficient for reasonable number of dimensions and full tensor data  $d \leq 6$  which is the setup of this numerical study.

The idea of this algorithm is to use a series of SVDs (or PODs) to separate the remaining tensor into a *transfer tensor* and a tensor of 1 order smaller until the last dimension is reached. The corresponding TT-SVD algorithm is given in algorithm 4. The main drawback of TT decomposition is the partial orthogonality of the transfer tensors ( $G_i$ ) thus making it hard to use for ROM.

---

**Algorithm 4: TT-SVD**


---

```

input :  $\mathcal{F} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ , truncation rank  $\mathbf{r}$  or prescribed error  $\varepsilon$ 
output:  $\mathcal{X}(i_1, \dots, i_d) = \sum_{\alpha_0, \dots, \alpha_d=1}^{\mathbf{r}} G_1(\alpha_0, i_1, \alpha_1) \cdots G_d(\alpha_{d-1}, i_d, \alpha_d)$ 

1 Compute the truncation parameter  $\delta = \frac{\varepsilon}{\sqrt{d-1}} \|\mathcal{F}\|_F$  ;
2 Temporary tensor:  $\mathcal{C} = \mathcal{A}$ ,  $r_0 = 1$  ;
   for  $i = 1, \dots, d$  do
      /* reshape( $\mathcal{C}$ ,  $r_{i-1} n_i$ ,  $\frac{\text{numel}(\mathcal{C})}{r_{i-1} n_i}$ ) */ 
       $\mathcal{C} = \mathcal{C}^{(i*)}$ ;                                /* */
      /* truncated SVD at given rank  $r_i$  */
       $\mathbf{U} \Sigma \mathbf{V}^\top = \text{tSVD}(\mathcal{C}, r_k, \delta)$  ;
       $\mathcal{G}_i = \text{reshape}(\mathbf{U}, [r_{i-1}, n_i, r_i])$  ;
       $\mathcal{C} = \Sigma \mathbf{V}^\top$  ;
   7  $\mathcal{G}_d = \mathcal{C}$ ;
   return  $\mathcal{X} = [\mathcal{G}_1, \mathcal{G}_2, \dots, \mathcal{G}_d]$ 

```

---

*Remark 1 (Hierarchical format)* In this paper we omit the hierarchical format as it does not provide any specific algorithm, only translates the other algorithms presented in a larger framework that contains them. Typically the decomposition itself is performed as any of these methods and a leaf to root truncation procedure is added to benefit from the format very efficient handling of large dimensions.

As a conclusion of this theoretical presentation, the main characteristics of the above formats are presented in Tab. 2 including common algorithms, storage cost and evaluation cost. In the next section, a comprehensive numerical study is provided.

Table 2: Synoptic table of tensor formats for order  $d$  tensor  $\mathcal{F} \in \mathbb{R}^{n \times \cdots \times n}$  with rank  $r$  or  $\mathbf{r} = (r, \dots, r)$ .

Format	Algorithm	Storage	Evaluation
Full	Native array format	$\mathcal{O}(n^d)$	0
Canonical	ALS, PGD	$\mathcal{O}(drn)$	$\mathcal{O}(dr)$
Tucker	ST-HOSVD, HOSVD	$\mathcal{O}(k^d + dkn)$	$\mathcal{O}((d+1)k^d)$
Tensor Train	TT-SVD, TT-POD	$\mathcal{O}(dk^2n)$	$\mathcal{O}((d-1)k^3)$
Recursive format	RPOD RSV	Similar to TT	Similar to TT

## 4 Experimental results

First, we remind of the criteria for measuring the error and compression. The approximation or decomposition error of  $\mathcal{T}$  is defined by

$$E = \frac{\|\mathcal{T}_{\text{exact}} - \mathcal{T}_{\text{decomp}}\|}{\|\mathcal{T}_{\text{exact}}\|}, \quad (17)$$

while the kind of norm is defined according to the nature of the tensor. The compression rate (in %) which is the storage cost of an approximation in a given format for a specific rank divided by the storage cost of the full format. It reads

$$CR = \frac{\text{Mem\_cost}(\mathcal{T}_{\text{decomp}})}{\text{Mem\_cost}(\mathcal{T}_{\text{exact}})} (\times 100 \text{ for \%}). \quad (18)$$

#### 4.1 pydecomp software

In order to evaluate and compare these techniques, an open source software was developed. It is freely available at [https://git.notus-cfd.org/llestandi/python\\_decomposition\\_library](https://git.notus-cfd.org/llestandi/python_decomposition_library). This library relies heavily on `numpy` and `lapack` for computing efficiency of projections and SVD/POD. On top of that, a few classes are build, including the above formats, and the low rank approximation of tensors in these formats is automated. A few benchmark functions are available, they can serve both as tutorial (the functions are documented in the code itself) and as actual comparison tool. Fig. 6 provides a graph describing the structure of the library. Ample discussion on the structure and genesis of the software is provided in [8]. For a standard order  $d$  tensor  $\mathcal{F} \in \mathbb{R}^{n \times \dots \times n}$  `pydecomp`

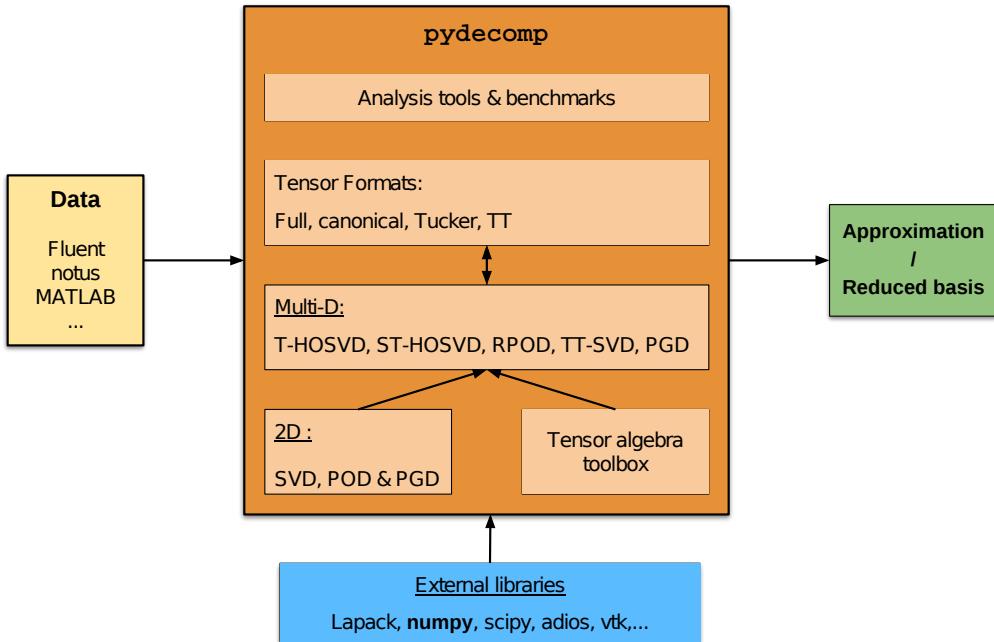


Fig. 6: `pydecomp` software architecture graph

complies with the general approximation characteristics of each format presented in table 2. For each of these format, the storage cost is computed exactly in `pydecomp` once the decomposition has been computed.

#### 4.2 Synthetic data

In this subsection we briefly recall numerical results reported in [43] for synthetic data, by which we mean data directly computed form a function's expression. The data is generated on uniform grids of  $n_1 \times \dots \times n_d$  that discretizes  $\Omega = [0, 1]^d$ . The following real test functions are used

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

In order to evaluate the separability of these three test functions with the studied methods, a relatively coarse grid of  $32 \times 32 \times 32$  is used. This first experiment is performed with a functional approach and POD, i.e. the  $L^2$  scalar product is used and numerical integrals are computed with a simple trapezoidal rule. The results are presented for all three functions in Fig. 7 in which one can compare the compression capacity of each methods for these simple functions. The steeper the slope, the higher compression power is observed.

