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Model reduction of multi-variable distributed systems through empirical projection spaces

F. van Belzen, S. Weiland and L. Özkan

Abstract—This paper considers the problem of finding optimal projection spaces for the calculation of reduced order models for distributed systems. The method of proper orthogonal decompositions is popular in the reduction of fluid dynamics models, but may become rather cumbersome for the reduction of systems in which the total dimension of physical variables is large. This paper aims to deal with this problem and proposes the construction of projection spaces from tensor representations of observed, measured or simulated data. The method is illustrated for the reduced order modeling of a tubular reactor.

Index Terms—Model Reduction, Proper Orthogonal Decompositions, Distributed systems

I. INTRODUCTION

An important class of distributed systems models the evolution of signals that evolve both in space as well as in time. Examples of such systems can be found in virtually all engineering disciplines including fluid dynamics, aerodynamics, seismology, etc. Usually, first principle models of these systems involve coupled sets of partial differential equations that are inferred from physical conservation laws. Today, many commercial and dedicated packages exist that allow an efficient simulation of such models. However, depending on the specific application, the number of finite elements or finite volumetric elements may be substantial and easily lead to large-scale models that require the solution of up to $10^6 - 10^8$ equations at every time step.

To reduce computation time and to enable the use of model based analysis and design tools, it then becomes necessary to construct reduced order models. The need for efficient reduction techniques of various types of distributed systems has been recognized by many authors in different domains of engineering. See, for example [5], [9], [10], [11].

A popular technique for model reduction of large-scale, possibly nonlinear distributed systems is the method of proper orthogonal decompositions (POD). The method is data-based in the sense that it determines optimal projection spaces in the spatial configuration space from data. The computed projection spaces aim to capture dominant (spatial) patterns that are present in the data and subsequently uses these spaces to carry out a Galerkin type of projection on the equation residual defined by the model. See, e.g., [2], [1], [3] for an account on these methods.

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This paper proposes a novel construction of a data-based spectral expansion of a spatial-temporal measurement. The prime motivation for this work lies in the observation that the choice of a suitable inner product on the space of multi-variable signals that evolve over a spatial domain is a rather delicate matter that, often, has no or little physical relevance. Yet, the choice of inner products in proper orthogonal signal decompositions is instrumental for the quality of reduced order models and spectral approximations of signals.

In this paper we propose a tensor-based approach to the problem of finding optimal bases in the joint space of independent and dependent variables of signals. The construction is based on a singular value decomposition of a tensor and is applied to an example of a tubular reactor.

II. PROBLEM STATEMENT

Consider a signal $s : \mathbb{X} \times \mathbb{T} \rightarrow \mathbb{Y}$ defined on a spatial configuration space $\mathbb{X} \subseteq \mathbb{R}^d$ and a temporal domain $\mathbb{T} \subseteq \mathbb{R}$ and that produces values in a q dimensional vector space $\mathbb{Y} = \mathbb{R}^q$. That is,

$$s(x, t) = \begin{bmatrix} s^{(1)}(x, t) \\ \vdots \\ s^{(q)}(x, t) \end{bmatrix}, \quad x \in \mathbb{X}, t \in \mathbb{T}. \quad (1)$$

We will say that the signal is *discrete* if both the spatial and temporal domains $\mathbb{X}$ and $\mathbb{T}$ in (1) are discrete and finite sets of possibly non-uniformly distributed disjoint points $\mathbb{X} = \{x_1, \dots, x_{L_1}\}$ and $\mathbb{T} = \{t_1, \dots, t_{L_2}\}$. We consider multi-variable signals, i.e., signals for which $q > 1$. For reasons of notational consistency we will set $L_3 = q$. Generally, the signal $s(x, t)$ is viewed as a solution trajectory of an arbitrary linear distributed system described by a Partial Differential Equation (PDE).

It is the aim of this paper to derive a model reduction strategy for this type of distributed systems that overcomes issues of robustness of the reduced model, computational efficiency and sensitivity towards scaling of physical variables present in existing methods.

