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Model Reduction of Systems with Traveling Waves using Projection methods ⋆

K.M. Nauta * **S. Weiland** ** **A.C.P.M. Backx** **

* *Eindhoven University of Technology, Eindhoven, The Netherlands, (e-mail: k.m.nauta@tue.nl).*
** *Eindhoven University of Technology, Eindhoven, The Netherlands*

Abstract: Proper Orthogonal Decomposition (POD) based projection methods are an important tool for the reduction of complex nonlinear models. Large reductions in model order can be frequently be obtained due to the exploitation of correlations between model states that exist for representative behavior of the model. However, when this model behavior includes traveling waves or shock fronts these methods perform less well as a large number of modes is required to capture this type of behavior. This paper investigates the use of correlation to pre-process simulation data such that bi-orthogonal projection can subsequently be applied to obtain a reduced model that is of low order.

1. INTRODUCTION

Medium and large-order dynamical systems are often inferred from discretization of spatially distributed physical phenomena. Such physical phenomena might exhibit various forms of spatial symmetry. In this paper we consider the application of a Proper Orthogonal Decomposition (POD) type method to reduce the order of models of systems with translation symmetry. In its standard form, the POD method uses simulation data of the system in the form of a collection of snapshots of the system state at each time instant to build an empirical covariance matrix. From this covariance matrix the empirical eigenmodes of the system are identified. The model equations are then projected on these eigenmodes to obtain the reduced system. However, this method performs poorly for simulation data that contains traveling waves or fronts. To remedy this, the simulation data is first aligned by applying spatial translation to the state at each time instance. This puts the data into the frame of reference of the traveling wave. The aligned simulation data is subsequently used to find the dominant modes of the wave profile.

Translation of data as a preprocessing step to POD was introduced by Kirby and Armbruster (1992) using a template fitting procedure. It was applied to periodic systems in Glavaski et al. (1998), Shah and Sorensen (2005). In the current paper the template fitting procedure is used to deal with non-periodic systems, which requires the use of extrapolation techniques. Furthermore, the wave profile is not considered to be known a-priori. The projection and reconstruction relations are chosen such that resulting projection is bi-orthogonal.

This paper is organized as follows: After introducing translational symmetry relations, the application of the standard POD method to these types of systems is used to motivate the approach whereby the basisfunctions are translated in the spatial domain. The main part of the paper is devoted to the alignment of non-periodic data on a bounded domain as a pre-processing step to POD. The followed approach is illustrated using an example based on a fixed-bed reactor.

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2. SYSTEMS WITH TRANSLATIONAL SYMMETRY

For systems with behavior that include traveling waves or shock fronts, the dynamics conform either exactly or approximately to a translation symmetry relation between temporal and spatial coordinates. To formulate this relation, we consider one dimensional phenomena in this paper. Consider signals that act on an infinite one dimensional spatial domain $\mathbb{X} = \mathbb{R}$ and let $\mathcal{Y}$ be a Hilbert space of functions defined on $\mathbb{X}$. We denote the corresponding inner product and norm in $\mathcal{Y}$ by $\langle \cdot, \cdot \rangle$ and $\|\cdot\|$, respectively. Correlation $\langle p, q \rangle / (\|p\| \|q\|)$ is denoted by $corr(p, q)$. Let $\mathcal{U}$ be a class of input signals $u : \mathbb{R}_+ \to \mathbb{R}^{n_u}$ and let $f : \mathcal{Y} \times \mathcal{U} \to \mathcal{Y}$ be a Lipschitz continuous function. We consider the system

$$\frac{\partial y}{\partial t} = f(y, u), \tag{1}$$

where $y(t) \in \mathcal{Y}$ and $u \in \mathcal{U}$. We write $y(t, x)$ for the evaluation of y at time t and location $x \in \mathbb{X}$. We will say that the system (1) admits a translational symmetry if there exists a continuous function $w : \mathbb{R} \to \mathbb{X}$ such that

$$y(t, x) = y(0, x - w(t)) \tag{2}$$

for all $x \in \mathbb{X}$, $t, \delta \in \mathbb{R}_+$. We call w the wave displacement function. Inserting (2) into (1) and using the existence of $w(t)$, (1) can be rewritten as

$$f(y, u) = -\frac{\partial y}{\partial x}\dot{w} = -\frac{\partial y}{\partial x} g(w, u), \tag{3}$$

with the function $g : \mathbb{R} \times \mathbb{R}^{n_u} \to \mathbb{R}$. Integrating (3) over x the first order system

$$\dot{w} = g(w, u) \tag{4a}$$

$$y(t, x) = y(0, x - w(t)) \tag{4b}$$

is obtained that exactly captures the dynamics of (1). In many cases the symmetry relation (2) only holds

approximately, as waves and fronts change shape while traveling. For us, this means that shifted time solutions are highly correlated. This is quantified by

$$corr(y(t,x), y(t+\delta, x - w(t+\delta))) > 1 - \epsilon \qquad (5)$$

for some δ and $0 < \epsilon << 1$. The reduction to a one dimensional system for the case when the exact relation (2) holds indicates that the potential for approximation by reduced order models for systems where (5) holds is large.