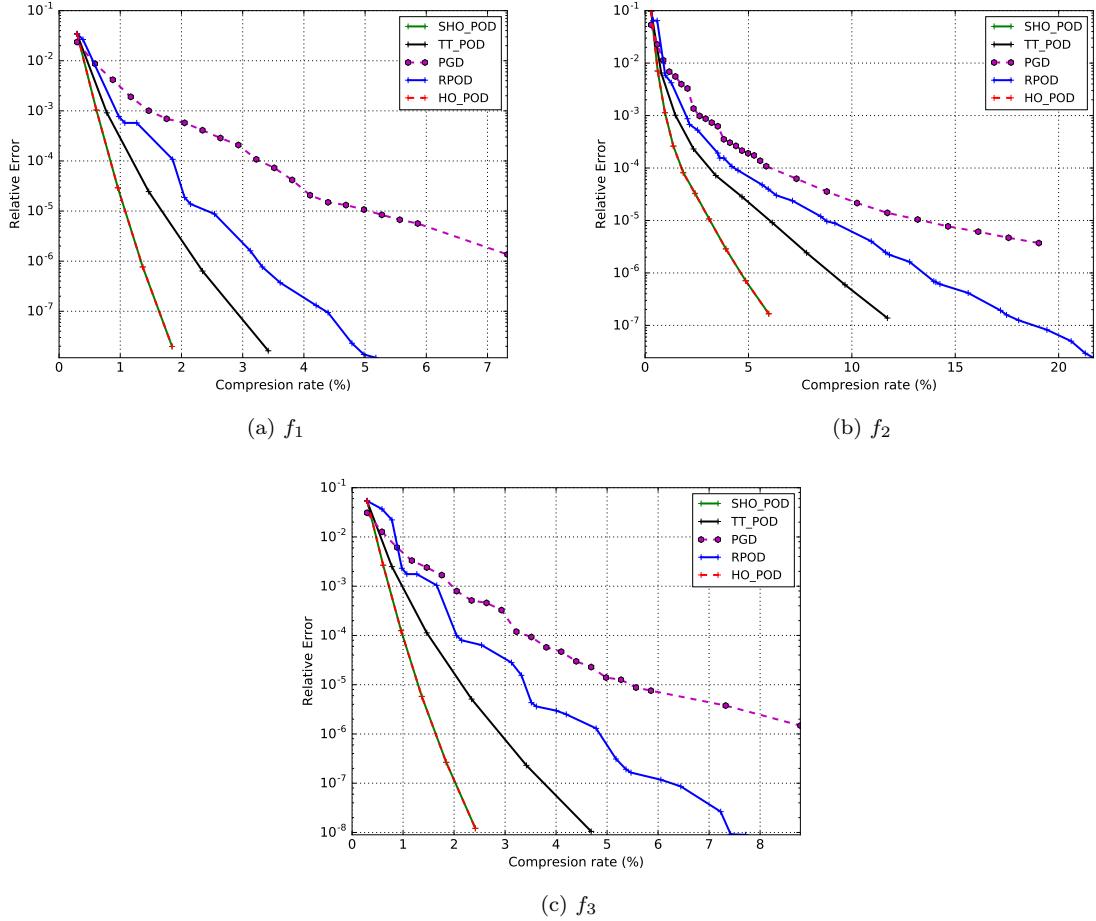


Fig. 7: Decomposition of 3 test functions with  $d = 3$  on a  $32^3$  grid with 5 discretization methods, using  $L^2$  integration and norm.

On these figures, one can see a group of very efficient methods (TT-POD and \*\*-HOPOD) i.e. the error reduces in a quasi exponential fashion. On the other end of the spectrum PGD (the functional CP decomposition algorithm) is the least efficient in all three cases. This can be attributed to the non-optimality of this method that is too important to be compensated by the storage  $d$ -linear efficiency. Additionally, this approach requires CPU times that are orders of magnitude bigger than the other methods and *grow exponentially* with the size of the problem. For this reason, we dismiss canonical decomposition (in both tensor and function form) from the following study as it is simply not able to compute a decomposition in a “reasonable” time.

On these simple examples, it is unclear whether RPOD is a good candidate or not, the decay of the error is not exactly exponential although the error is orders of magnitude smaller than PGD. Still, further analysis as shown in [43] confirms that for all tested configurations, in terms of CR, recursive methods consistently perform below Tucker and tensor train methods in spite of a much longer CPU time (more than 5 *times* more, see [43, Relative CPU time paragraph]). In addition to that, the complex tree data structure and the non-orthogonality of the collection of vectors leads to dismissing RPOD for further study of the numerical efficiency in this article.

Two decomposition methods (ST-HOPOD and T-HOPOD) have been tested for the Tucker format. As expected (see [28]), the results obtained are almost identical , in particular in terms of compression rate, then the only criterion left as to which one to use is computing time. As shown in [8], Sequentially truncated decomposition is, on average, 4 times faster than truncated decomposition. Thus in the following sections, the study focus on ST-HOPOD only for Tucker decomposition.

Now that the most efficient methods have been selected, TT-SVD and ST-HOSVD are applied to decompose data obtained through experiments, both numerical and physical. The goal of the following sections is to provide insight for efficient data reduction and qualitative analysis of their use.

This study is restricted to relatively small dataset i.e. in the order of 1GB so that decomposition as well as postprocessing is reproducible on a laptop. Three different cases are studied. Two are scalar data of only one variable, that is to say  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  as it is the simpler case, one from numerical and one from actual experiment. The third example addresses the multiple variables of the vectorial case i.e. some of the many ways to approximate the discretization of  $f : \mathbb{R}^d \rightarrow \mathbb{R}^p$ .

### 4.3 A scalar simulation : 2D lid driven cavity at high Reynolds number

A direct numerical simulation (DNS) of the 2D singular lid driven cavity problem in streamfunction-vorticity formulation with high accuracy (NCCD 6th order scheme, see [50] for implementation details of T.K. Sengupta code and analysis of the flow). High Reynolds numbers are studied, here we focus on range  $Re \in [10000, 10100]$  with a spacing of 20. Time steps are very small,  $dt = 10^{-3}$  thus snapshots sampling is coarser :  $\delta t = 0.2$  in order to capture longer time series and especially limit cycles. To capture the flow behavior from initial quiescent state to the limit cycle, simulation must run from  $t = 0$  to a few thousands which represent too many snapshots, indeed, each snapshots requires 0.5MB of memory thus leading to 5GB minimum per simulation). Consequently, for this analysis, a narrow range of the limit cycle is sampled from  $t = 1900.2$  to 1940, leading to 200 snapshots per  $Re$ . Finally, a relatively coarse space grid of  $257 \times 257$  is chosen for easier handling as we have shown that the number of modes is only weakly affected by grid density. In conclusion, after interfacing `pydecomp` with LDC code, an order 3 tensor  $\mathcal{T}$  of shape  $66049 \times 201 \times 6$  is obtained. In this case, space is given as a single dimension and is referred to as *vectorized*. As it is not clear whether it is preferable to decompose using this layout, the “fully” separated decomposition is also studied. In this case, space is seen as two separate dimensions leading to an order 4 tensor of shape  $257 \times 257 \times 201 \times 6$  which is called *reshaped*. Both approaches are compared in Fig. 8. Note that the data is not preprocessed, i.e. no centering of trajectories is performed before applying the decomposition algorithms.

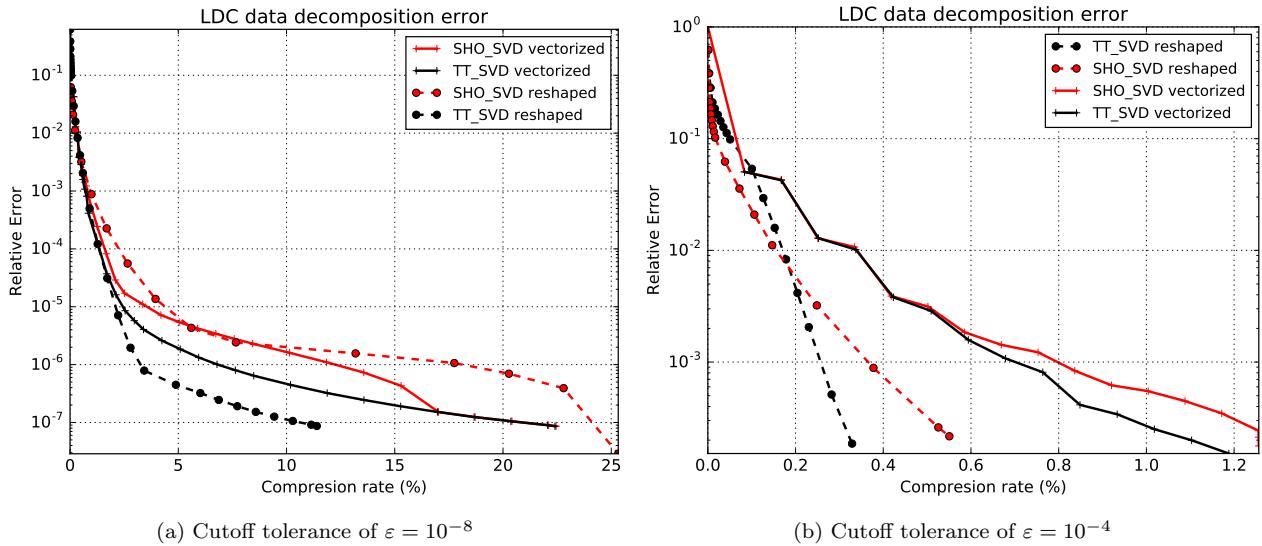


Fig. 8: Lid Driven Cavity Simulation within the stable limit cycle time range, see [50, 51], input tensor is of shape  $6 \times 201 \times 66049$ .  $t = 1900$  to 1940 with a stepping of 0.2, space is a  $257 \times 257$  grid that can be **vectorized** (solid lines) i.e. taken as a long vector of size 66049. Space treated as 2 dimension is referred as **reshaped** (dashed lines). Reynolds is a parameter dimension with  $Re \in [10000, 10100]$  and a stepping of 20.