III. SPECTRAL DECOMPOSITIONS AND EMPIRICAL PROJECTION SPACES

As mentioned in the introduction, POD is a popular model reduction method for distributed systems. It is based on the construction of spectral expansions of signals in terms of empirical basis functions that are derived from suitable measurements or simulated data. Two different strategies to construct data-based spectral expansions for multivariable signals as in (1) exist. These are *single variable* and *lumped*

variable expansions. Both strategies will be reviewed in this section and the computation of the corresponding POD basis functions will be discussed. We end with some remarks on the performance of these techniques.

A. Spectral Expansions

In single-variable expansions each component of s is expanded individually. Specifically, for each of the components $j = 1, \dots, q$ in (1) it is assumed that, for any time instant $t \in \mathbb{T}$, the component function $s_j(\cdot, t)$ belongs to a Hilbert space $\mathcal{H}_j$ of functions mapping $\mathbb{X}$ to $\mathbb{R}$ with the usual algebraic structure of function addition and scalar multiplication and with corresponding inner product $\langle \cdot, \cdot \rangle_j$. Then, if $\varphi_{\ell_j}^{(j)} : \mathbb{X} \rightarrow \mathbb{R}$ is a (countable) orthonormal set of basis functions of $\mathcal{H}_j$, then (1) admits an expansion of the form

$$s(x, t) = \begin{bmatrix} \sum_{\ell_1} a_{\ell_1}^{(1)}(t) \varphi_{\ell_1}^{(1)}(x) \\ \vdots \\ \sum_{\ell_q} a_{\ell_q}^{(q)}(t) \varphi_{\ell_q}^{(q)}(x) \end{bmatrix}.$$

Here, the coefficients are uniquely determined by $a_{\ell_j}^{(j)}(t) = \langle s^{(j)}(\cdot, t), \varphi_{\ell_j}^{(j)} \rangle_j$.

If $r = (r_1, \dots, r_q)$ is a vector of integers then the *truncated expansion* of order r is defined by the signal $s_r(x, t)$ whose j th entry is given by the finite expansion

$$s_r^{(j)}(x, t) = \sum_{\ell_j=1}^{r_j} a_{\ell_j}^{(j)}(t) \varphi_{\ell_j}^{(j)}(x).$$

For lumped variable expansions it is assumed that for any $t \in \mathbb{T}$ the function $s(\cdot, t)$ belongs to a Hilbert space $\mathcal{H}$ of functions mapping $\mathbb{X}$ to $\mathbb{Y}$ with corresponding inner product $\langle \cdot, \cdot \rangle$. For any (countable) orthonormal set of basis functions $\varphi_\ell : \mathbb{X} \rightarrow \mathbb{Y}$, of $\mathcal{H}$ the signal s is represented as

$$s(x, t) = \sum_{\ell} a_{\ell}(t) \varphi_{\ell}(x), \quad x \in \mathbb{X}, \quad t \in \mathbb{T}.$$

Here, the time-varying coefficients are uniquely determined by $a_{\ell}(t) = \langle s(\cdot, t), \varphi_{\ell} \rangle$.

Again, for a fixed integer r , the truncated lumped expansion is given by the signal

$$s_r(x, t) := \sum_{\ell=1}^r a_{\ell}(t) \varphi_{\ell}(x)$$

and consists of the orthogonal projection of s on the span of the first r basis functions.

B. Basis Choice

The method of proper orthogonal decompositions defines the basis functions in the single variable and lumped variable expansions as follows. In either case, the basis functions depend on a measurement (1) that is assumed to be given.

Specifically, for the single variable expansion a data correlation operator $\Phi_j : \mathcal{H}_j \rightarrow \mathcal{H}_j$ is defined for each

$j = 1, \dots, q$ with respect to a given signal (1) according to

$$\langle \psi_1, \Phi_j \psi_2 \rangle := \int_{\mathbb{T}} \langle \psi_1, s^{(j)}(\cdot, t) \rangle \langle \psi_2, s^{(j)}(\cdot, t) \rangle dt$$

for $\psi_1, \psi_2 \in \mathcal{H}_j$. Then Φ_j is a well defined linear, bounded, self-adjoint and non-negative operator on $\mathcal{H}_j$. The collection $\{\varphi_{\ell}^{(j)} \mid \ell = 1, 2, \dots\}$ of ordered normalized eigenfunctions of Φ_j then defines an orthonormal basis of a subspace in $\mathcal{H}_j$. That is, let $\varphi_{\ell}^{(j)} : \mathbb{X} \rightarrow \mathbb{Y}$ be the function that satisfies $\|\varphi_{\ell}^{(j)}\| = 1$ and