3. MODEL REDUCTION USING POD

In its standard form, the POD method uses a Galerkin projection to arrive at the reduced order system. First, the more general Petrov-Galerkin projection for systems of type (1) will be formulated. Suppose that $\{\phi^{(i)}\}_{i\in\mathbb{Z}_+}$ is a complete basis of $\mathcal{Y}$. Let $\{\psi^{(i)}\}_{i\in\mathbb{Z}_+}$ be a basis for the corresponding dual space $\mathcal{Y}^*$ and let $(\cdot,\cdot) : \mathcal{Y} \times \mathcal{Y}^* \to \mathbb{R}$ denote the inner product of the Hilbert space with its dual. Hence, for every $y \in \mathcal{Y}$ we have

$$y = \sum_{i\in\mathbb{Z}_+} a_i \phi^{(i)} \quad \text{where} \quad a_i = (y, \psi^{(i)}) \qquad (6)$$

In particular $(\phi^{(i)}, \psi^{(j)}) = \delta_{ij}, \forall i, j \in \mathbb{Z}_+$. Given a pair of dual bases $\{\phi^{(i)}\}$, $\{\psi^{(i)}\}$ we consider the m-th order approximation

$$\hat{y}_m = \sum_{i=1}^{m} a_i \phi^{(i)} \qquad (7)$$

for any $y \in \mathcal{Y}$. In particular, for y satisfying (1) we get

$$\hat{y}_m(t) = \sum_{i=1}^{m} a_i(t) \phi^{(i)}(x) \qquad (8)$$

where the coefficients a_i are obtained from a Petrov-Galerkin projection of (1) in the sense that

$$\dot{a}_j(t) = (f(\sum_{i=1}^{m} a_i(t)\phi^{(i)}(x), u), \psi^{(j)}) \qquad (9)$$

where $j = 1, \ldots, m$. Using the definitions

$$\Phi := [\phi^{(1)}, .., \phi^{(m)}], \quad \Psi := [\psi^{(1)}, .., \psi^{(m)}]$$

and letting $\circ$ be defined such that $\Phi \circ a$ refers to (8) and $\Psi \circ f$ refers (20), the reduced order model can be written in more compact notation:

$$\dot{a}(t) = \Psi \circ f(\Phi \circ a, u) = \hat{f}(a, u) \qquad (10a)$$

$$\hat{y}_m(t) = \Phi \circ a \qquad (10b)$$

The POD method uses sampled solution trajectories of finite dimension $\mathcal{Y}_s \subset \mathcal{Y}$ of the original system to determine an orthogonal basis (i.e. $\psi^{(i)} = \phi^{(i)}$ that leads to an accurate approximation of (1) by (10) for these trajectories. Suppose that p observations $\{y^{(1)}, \ldots, y^{(p)}\}$ with $y^{(i)} \in \mathcal{Y}$ are available. These are often referred to as snapshots of the signal. We call an orthonormal basis $\{\phi^{(i)}\}$ a POD basis of $\mathcal{Y}$ (w.r.t this data) if the error

$$\gamma = \sum_{i=1}^{p} \|y^{(i)} - \hat{y}_m^{(i)}\| \qquad (11)$$

is minimal for any truncation level m. We consider a finite number of time observations

$$y^{(t_1)}, \ldots, y^{(t_p)} \qquad (12)$$

as data. It can be shown, e.g. Holmes et al. (1996), that the POD basis is derived from the solutions of the eigenvalue problem

$$R\phi^{(i)} = \lambda_i \phi^{(i)} \qquad (13)$$

where $R : \mathcal{Y} \to \mathcal{Y}$ is obtained from autocorrelation of the observations

$$\langle \zeta_1, R\zeta_2 \rangle = \sum_{j=1}^{p} \sum_{i=1}^{p} \langle \zeta_1, y^{(t_i)} \rangle \langle \zeta_2, y^{(t_j)} \rangle \qquad (14)$$

Each $\phi^{(i)} \in \mathcal{Y}$ is referred to as a *POD mode*.

In practice, for any Galerkin-type projection method, first solutions are obtained for a high-order but finite dimensional system. This system is obtained by discretizing $\mathcal{Y}$ into a finite (but huge) dimensional vector space $\mathcal{Y}_b \subset \mathcal{Y}$ using for example the method of lines at n spatial points. In this case the operators $(\Psi : \mathbb{R}^n \to \mathbb{R}^m, \Phi : \mathbb{R}^m \to \mathbb{R}^n)$ become matrices, the inner product is the Euclidian product and $\circ$ is now matrix multiplication.