This data is highly separable, all four configuration reach machine precision with relatively low compression rates 10% to 25%. Indeed both decomposition methods and both data layouts display exponential decay of the error as function of the compression rate. This is particularly visible when the error  $E > 10^{-5}$  in the top graph Fig. 8a. For lower truncation one can see an abrupt change of slope which can attributed to reaching “noisy” data. Indeed, this phenomenon is observed on most actual datasets.

Next, one can observe that all four methods display comparable accuracy for moderate accuracy ( $E \gtrsim 10^{-3}$ ), which means that the choice must be driven by the goal of the decomposition. For optimal storage, one is advised to prefer TT-SVD for both layout although vectorized layout allows the user to reduce the truncation error by almost a decade. Finally, the latter offers, by far, the best CR=10% for maximum accuracy as compared to the roughly 20% of concurrent methods. Regarding ST-HOSVD, the observation regarding layout is the opposite of TT-SVD as compression efficiency is (slightly) reduced with reshaping.

*Remark 2 (Handling of the space dimension)* As shown for this example, the compression rate is weakly influenced by the space layout. This confirms the intuition that the amount of information contained in space does not depend on its layout. However, we can see that it is not entirely true since differences appear early on, one can merely affirm that the qualitative separability of the field does not depend on the layout. In specific cases such as quasi 2D problems (not shown here, e.g. thin plate simulation), the third dimension *must* be separated as it represents a huge gain to treat it separately. Indeed it can be seen as an identity function.

The rank, however, is drastically influenced by this choice as one can see in table 3. The same cutoff value of  $\varepsilon = 10^{-4}$  has been used with each method and the truncation error is virtually the same. It is important to notice that in spite of the sequential nature of these methods the ranks of time and  $Re$  are unmoved by the layout choice.

Table 3: LDC decomposition ranks with the same prescribed cutoff value  $\epsilon = 10^{-4}$  (last point in Fig. 8b).

Data layout	Vectorized	Reshaped
ST-HOSVD	[15,18,6]	[59,63,18,6]
TT-SVD	[15,6]	[59,15,6,]

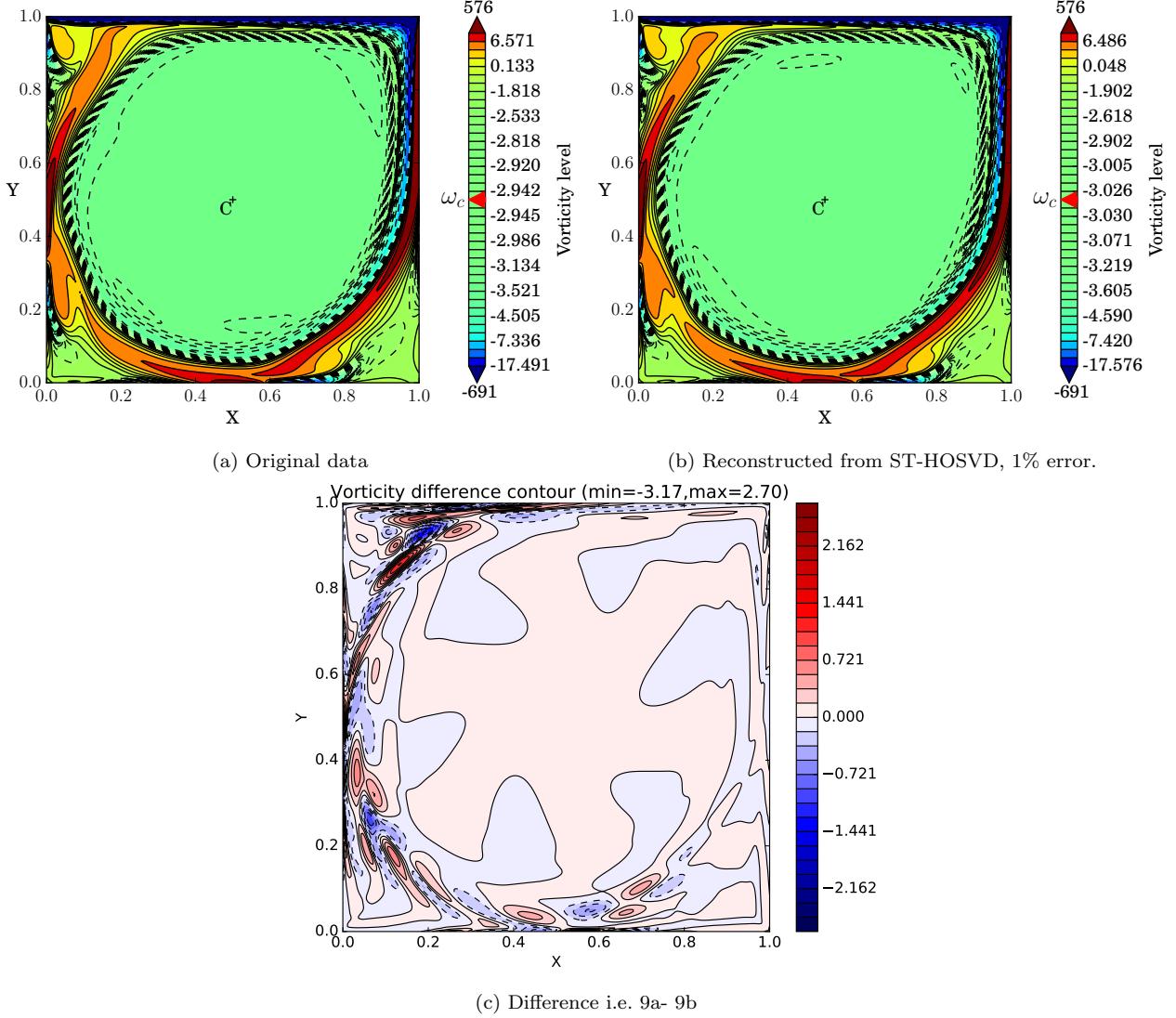


Fig. 9: Vorticity field of the lid driven cavity at  $Re=10000$ ,  $t=1900s$  decomposition is reconstructed compared with 1% relative error in Frobenius norm i.e. rank=(10,10,3) and compared to original dataset. Isolines are plotted as well as colormap, they are exponentially spaced from the center of the square value, solid is superior to  $\omega(C)$  while dashed lines are inferior. This is to make comparison with centered data.

Yet, spatial decomposition rank is drastically changed, being multiplied 4 times for each one in ST-HOSVD. It is interesting to notice that only the first rank in TT-SVD is big, the second one remains the same as for the vectorized layout. It can be interpreted that the space spanned by space dimensions 1 and 2 (embedded at the second stage of the algorithm) remains the same no matter the layout thus leading the same value of 15.

Now, we shift our attention to Fig. 8b. In this cases, we are interested in the ability of these methods to compress the data with moderate accuracy. The superiority of the reshaped representation of space is blatant as it proposes a much finer range of compression since many approximation levels are to be found for  $CR \leq 0.1$  while the storage requirement is halved compared to *vectorized*. This phenomenon is enforced by relatively low spatial ranks as compared with  $n_x$  and  $n_y$  (see Table 3). In terms of compression power, this largely overcomes the highly intertwined nature of both space axes i.e. the rich flow behavior lies in complex 2D structure that in spite of not being represented well in the reshaped layout is overcome by rank truncation.