$$\Phi_j \varphi_{\ell}^{(j)} = \lambda_{\ell} \varphi_{\ell}^{(j)}$$

where λ_{ℓ} is the ℓ th largest eigenvalue of Φ_j . Then $\{\varphi_{\ell}^{(j)}\}$ is a collection of orthonormal functions provided that the eigenvalues λ_{ℓ} are disjoint (for non-disjoint eigenvalues the eigenfunctions of Φ_j can be chosen to be orthonormal). This specific basis is optimal for the given data in the sense that $\int_{\mathbb{T}} \|s^{(j)}(\cdot, t) - s_r^{(j)}(\cdot, t)\|^2 dt$ is minimal for all truncation levels r_j and for all $j = 1, \dots, q$.

If $\mathbb{X}$ consists of L_1 disjoint samples, the spaces $\mathcal{H}_j$ become L_1 dimensional and Φ_j is a non-negative definite matrix of dimension $L_1 \times L_1$ defined by $\Phi_j = S_j D S_j^T$ where $[S_j]_{\ell_1, \ell_2} = s^{(j)}(x_{\ell_1}, t_{\ell_2})$ is sometimes referred to as a *snapshot matrix* and $D = D^T > 0$ is a positive definite matrix that reflects the inner product in $\mathcal{H}_j$.

Similarly, for the lumped variable expansion, a POD basis is defined by the eigen functions φ_{ℓ} of the data correlation operator $\Phi : \mathcal{H} \rightarrow \mathcal{H}$ defined by

$$\langle \psi_1, \Phi \psi_2 \rangle := \int_{\mathbb{T}} \langle \psi_1, s(\cdot, t) \rangle \langle \psi_2, s(\cdot, t) \rangle dt; \quad \psi_1, \psi_2 \in \mathcal{H}.$$

As before, this basis is optimal in the sense that $\int_{\mathbb{T}} \|s(\cdot, t) - s_r(\cdot, t)\|^2 dt$ is minimal for all truncation levels r . Under the condition that $\mathbb{X}$ consists of L_1 disjoint samples, the Hilbert space $\mathcal{H}$ becomes finite dimensional and Φ is a non-negative definite matrix of dimension $L \times L$ where $L = L_1 L_3 = L_1 q$. In this case, the computation of a POD basis is therefore algebraically equivalent to an eigenvalue decomposition problem.

C. Discussion

Both methods discussed in this section have disadvantages. Main disadvantage of the single-variable method is that relationships in vector valued physical quantities (such as velocities and forces) are decoupled. This may cause a loss of accuracy and robustness in the reduced model [12].

One of the main problems that arises with lumped-variable decompositions is that for finely meshed configuration spaces $\mathbb{X}$ (i.e., large L_1) and systems that describe relationships between many physical components (i.e., large L_3) the product $L = L_1 L_3$ may become a significant number which makes the computation of eigenvectors of Φ a difficult task. Another problem with this method is that the accuracy of the approximation s_r of s crucially depends on the choice of the inner product of $\mathcal{H}$. Especially for systems with many physical variables a proper choice of inner product is non-trivial.

IV. MULTIVARIABLE EXPANSIONS USING TENSOR DECOMPOSITIONS

A. Tensor expansions

To simplify exposition, we define tensor expansions only for discrete signals (1). Assume that the set of dependent variables $\mathbb{Y}$ is a linear and finite dimensional vector space over the real numbers and let this space be equipped with the structure of an inner product $\langle \cdot, \cdot \rangle$. We denote this space by Y . For an arbitrary triple $(x_{\ell_1}, t_{\ell_2}, y_{\ell_3}) \in \mathbb{X} \times \mathbb{T} \times \mathbb{Y}$ define

$$s_{\ell_1 \ell_2 \ell_3} := \langle s(x_{\ell_1}, t_{\ell_2}), y_{\ell_3} \rangle$$