Fig. 9 shows that even with moderate accuracy of 1% error the reconstructed data is largely usable for qualitative analysis. This is very interesting for long term storage as the required space for this dataset is reduced to 0.2% of the original 634MB i.e. 1.2MB. Fig. 9a shows the original vorticity field of  $Re = 10000$  at  $t = 1900$

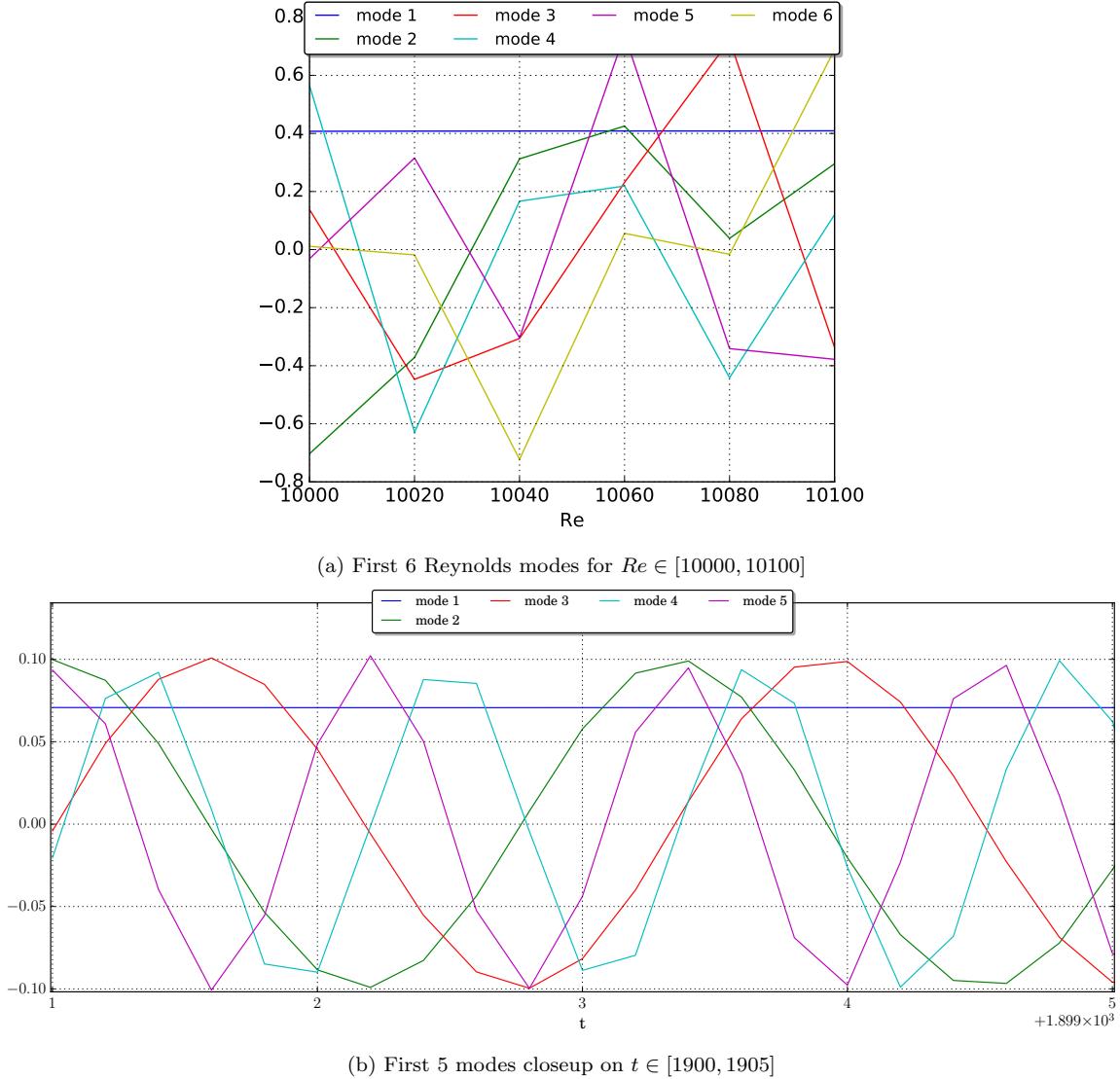


Fig. 10: Time and Reynolds modes of lid driven cavity during limit cycle ( $t \in [1900, 1905]$ ) in for  $Re \in [10000, 10100]$ .

while Fig. 9b proposes the same field from reconstructed ST-HOSVD in the vectorized layout and Fig. 9c is the difference between these two fields. One can see that the structures are well captured as well as the minimum and maximum value. The central region vorticity level is off by a few percent. However the lower amplitude structures are captured with less accuracy. Finally, the difference map shows that locally, the relative error remains small. As one would expect, most of the error is contained in large gradient regions near the boundaries of the domain.

Very limited physical hindsight is can be drawn by observing “reshaped” space modes along X and Y which is why they are not shown here. the central region is mostly flat with varying mean values while the extremities of the domain show large spikes and modes Y present small scale oscillations in addition to larger structures near  $y = 1$ . The “vectorized” modes (not shown) are similar to the one given in space time decompositions in [51] and can be used for physical hindsight.

Finally, in order to acquire a better grasp of the decomposition obtained, Fig. 10 shows the first modes associated with  $Re$  and time. In both cases, the first mode plays a special role of virtually applying a constant offset, it can be referred as a *mean mode*. Indeed this kind of mode is observed whenever the data has not been centered beforehand, the decomposition “naturally” separate the mean field from the fluctuations. A simple averaging of the data suppresses it and it is often advocated to do so in the literature as it should improve the decomposition. Next, Fig. 10b displays well organized modes, these pairs of modes (2-3, 4-5) are separated by a phase shift of  $\pi/4$  and the frequency of pair 2 is double the frequency of pair 1. This pattern is studied in greater details in [51], yet it interesting to note that the same pattern is observed for multivariate decomposition involving  $Re$  as a parameter as well as usual bivariate POD. It is then possible to infer that the time behavior is the same for each  $Re$  in the chosen range. At the other end of the regularity spectrum, one finds  $Re$  associated modes in Fig. 10a. These modes appear to be a mean to exclude each other from combinations, no clear pattern emerges. This observation indicates low feasibility for  $Re$  based interpolated ROM.

#### 4.4 Experimental data : droplets evaporation

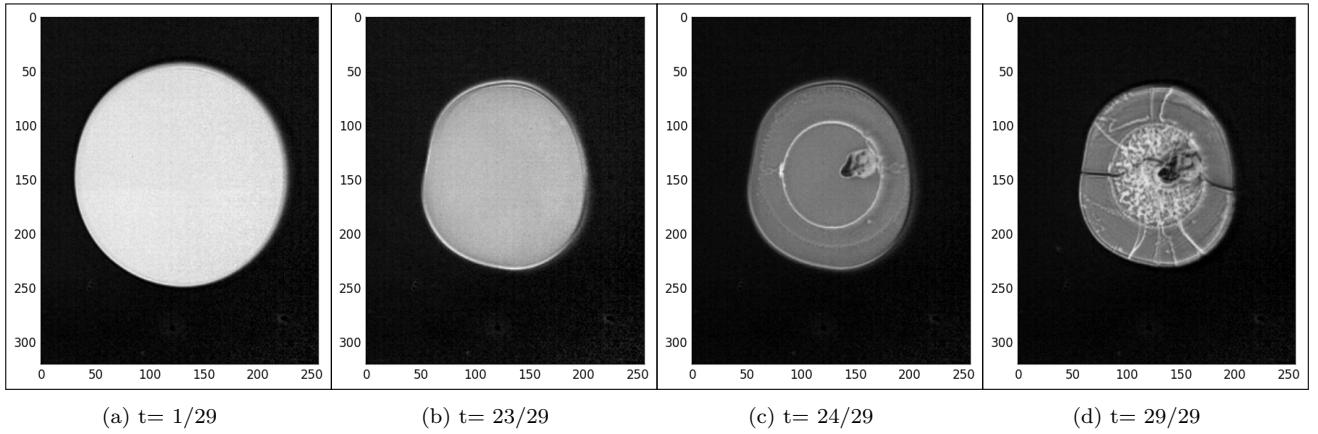


Fig. 11: Visualization of 4 snapshots of the density field at the 21<sup>st</sup> tabulated wavelength. Data kindly provided by C. Pradère (I2M Bordeaux).

In this second example, a scalar field obtained by a lab experiment is studied. The goal here is to emphasize that very little prior knowledge of the data is necessary to perform decomposition contrary to analysis. This dataset was kindly provided by C. Pradère, from I2M-TREFLE laboratory. It is a study of droplets evaporation during 29 timesteps with recording at 51 different wavelength to evaluate the density field. The camera resolution is  $320 \times 356$ , no further detail on the technology used is required. Finally, a matlab “.mat” binary file off 800MB is given. `pydecomp` provides a simple interface for inputting such files that yields a  $29 \times 51 \times 320 \times 356$  tensor.

*Phenomenon* Fig. 11 provides insight on the phenomenon studied, the circular drop at initial time evaporates and shrinks gradually up to frame 23. Cracks appear at  $t=24$  (different wavelength may not show these cracks) and the droplet is completely shattered at  $t=29$ . One may infer that the droplet has solidified but this information (not given by C. Pradère) is not necessary for data decomposition.

The data is obtained experimentally and it is likely that many physical phenomena are happening simultaneously during the experiment. Then, one has to assess the separability of the array. In the absence of any information about the parameter spaces at stake, the Frobenius norm based decomposition is used. Fig. 12 shows that with both ST-HOSVD and TT-SVD, very little compression is achieved. Indeed, Fig. 12a shows that more than 60% compression rate is needed to reach a relative error of 1%. Yet, one can see that the error drops (actually down to machine error) with a compression rate slightly below 100% which means that the density field is represented “*exactly*” with a slight datasize reduction. Fig. 12b shows that attempts at vectorizing data provide no improvement in the error decay rates. This zoomed in view, informs us that a reduction to a few percents of error is attained

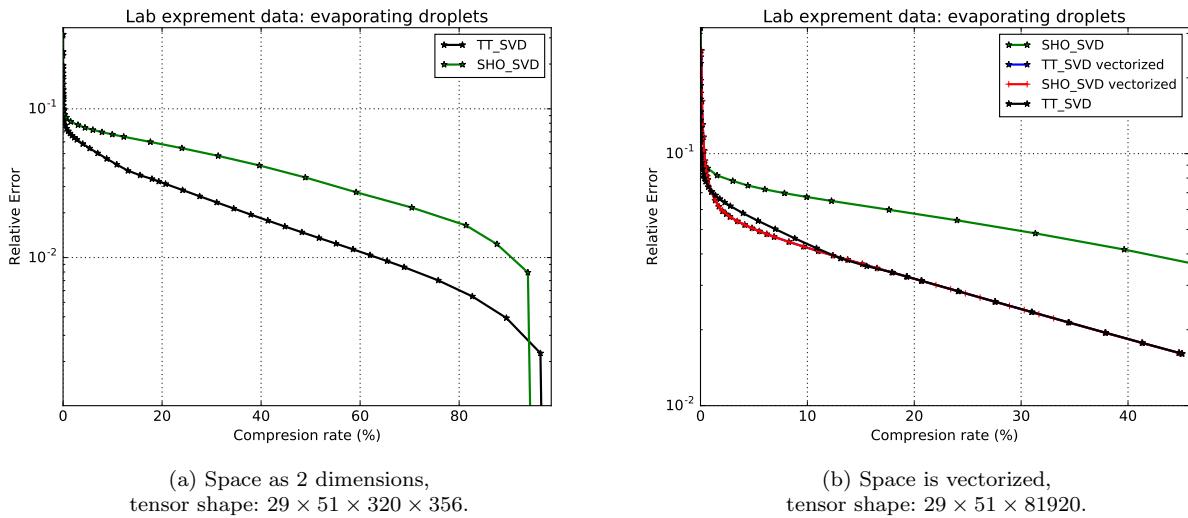


Fig. 12: Decomposition of experimental data kindly provided by C. Pradère (I2M Bordeaux). The density is given as a function of time, wavelength and space

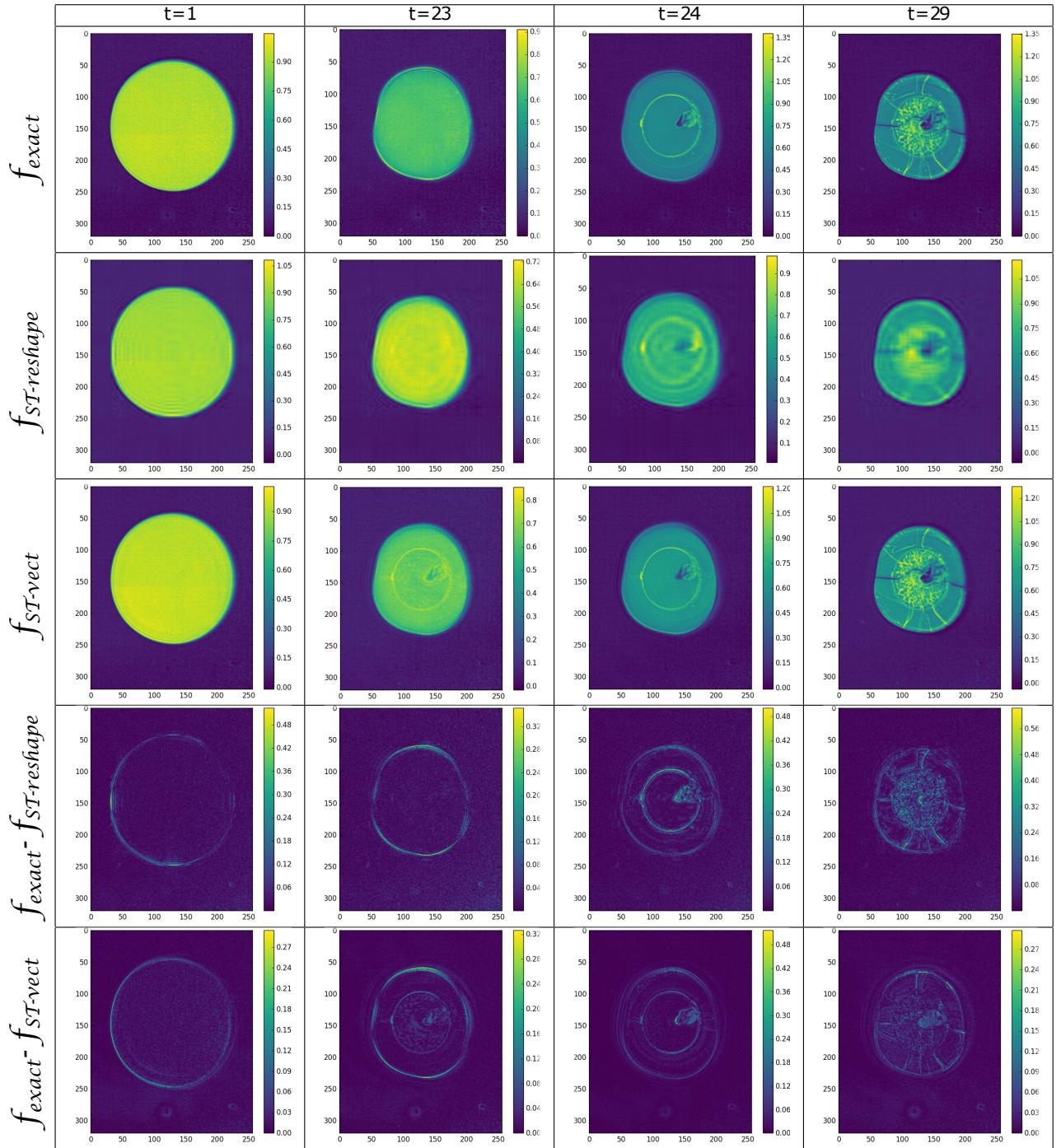


Fig. 13: Synoptic view of reconstructed ST-HOSVD decompositions of the density field, tolerance,  $\varepsilon = 10^{-2}$ , wavelength 21. Each line represent a different dataset, from top to bottom:  $f_{\text{exact}}$ ,  $f_{\text{ST},\text{reshape}}$ ,  $f_{\text{ST},\text{vectorized}}$ , difference ( $f_{\text{exact}} - f_{\text{ST},\text{reshape}}$ ) and difference ( $f_{\text{exact}} - f_{\text{ST},\text{vectorized}}$ ).

within a few modes. Thus some of the behavior is separable. But the complexity of this phenomenon lies in nonlinear physics, such as transport or phase change, that are known to cause poor error decay of the SVD/POD.

Finally, Fig. 13 provides a synoptic view of the ST-HOSVD decompositions with a prescribed error of  $10^{-2}$  in both vectorized and reshaped layout. This means an actual error of 6% for the *vectorized* layout with a compression rate of 1.5%. The *separated space* global error is 9% for a compression rate of 0.3%. This partial choice of low accuracy high compression is aimed at showing that this kind of representation is sufficient for qualitative analysis. First, in spite of high global error level, the sequence of droplet evaporation is well captured by both methods, the crack appears at the expected frame in each decomposition. The main difference between the two layout lies in the sharpness of the spatial representation, indeed the vectorized approach produces a sharp edged representation while the separated space dimension lead to a “blurry” phenomenon. This is confirmed by the bottom frames, in which one clearly sees that the error is located at high density gradient regions. In conclusion vectorized layout

produces less efficient decomposition but allows for a sharp and easy to interpret reconstructed field while the separated space dimensions yields a blurry image, yet with lower global error.