where $1 \leq \ell_1 \leq L_1$, $1 \leq \ell_2 \leq L_2$ and $1 \leq \ell_3 \leq L_3 = q$ and where y_{ℓ_3} ranges over the standard unit vectors in $\mathbb{Y}$. Then $s_{\ell_1 \ell_2 \ell_3}$ defines a multi-way array $[[s]] \in \mathbb{R}^{L_1 \times L_2 \times L_3}$ that stores the values of s on all sample points. At a more abstract level, $[[s]]$ defines a multi-linear functional $S : X \times T \times Y \rightarrow \mathbb{R}$ on the finite dimensional vector spaces $X = \mathbb{R}^{L_1}$, $T = \mathbb{R}^{L_2}$ and $Y = \mathbb{R}^{L_3}$ defined by

$$S := \sum_{\ell_1=1}^{L_1} \sum_{\ell_2=1}^{L_2} \sum_{\ell_3=1}^{L_3} s_{\ell_1 \ell_2 \ell_3} e_{\ell_1}^{(1)} \otimes e_{\ell_2}^{(2)} \otimes e_{\ell_3}^{(3)} \quad (2)$$

Here, $\{e_{\ell_1}^{(1)}\}_{\ell_1=1}^{L_1}$, $\{e_{\ell_2}^{(2)}\}_{\ell_2=1}^{L_2}$ and $\{e_{\ell_3}^{(3)}\}_{\ell_3=1}^{L_3}$ denote the bases of standard unit vectors in X , T and Y , respectively, and $E := e_{\ell_1}^{(1)} \otimes e_{\ell_2}^{(2)} \otimes e_{\ell_3}^{(3)}$ is a so called *rank-1 tensor* defined by the product $E(x, t, y) := \langle e_{\ell_1}^{(1)}, x \rangle \langle e_{\ell_2}^{(2)}, t \rangle \langle e_{\ell_3}^{(3)}, y \rangle$ where $(x, t, y) \in X \times T \times Y$ and the inner products are taken in X , T and Y respectively. Thus, S is a linear functional in each of its three arguments but S is non-linear on the product space of its domain. Multi-linear functionals defined on the Cartesian product of N vector spaces are called *order N tensors*. Hence, S is an example of an *order-3 tensor*. Note that, by construction, $S(e_{\ell_1}^{(1)}, e_{\ell_2}^{(2)}, e_{\ell_3}^{(3)}) = s_{\ell_1 \ell_2 \ell_3}$.

A change of basis for the representation of the tensor (2) is implied by a basis change in X , T or Y and is carried out as follows. If

$$\{\varphi_{\ell_1}^{(1)}\}_{\ell_1=1}^{L_1}, \{\varphi_{\ell_2}^{(2)}\}_{\ell_2=1}^{L_2}, \{\varphi_{\ell_3}^{(3)}\}_{\ell_3=1}^{L_3} \quad (3)$$

denote arbitrary but orthonormal bases of X , T and Y , respectively, then S admits the representation

$$S = \sum_{\ell_1=1}^{L_1} \sum_{\ell_2=1}^{L_2} \sum_{\ell_3=1}^{L_3} \hat{s}_{\ell_1 \ell_2 \ell_3} \varphi_{\ell_1}^{(1)} \otimes \varphi_{\ell_2}^{(2)} \otimes \varphi_{\ell_3}^{(3)}$$

with respect to the bases (3) where $\hat{s}$ denote the elements of S with respect to the new basis, i.e. $\hat{s}_{\ell_1 \ell_2 \ell_3} = S(\varphi_{\ell_1}^{(1)}, \varphi_{\ell_2}^{(2)}, \varphi_{\ell_3}^{(3)})$. A rank $r = (r_1, r_2, r_3)$ -truncation of S with respect to the basis (3) is the tensor

$$S_r = \sum_{\ell_1=1}^{r_1} \sum_{\ell_2=1}^{r_2} \sum_{\ell_3=1}^{r_3} \hat{s}_{\ell_1 \ell_2 \ell_3} \varphi_{\ell_1}^{(1)} \otimes \varphi_{\ell_2}^{(2)} \otimes \varphi_{\ell_3}^{(3)}. \quad (4)$$

Hence, S_r is the restriction of S to the Cartesian product of the first (r_1, r_2, r_3) basis elements of X , T and Y .