#### 4.5 A vectorial simulation : breaking wave

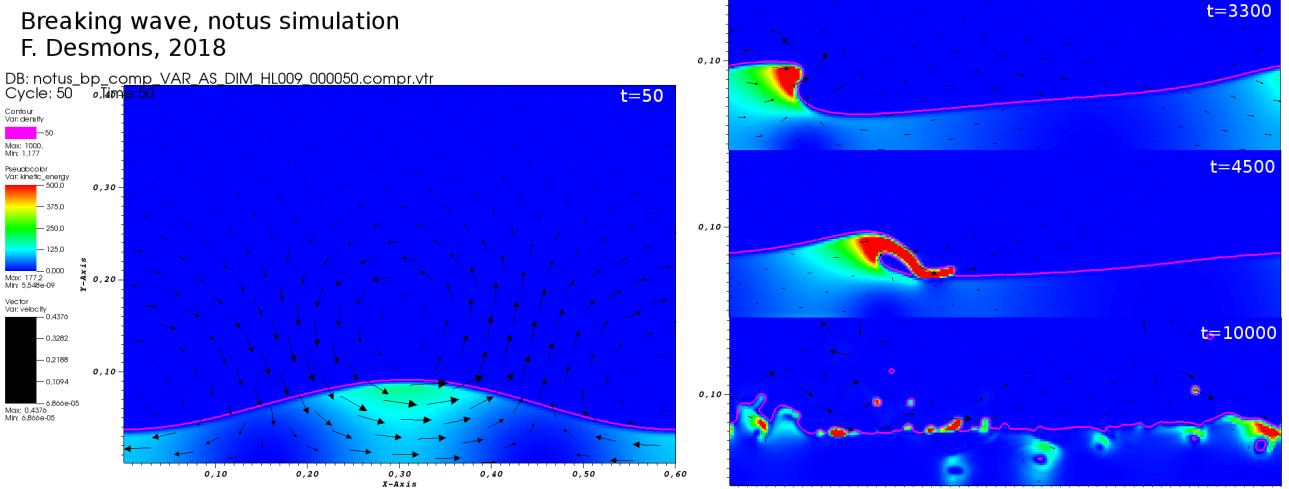


Fig. 14: Breaking wave simulation (by F. Desmons) computed with `notus` CFD code developed at I2M Bordeaux, wave height of 9cm and length of 10cm. The wave is going rightward from the initial state (left frame), crosses the periodic boundary (top right), breaks at  $t \approx 4500$  follows to an unphysical chaotic state. Pink lines represent the water/air interface, arrows size are proportional to the velocity amplitude and the colormap accounts for kinetic energy.

In this last example, we study a 2D simulation of a breaking wave which provides 5 output variables : density, pressure, vorticity, velocity along each dimension. It is not intended to be a state of the art breaking wave physics simulation, the goal here is to provide a complex physics two phases flow computed with a validated HPC code : `notus-cfd`.

The Navier Stokes equation with two fluids is solved thanks to a level set methods with a velocity-pressure scheme. The spatial domain  $\Omega = [0, 0.6] \times [0, 0.6]$  is discretized on a  $256 \times 256$  cartesian grid, while the time is solved with small times steps which are sampled in 201 equispaced snapshots. The third parameter is the ratio wave height over wave length, the latter being fixed for the whole set of simulation to 10cm, 3 heights are given: 9, 10 and 11 cm. In each case, the boundary conditions are periodic and the velocity field is initiated with an adapted velocity. Finally, the density field is equal to 1000 in the liquid phase and 1 in the gas phase. For stability reasons, the transition is smoothed on a few cells. Simulation with wave height of 9cm is provided in Fig. 14 where one can see four typical snapshots of the breaking wave.

*Data layout* The previous examples have shown that in spite of providing sharper spatial description, a vectorized space is not the most efficient configuration in terms of storage cost. Additionally, the physics of the studied problem clearly has two separate domains, air and water which remain in the same region with respect to coordinate Y. Only a small portion of the Y range is affected by phase change. For these reasons, a space separated layout is used. Furthermore, this dataset provides 5 different output fields which are correlated since they solve the same Navier-Stokes equation system. But, they possess very different mathematical properties, for instance, density field is representing as sharply as possible an inherently discontinuous field whereas the pressure field is naturally smooth and continuous in spite of following the same interface. The velocity field is represented by two scalar values but has been solved at the same time. Finally, the vorticity field is post-processed from velocity but the field itself is much sharper due to the rotational operator, thus making decomposition less efficient. In conclusion, two data layouts are studied, both with separated X and Y axes.

- Output data for each variables are processed sequentially. Five order 4 tensor of shape  $3 \times 201 \times 256 \times 256$  are decomposed.
- Output data for each variable is assembled into a new dimension that intends to account for embedded correlation among variables. One order 5 tensor of shape  $5 \times 3 \times 201 \times 256 \times 256$  is decomposed.

*Scalar product* As for any decomposition problem, choosing the base scalar product and associated norm is thought carefully. In this case, two parameters, output vector in case b. and wave height, impose the use of  $l^2$  scalar product. Thus SVD based decomposition is preferred with TT-SVD and ST-HOSVD.

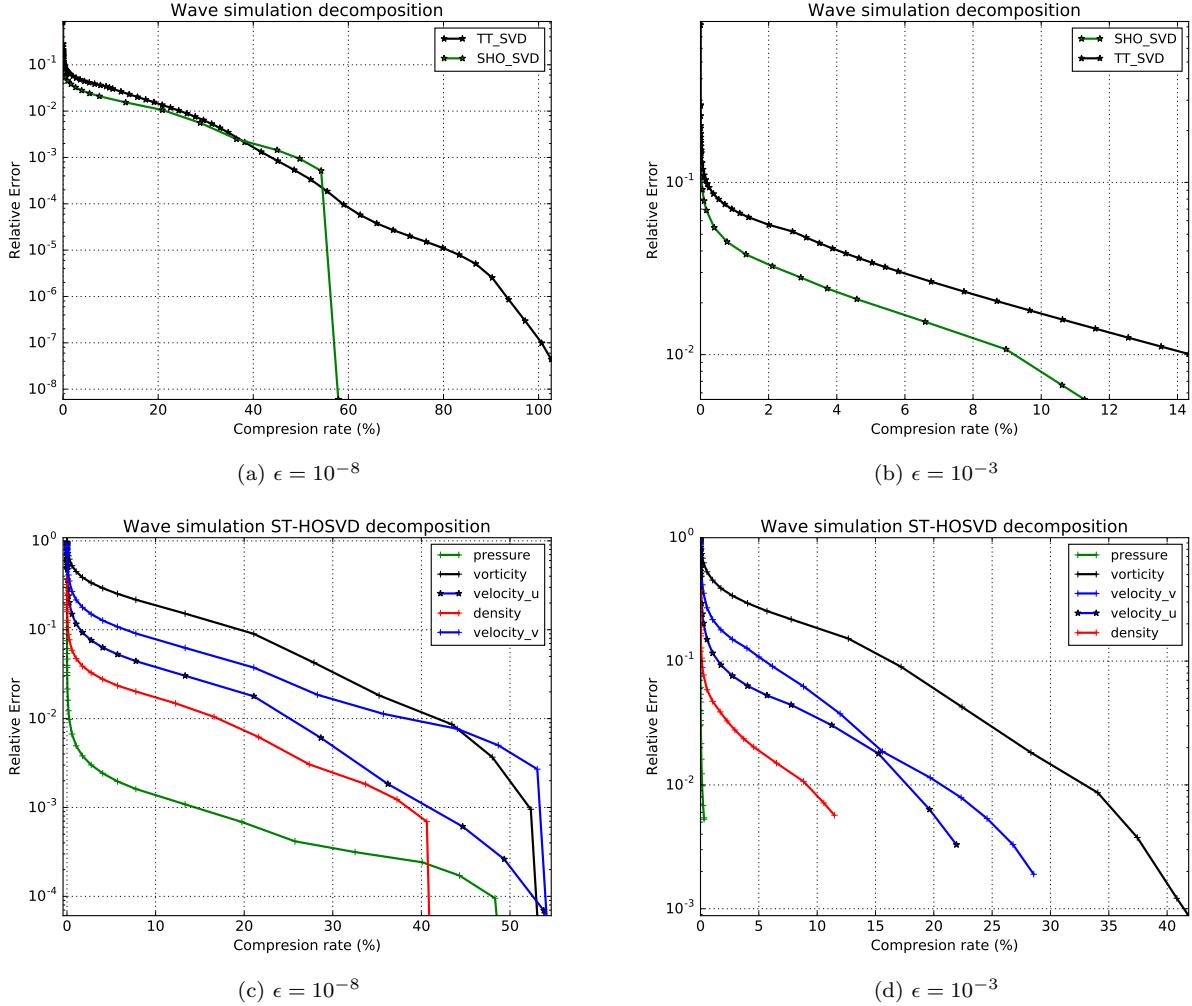


Fig. 15: Compression of breaking wave simulation data from `notus`. Parameters : 5 output variables, 3 wave heights,  $n_t = 201$ ,  $n_x = 256$ ,  $n_y = 256$ . Top frames are decomposition with output variable taken as an additional dimension with  $n = 5$  (case b.), bottom frames is the same dataset but each variable is seen as a separate scalar decomposition problem (case a.).

*Low rank approximation analysis* Fig. 15 provides the error versus compression rate graphs for layouts a. and b., we focus first on the top frames. Separability of the dataset with layout b. sits in the separable range. Indeed, a sharp decay of the error is observed for large scale evolution i.e. for error levels down to a  $E = \mathcal{O}(10^{-2})$ . Then, a clear inflection is observed around 0.5% compression rate for both methods. Yet, it still appears that the error decay follows an exponential trail. Note that ST-HOSVD yields the best approximation at low compression levels (see Fig. 15d) and represents to machine error the data with a compression rate of 60% as seen in Fig. 15c. No such convergence is observed for TT-SVD.

Regarding separate decompositions of variables through ST-HOSVD, lower frames of Fig. 15, it is observed in Fig. 15c that every single variable is represented to machine error within 50% of the original data size (per variable). It is actually uncommon for complex simulation data to present an “exact” tucker rank. Still, here, for each variable, machine error is reached for a tucker rank of  $r = (3, 201, \approx 130, 256)$ . Next, for small truncation error levels, all variables decrease at the same slope, only the extent of the initial drop varies. Fig. 15d provides a bigger truncation criterion in order to better grasp the moderate accuracy decomposition. Large differences between variables are observed, with pressure field being extremely separable while the vorticity field occupies the other end of the spectrum. Table 4 emphasizes the great variation of ranks among variables for an identical tolerance.

In conclusion, if one is interested specifically in an “easily” separable field, then the best choice is to treat variables separately. On the other hand, when interested in several variables, it is a better option to compress all the data together.

*Remark on graphs discrepancies* One may notice that these graphs are not exactly the same, this is because the truncation value  $\epsilon$  is applied to the ST-HOSVD itself i.e. to each SVD. This leads to some mode combination to disappear from the larger  $\epsilon$  although the actual projection norm is of the same order as  $\epsilon$ . For instance let us

Field	Rank
density	[3,174,58,147]
pressure	[3,52,14,44]
velocity_u	[3,184,79,256]
velocity_v	[3,179,101,158]
vorticity	[3,195,114,246]

Table 4: Breaking wave approximation ST-HOSVD ranks with prescribed cutoff value  $\varepsilon = 10^{-3}$  (last point in Fig. 15d).

pretend that  $\varepsilon = 10^{-3}$  yields a rank (3,7,27,35), there is no warranty that modes (3,8,27,32) from the full rank decomposition is associated with a weight  $\omega_{3,8,27,32} < \varepsilon$ .

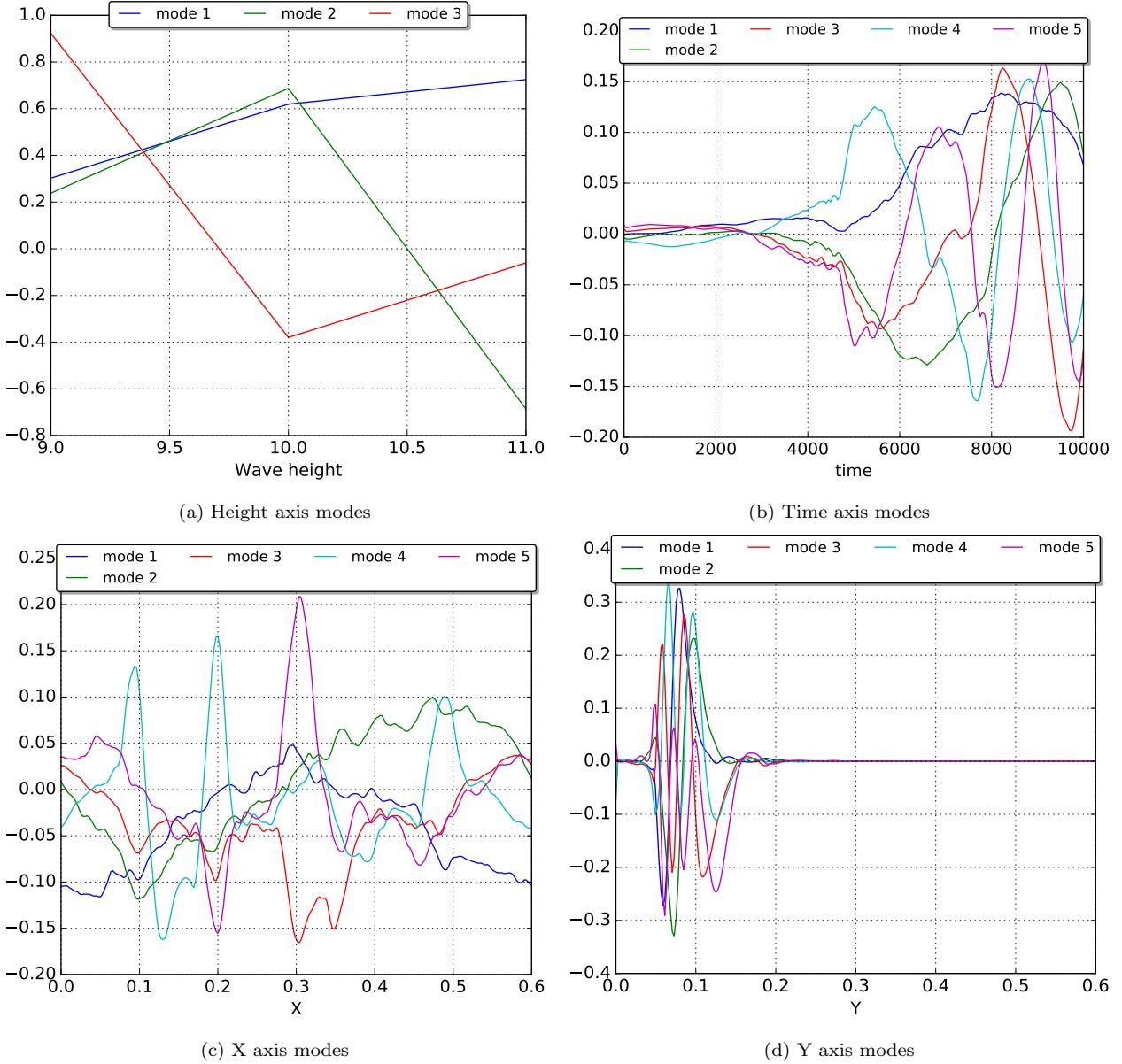


Fig. 16: The first vorticity modes for separated variables layout.

*Breaking wave vorticity modes* The physics at stake in this example is different than the previous ones, then we look at the first five modes of each dimension (see Fig. 16) for the vorticity field. The top left frame, Fig. 16a, shows the modes associated with the initial height of the wave. No clear pattern is distinguishable and the sharp variation mostly indicates that they would be better considered as discrimination function rather than modes in the usual sense. Consequently, there is very little prospect for interpolated ROM on this parameter when the user have only

3 instances available. Times modes (Fig. 16b) can be interpreted as being activated by the breaking of the wave (time range is approximately [3300,4500]) and further agitation. As expected, space modes along dimensions X and Y produce remarkably contrasted patterns. On one hand, X modes describe global agitation with distinct patterns at impact ( $x = 0.2$ ) and splash region ( $x = 0.3$ ). On the other hand Y modes show an intense activity near the interface and close to 0 value elsewhere. The same pattern is observed for other variables (not shown) but vorticity provides the most readable graphs.

*Reconstructed fields* Finally, a quick overview of the reconstruction is given by means of the density field and levelset reconstruction. Indeed, this is a very sensitive variable and it is required to capture correctly the interphase for any interpretation of the stored results. Fig. 17 shows the same snapshots as Fig. 14 where the black solid line is the original isoline 50 of the density field and the green dotted line is its reconstructed counterpart from ST-HOSVD( $\varepsilon = 10^{-3}$ ). The background color maps the difference between both density fields. In spite of marked error field, the reconstructed levelset fits perfectly with the original one, no bubble is omitted and the shapes are well captured. Still, some parts of the density field are negative (intense blue color in the air corresponds to  $\rho < -20$ ). This is obviously non physical and this issue should be addressed in order to prevent misinterpretation for cases in which the analysis is more complicated.

It should be noted that with this precision of  $\varepsilon = 10^{-3}$ , it is almost *impossible to distinguish* the reconstructed field from the original mode. Some slight oscillations may be spotted but are easily discarded by the observer as their amplitude is a few percent of the maximum field value.

## 5 Discussion and Conclusion

This paper presents as briefly as possible the main techniques for multidimensional data decomposition and approximation. Then they are applied to physics problem and analysis for both numerical and physical experiments. In short, this paper is an attempt at answering the following question.