Given basis functions (3) for X , T and Y , a spectral expansion of the original signal s can be defined as follows

$$s(x_i, t_j) = \sum_{\ell_1=1}^{L_1} \sum_{\ell_2=1}^{L_2} \sum_{\ell_3=1}^{L_3} \hat{s}_{\ell_1 \ell_2 \ell_3} \begin{bmatrix} \langle \varphi_{\ell_3}^{(3)}, e_1^{(3)} \rangle \\ \vdots \\ \langle \varphi_{\ell_3}^{(3)}, e_q^{(3)} \rangle \end{bmatrix} \begin{bmatrix} \langle \varphi_{\ell_1}^{(1)}, e_i^{(1)} \rangle \langle \varphi_{\ell_2}^{(2)}, e_j^{(2)} \rangle \end{bmatrix}$$

Now define

$$\begin{bmatrix} b_{\ell_1}^{(1)}(t_j) \\ \vdots \\ b_{\ell_1}^{(q)}(t_j) \end{bmatrix} = \sum_{\ell_2=1}^{L_2} \sum_{\ell_3=1}^{L_3} \hat{s}_{\ell_1 \ell_2 \ell_3} \langle \varphi_{\ell_2}^{(2)}, e_j^{(2)} \rangle \begin{bmatrix} \langle \varphi_{\ell_3}^{(3)}, e_1^{(3)} \rangle \\ \vdots \\ \langle \varphi_{\ell_3}^{(3)}, e_q^{(3)} \rangle \end{bmatrix}$$

Then the spectral expansion of s becomes

$$s(x_i, t_j) = \sum_{\ell_1=1}^{L_1} \begin{bmatrix} b_{\ell_1}^{(1)}(t_j) \\ \vdots \\ b_{\ell_1}^{(q)}(t_j) \end{bmatrix} \langle \varphi_{\ell_1}^{(1)}, e_i^{(1)} \rangle$$

and its rank $r_1 \leq L_1$ approximation is again defined by truncation. Here $1 \leq i \leq L_1$ and $1 \leq j \leq L_2$.

B. Tensor basis choice

We propose the construction of suitable bases for X , T and Y in such a manner that a coordinate change of the tensor S with respect to this bases achieves that the truncated tensor S_r defined in (4) with $r_1 \leq L_1$, $r_2 \leq L_2$, $r_3 \leq L_3$ will minimize the error $\|S - S_r\|$ in a suitable tensor norm. Although we consider the order-3 tensor (2) in this section, the theory applies to higher order tensors as well.

A POD basis for X , T and Y can now be defined

Definition IV.1 We call the basis (3) of S optimal for a given truncation level $r = (r_1, r_2, r_3)$ if the truncation error $\|S - S_r\|$ is minimal. We refer to the bases $\{\varphi_{\ell_1}^{(1)}\}_{\ell_1=1}^{L_1}$, $\{\varphi_{\ell_2}^{(2)}\}_{\ell_2=1}^{L_2}$, $\{\varphi_{\ell_3}^{(3)}\}_{\ell_3=1}^{L_3}$ as a tensor POD basis if the relative truncation error

$$\frac{\|S - S_r\|}{\|S\|} \leq \epsilon$$

where ϵ is a user-defined error bound.

For order-2 tensors (matrices), optimal bases $\{\varphi_{\ell_1}^{(1)}\}$ and $\{\varphi_{\ell_2}^{(2)}\}$ are obtained from the left and right singular vectors in a singular value decomposition of the matrix. In that case, the truncated tensor (4) achieves a minimal error for any truncation level r when $\|S - S_r\|$ is measured in either the induced norm or the Frobenius norm. For higher-order tensors, the computation of orthonormal bases such that the approximation error $\|S - S_r\|$ is minimal is not straightforward. Different methods exist, including the Higher-Order Singular Value Decomposition (HOSVD) [13] and the Tensor SVD [14].

The HOSVD is a well-known method in signal processing. It gives an extension of the matrix SVD by considering all possible unfoldings of tensors. For an order- N tensor, the idea is to replace the multilinear structure of the tensor by N unfoldings, each of which defines a bilinear structure (a matrix). An SVD is computed for each unfolding which defines the HOSVD basis. See [13] for more details.

The Tensor SVD has been advocated in [14] and is an alternative method for constructing a singular value decomposition for tensors. The first singular value can be defined as follows. Let

$$\mathcal{S}_1 := \{(x, t, y) \in X \times T \times Y \mid \|x\| = \|t\| = \|y\| = 1\}.$$

be the Cartesian product of unit vectors in X , T and Y and define

$$\sigma_1(S) = \sup_{(x,t,y) \in \mathcal{S}_1} |S(x, t, y)|. \quad (5)$$

We call (5) the first level singular vectors of the tensor S . Since $\mathcal{S}_1$ is compact, an extremal solution of (5) exists and is attained by a triple $(\varphi_1^{(1)}, \varphi_1^{(2)}, \varphi_1^{(3)}) \in \mathcal{S}_1$.

The following theorem shows that the first singular value and singular vectors can be used to find the optimal rank-one approximant to the tensor in Frobenius norm. The proof can be found in [7].

Theorem IV.2 The tensor $S_1^* := \sigma_1(S) \varphi_1^{(1)} \otimes \varphi_1^{(2)} \otimes \varphi_1^{(3)}$ is the optimal rank-1 approximation of S in the sense that $\|S - S_1^*\|$ is minimal among all rank 1 approximations of S . Here $\|S\|^2 := \sum s_{\ell_1, \dots, \ell_3}^2$ is the Frobenius norm.

Theorem IV.2 is particularly useful to define an algorithm of successive rank-1 approximations of a given tensor $S \in \mathcal{T}_N$. Indeed, for given $S \in \mathcal{T}_N$, let $S_1^* := S_{(1, \dots, 1)}^*$ denote the optimal rank-1 tensor as defined in Theorem IV.2. The error $E_1 := S - S_1^*$ then belongs to $\mathcal{T}_N$ and is minimal in Frobenius norm when ranging over tensors $S - S_1$ with $S_1 \in \mathcal{T}_N$ of rank-1. For successive values of $k > 1$, apply Theorem IV.2, to the error tensor E_{k-1} to define S_k^* as the optimal rank-1 tensor that minimizes the criterion $\|E_{k-1} - S_k\|$ over all rank-1 tensors $S_k \in \mathcal{T}_N$. Then set $E_k := E_{k-1} - S_k^*$.

Definition IV.3 Given $S \in \mathcal{T}_N$, the k th order successive rank-1 approximation of S is the tensor

$$S^{(k)} := S_1^* + \dots + S_k^* \quad (6)$$

where $S_1^*, \dots, S_k^*$ are optimal rank-1 approximations of S , $E_1, \dots, E_{k-1}$, respectively, as defined in the previous paragraph.

This construction causes approximations that are strictly improving with the order k :

Theorem IV.4 If $S^{(k)}$ denotes the k th order successive rank-1 approximation of a tensor S then

$$\|S - S^{(k+1)}\| \leq \|S - S^{(k)}\|$$

for all k .

Proof: The Frobenius norm of the error $E_k = T - T^{(k)}$ satisfies the recursion $\|E_k\|_F^2 = \|E_{k-1}\|_F^2 - \sigma_1^2(E_{k-1})$ with $\|E_1\|_F^2 = \|T\|_F^2 - \sigma_1^2(T)$. In particular so that the norm of successive errors is non-increasing. ■

We refer to [6], [4], [8] for more details on the Tensor SVD and the computation of Successive Rank One approximations.

Using either the HOSVD or successive rank-one approximations, a tensor POD basis can be computed from a data set. The computational efficiency is determined by L_1 , L_2 and L_3 and not by products, as with the lumped-variable method. Furthermore, the selection of inner product for the dependent variables is now independent from the selection of an inner product for the dependent variables, this will make the method less sensitive to the scaling of individual physical variables. Finally, the spectral expansion used does not separate dependent variables, as in the single-variable expansion case. This will ensure that the coupling between physical variables is kept intact. Figure 1 shows how the three different methods that have been discussed so far deal with a finite-dimensional collection of snapshot data.