*“Which one of the numerous decomposition method should be used for low rank approximation of mechanics data?”*

To do so, a decomposition library, `pydecomp`, has been developed. It takes advantage of python numerous libraries for scientific computing, visualization and data I/O handling. Benchmark cases are proposed in the library to test and compare each of the available methods : PGD, RPOD, T-HOSVD, ST-HOSVD and TT-SVD in both discrete and continuous formulation (SVD and POD can be exchanged freely as they are essentially equivalent).

In section 4.2, these benchmarks have been put to use. The conclusion is that PGD cannot be used as a multidimensional decomposition method for it is extremely slow and compression power is insufficient. Yet, it should not be dismissed completely as it makes a relatively efficient 2D iterative methods. Indeed, it allows the user to compute only the required modes contrary to standard SVD/POD algorithm. The T-HOSVD has been dismissed as its results are indistinguishable from ST-HOSVD while being several times slower for large datasets. RPOD has also been classified as not suitable for three reasons. First, its decomposition performance is far poorer than TT-SVD and ST-HOSVD, second, the computing time is much higher than its contenders (about 5 time more). Third, the recursive nature of the methods does not translate naturally in the same way as other scientific computing algorithms and leads to shallow and wide trees that are slow to scan. Discussion (supported by [43,8]) on scalar product selection has lead to the conclusion that default should be “blind” eulerian scalar product, especially for Cartesian grids. However, some cases could benefit from  $L^2$  scalar product such as Gaussian quadrature points, or contexts in which the physics is well known and requires a special scalar product such as integrating a vector field using  $H^1$  norm.

In sections 4.3 to 4.5, a close attention was given to the two most efficient methods for tackling actual data. Two scalar fields were used, one from an experiment, the other from a DNS simulation. The experimental data, taken from a droplet drying with 4 parameters (time, wavelength, 2D space) was found weakly separable with both methods. This is attributed to the nonlinear nature of the studied physics. Yet the reconstructed field for a tolerance of  $\varepsilon = 10^{-2}$  seems sufficient for qualitative interpretation. The high error levels seem to lie in the cracks representation as shown in the brief analysis of the modes. The DNS data (LDC) was chosen to present regularities that were accurately captured. In each of these methods two data layouts for space decomposition were studied, one separates X and Y dimension while the other vectorize so that space is viewed as a single dimension. For both datasets, the separate dimension produces lower compression rate for a fixed error level but the inherent bi-dimensionality of the structure is captured with less accuracy (to the human eye) in spite of lower error. Indeed mode combination leads to oscillations that reduce when the rank is increased. The last example was a breaking wave simulation computed using `notus CFD`. It proved the versatility of `pydecomp` implementation in handling data from several sources with different characteristics. It was shown that different variables from a single simulation present remarkably diverse separability levels. As expected, the smoother the field, the more separable it is. Another layout question was raised for this example, wondering whether these output variables should be treated as a distinct problems or as a single variable. Once again, there is no definitive answer and the user must adapt the layout to their need. The global decomposition allows easy handling but the compression rate is dominated by the least separable variable. Thus, for this case, a distinct processing of each variable is preferable. Moreover, it was observed that for this (complex) dataset tensor has a finite Tucker rank at machine error.

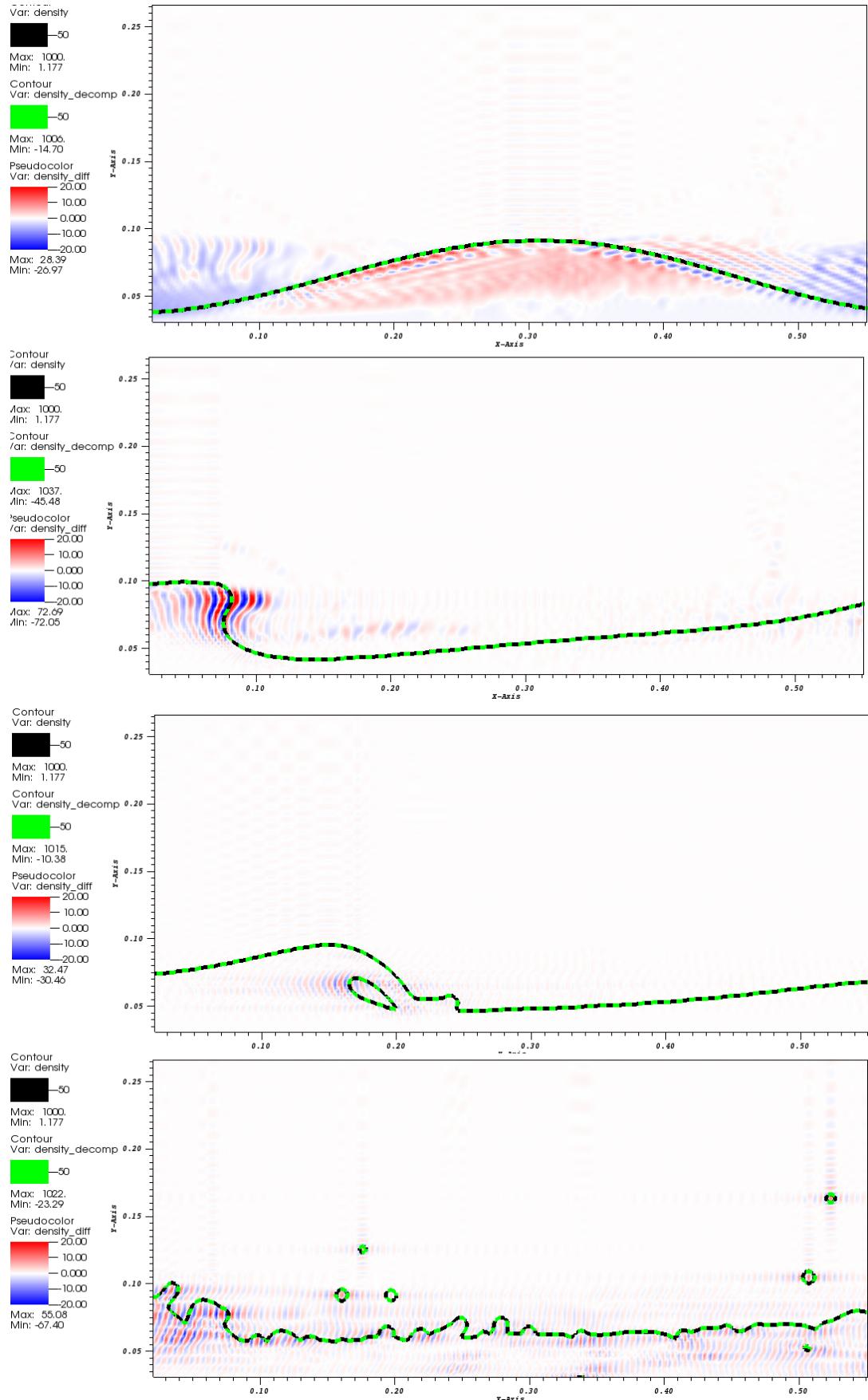


Fig. 17: Levelset 50 of the reconstructed density field at 4 time steps (same as Fig. 14) with the difference field between the original and reconstructed data.

In conclusion the low ranks approximation methods presented in this article constitute a tool that should not be overlooked in modern day scientific computing as it allows both cheaper storage (orders of magnitudes) and enables modal analysis.

## Future work

Among the many extensions of the present work, three promising items deserve further work.

First the integration of Hierachical format (HT) and decomposition will be necessary in the long run as it offers a number of interesting properties. The most prominent one being its ability to represent exactly and with very limited memory overload all other formats as well as their associated decompositions as long as adequate truncation algorithm is used (see [25,48]). It also allows one to build fully orthogonal basis (through reorthogonalization process) contrary to TT and at the same time allows very efficient maxvol/blackbox algorithms for handling large datasets (see [34,32]). HT should be thought of as very efficient method for handling cases in which  $d \gg 1$ .

This kind of sampling can be related to the way deep learning (DL) algorithms are trained. In fact there are many ways to link DL and tensor reduction, both methods can be seen as a way to produce approximation of high dimensional spaces through some training phase (optimization process). The main divide between these two approaches is that tensor reduction as presented here is always a linear process while DL is build for non-linear problems. In many cases DL relies on tensors and tensor calculus which makes it a perfect candidate to take advantage of the reduction techniques. For instance, Daulbaev et al. [52] recently proposed a Deep Neural network training methods that uses maxvol algorithm (from TT). Many others have proposed mixed formulation using both tensors and DL. Consequently a `tensorflow` API within `pydecomp` will provide a new range of application of `pydecomp`, similar to Novikov et al. work [53].

The last axis of extension of this work is to apply these techniques to PDE in more ways. This includes studying the effect of scalar product to improve convergence and select specific properties such as  $H^1$  norm for transport problems [54] but in the context of multidimensional problems. This is also intended at building multiparameter ROM (as proposed by the authors in [55]) and improving its stability.

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