Fig. 1. Overview of different approaches, t denotes time and x denotes position. For single-variable POD a matrix SVD is computed for each dependent variable separately, for lumped-variable POD one SVD of a large snapshot matrix is computed and for the tensor approach one decomposition of an order 3 tensor is computed.

V. APPLICATION FOR A TUBULAR REACTOR

We consider an application of the tensor decomposition in the reduced order modeling of a non-isothermal tubular reactor, where a first order irreversible exothermic reaction takes place [15]. The reactor is illustrated in Figure 2 and involves three jacket temperature controllers along the tube.

A. The model

The jacket temperatures T_{j1} , T_{j2} and T_{j3} are considered to be three independent inputs that serve as control variables. At the inlet side of the reactor, the temperature and concentration of the reactant are two additional inputs. The mathematical model of the reactor describes the evolution of the state vector $s(z, t) = \text{col}(T(z, t), C(z, t))$, i.e. the (normalized) temperature $T(z, t)$ and the (normalized)

Fig. 2. Tubular reactor

P_{eh}	P_{em}	L_e	D_a	γ	ν	μ
5	5	1.0	0.875	15	0.84	13.0

TABLE I
PHYSICAL PARAMETERS

concentration $C(z, t)$ of the reactant at an arbitrary location $z \in [0, 1]$ of the reactor and at arbitrary time instants $t \geq 0$. The model is given by the partial differential equations

$$\begin{aligned} \frac{\partial T}{\partial t} &= \frac{1}{P_{eh}} \frac{\partial^2 T}{\partial z^2} - \frac{1}{L_e} \frac{\partial T}{\partial z} + \nu C e^{\gamma(1-\frac{1}{T})} + \mu(T_{wall} - T) \\ \frac{\partial C}{\partial t} &= \frac{1}{P_{em}} \frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z} - D_a C e^{\gamma(1-\frac{1}{T})} \end{aligned}$$

subject to the boundary conditions

$$\text{at } z = 0 : \begin{cases} \frac{\partial T}{\partial z} = P_{eh}(T - T_i) \\ \frac{\partial C}{\partial z} = P_{em}(C - C_i) \end{cases} \quad \text{at } z = 1 : \begin{cases} \frac{\partial T}{\partial z} = 0 \\ \frac{\partial C}{\partial z} = 0 \end{cases}$$

Here, the wall temperature T_{wall} is given by

$$T_{wall}(z, t) = \begin{cases} T_{j1}(t) & \text{if } 0 \leq z \leq 1/3 \\ T_{j2}(t) & \text{if } 1/3 \leq z \leq 2/3 \\ T_{j3}(t) & \text{if } 2/3 \leq z \leq 1 \end{cases}$$

. The physical parameters of the model are given in Table I.

B. The data

A steady state operating condition has been determined for the model by carrying out an optimization on the three jacket temperatures $u(t) = \text{col}(T_{j1}(t), T_{j2}(t), T_{j3}(t))$ under the assumption that the temperature and concentration inlets are given by the normalized values of the disturbances $d(t) = \text{col}(T_i(t), C_i(t)) = \text{col}(1, 1)$ for $t \geq 0$. The optimization has been performed by minimizing a criterion function that expresses a trade-off between a minimal energy consumption in the reactor and a maximal production (i.e., a minimum of reactant concentration) under the constraint that the temperature in the reactor does not exceed a certain upper limit [16]. This resulted in optimal steady state jacket temperatures $u^* = \text{col}(0.9970, 1.0475, 1.0353)$ and corresponding steady state temperature and concentration profiles $(T^*(z), C^*(z))$ as shown in Figure 3. This optimal steady state operating condition turns out to be asymptotically stable. However with a very small region of attraction. Indeed, a 3% perturbation on the steady state inlet temperature or inlet concentration of the reactant brings the state $s(z, t)$ of the reactor in a periodic limit-cycle.

Fig. 3. Steady state profiles for temperature and concentration

Fig. 4. Time-evolution of temperature and concentration from snapshot data at point $z = 0.5$ (left), inlet temperature and concentration used for reduced model validation (right).

For this, the spatial configuration of the reactor has been discretized on a uniform spatial grid of 100 points and we applied the method of lines to approximate solutions of the distributed model by a discrete iteration of the sampled state vector $\hat{s}(t) := \text{col}(T(z_1, t), \dots, T(z_{100}, t), C(z_1, t), \dots, C(z_{100}, t))$ with the steady state profile as initial condition and with the perturbed inputs $T_{j1}(t) = T_{j2}(t) = T_{j3}(t) = 1$ and

$$T_i(t) = \begin{cases} 1 & \text{if } t < 5 \\ 1.038 & \text{if } t \geq 5 \end{cases}, \quad C_i(t) = 1$$

State data $s(z, t)$ has been collected on the discretized spatial samples z_i and at 5000 equidistant time samples in the interval $0 \leq t \leq 20$. The evolution over time of temperature and concentration at point $z = 0.5$ can be seen in Fig. 4 (left).

C. Reduced order model performance

To assess the performance of the reduced order models, a data set is generated as described in Sec. V-B, except for the inlet temperature and inlet concentration, which are disturbed as follows

$$\begin{aligned} T_i(t) &= \begin{cases} 1 & \text{if } t < 4, t > 18 \\ 1 + 0.04e^{0.045(t-4)} \sin(2(t-4)) & \text{if } 4 \leq t \leq 18 \\ + 0.01 \sin(5(t-4)) & \end{cases} \\ C_i(t) &= \begin{cases} 1 & \text{if } t < 4 \\ 1 + 0.015 \sin(5t) + 0.02 \sin(t) & \text{if } 4 \leq t \leq 18 \\ 1.02 & \text{if } t > 18 \end{cases} \end{aligned}$$

Figure 4 (right) shows these inlet trajectories.

We will compare the performance of the single-variable, lumped-variable and tensor approaches, where in the tensor approach basis functions are generated using both the Higher Order Singular Value Decomposition (HOSVD) [13] and

Fig. 5. Time evolution of temperature of single-variable reduced model (left) and lumped-variable reduced model (right).

Fig. 6. Time evolution of temperature of tensor-based reduced model with basis functions computed using HOSVD (left) and tensor-based reduced model with basis functions computed using successive rank-one approximations (right).

Successive Rank One approximations. The orders of the reduced models are chosen to be comparable. For the single-variable approach the order is chosen to be (4, 4), the lumped-variable reduced order model has order 8, and both tensor-based reduced order models have order (4, 4).

Figures 5 and 6 show the time evolution of temperature at point $z = 0.5$ for the four different reduced models. The time evolution of concentration shows similar behavior for each of the reduced models. The performance of the single-variable reduced model is inferior to the performance of the other models, see also Table II. This table gives the relative error of the total signal $s(z, t)$ in Frobenius norm and the worst-case errors of temperature and concentration. The table shows that the performance of the three remaining reduced models is comparable.

TABLE II
REDUCED MODEL SIMULATION ERROR RESULTS

Method	$\frac{\ W - \hat{W}\ _F}{\ W\ _F}$	$\ T - \hat{T}\ _\infty$	$\ C - \hat{C}\ _\infty$
Single	0.142	0.43	0.74
Lumped	0.024	0.17	0.19
Tensor - HOSVD	0.027	0.30	0.11
Tensor - Succ. RI	0.029	0.32	0.12

VI. CONCLUSIONS AND FUTURE WORK

This paper considered the construction of reduced order models for multi-variable distributed systems. We have intro-

duced a new method for the construction of projection spaces from measurement or simulation data of these processes. These projection spaces exploit the multi-linear nature of the snapshot data and are used in the POD framework to obtain reduced order models. For applications of high dimensionality or models that involve many physical variables, the computation of these projection spaces is much more efficient than the computation of projection spaces in existing methods. Furthermore, the proposed approach allows inner products for dependent and independent variables to be chosen independently. The tensor-based method has been applied to a tubular reactor model and compared to single-variable and lumped-variable techniques for obtaining reduced order models.

The simulation results support earlier findings in that the lumped-variable spectral expansions perform better than single-variable expansions. For this example, the performance of the tensor-based approach introduced in this paper is comparable to the performance of the lumped-variable approach. This makes the tensor approach an interesting alternative in applications with high dimensionality or with a large number of physical variables.

In the near future, we plan to test the tensor approach on more complex examples and compare different methods for computing tensor decompositions to assess accuracy, computational effort and reliability.

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