When the POD method as outlined above is applied to systems with translational symmetry, the result is a harmonic decomposition, see Kirby and Armbruster (1992). In this case, the number of modes required to approximate y is generally large. To illustrate this, the POD method as outlined above is applied to a example system with translational symmetry. Consider, for example, a system that represents a traveling unit pulse that exhibits the following response:

$$y(x,t) = 1(x - t) \qquad (15)$$

where $1(\cdot) : \mathcal{Y} \to \mathcal{Y}$ is a function that is defined as

$$1(x) = \begin{cases} 1 \text{ for } x = 0 \\ 0 \text{ for } x \neq 0 \end{cases}$$

If the vector y is sampled at n uniform temporal $(t_i = 0, .., n)$ and spatial $(x_i = 0, .., n)$ intervals, the snapshot matrix is simply:

$$T_{snap} = I_n \qquad (16)$$

The eigenspectrum of the identity matrix is flat. Therefore the POD method will perform poorly as a large reduced model order m is required to attain a desired accuracy $(\gamma = n - m)$. This poor performance is not limited to the example system but occurs whenever dynamics which conform to translational symmetry are dominant in the model response. To improve the performance, adaptation of the POD method is required.

4. PROJECTION FOR SYSTEMS WITH SYMMETRY

To take advantage of the translational symmetry relation an alternative parameterization of the state vector was proposed , see Kirby and Armbruster (1992). Define $\phi_{w_i}^{(i)}(x) := \phi^{(i)}(x - w_i)$ and let y be parameterized by the functions $\{\phi^{(i)}\}$ and the coefficients a_i, w_i as

$$y(t,x) = \sum_{i\in\mathbb{Z}_+} a_i(t) \phi_{w_i}^{(i)}(x) \qquad (17)$$

Inserting this parameterizations into the original system equation (1)

$$\sum_{i\in\mathbb{Z}_+} \dot{a}_i(t)\phi_{w_i}^{(i)}(x) - \dot{w}_i(t)a_i(t)\frac{\partial\phi_{w_i}^{(i)}}{\partial x}(x) = f(\sum_{i\in\mathbb{Z}_+} a_i(t)\phi_{w_i}^{(i)}(x), u) \quad (18)$$

is obtained. Now let $m \in \mathbb{Z}_+$ be a finite integer. We introduce the following assumption:

Assumption 1. Let the functions $\phi^{(i)}$ and a_i, w_i for $i = 1, .., m$ be such that the functions in the set

$$\{\phi_{w_i}^{(i)}(t), -\frac{\partial\phi_{w_i}^{(i)}}{\partial x}(t)a_i(t)\}_{i\in 1,\ldots,m} \quad (19)$$

are linearly independent.

If this assumption holds, the functions in (19) form a basis for the space $\mathcal{V} \subset \mathcal{Y}$. The associated dual basis is given for the space $\mathcal{V}^*$ by $\{\psi^{(i)}\}_{i\in 1,..,2m}$. Projecting onto the dual space $\mathcal{V}^*$, the time derivatives of the coefficients and phases can be obtained from

$$\dot{a}_j(t) = (f(\sum_{i=1}^{m} a_i(t)\phi_{w_i}^{(i)}(x), u), \psi^{(j)}) \quad (20)$$

$$\dot{w}_j(t) = (f(\sum_{i=1}^{m} a_i(t)\phi_{w_i}^{(i)}(x), u), \psi^{(j+m)}) \quad (21)$$

for $j = 1, .., m$. Defining

$$\Phi_w := [\phi_{w_1}^{(1)}, .., \phi_{w_m}^{(m)}] \qquad \Psi_w := [\psi^{(1)}, .., \psi^{(m)}]$$
$$a := col(\{a_i\}_{i\in 1,..,m}) \qquad w := col(\{w_i\}_{i\in 1,..,m})$$

the reduced model is now given by

$$\begin{pmatrix}\dot{a}\\ \dot{w}\end{pmatrix} = \Psi_w \circ f(\Phi_w \circ a, u) = \hat{f}(a, w, u) \quad (22)$$

If a single phase is present (i.e. $w_i = w \in \mathbb{R}, \forall i \in \mathbb{Z}_+$), this can be simplified significantly for unbounded domains or periodic functions by putting the system (1) into the frame of reference of the traveling wave and using orthogonal projection Glavaski et al. (1998).

We now consider the case of the bounded spatial domain $\mathbb{X} = \mathbb{X}_b : x \in [x_{min}^b, .., x_{max}^b]$ with the associated Hilbert space $\mathcal{Y}_b$. Define the domain $\mathbb{X}_w : x \in [x_{min}^w, .., x_{max}^w]$ with the Hilbert space $\mathcal{Y}_w$ such that it encompasses $\mathbb{X}_b$, i.e. $\mathbb{X}_b \subset \mathbb{X}_w$. Let the functions $\{\phi^{(i)}\}$ form a basis for $\mathcal{Y}_w$ and let the functions $\{\phi_{b,w}^{(i)}\}$ be defined as

$$\phi_{b,w_i}^{(i)}(x) := \phi^{(i)}(x - w_i) \quad \text{for all} \quad \{x, w_i | x \in \mathbb{X}_b, x - w_i \in \mathbb{X}_w\} \quad (23)$$

Assumption 2. We assume that for within a certain time interval $t_0 \le t \le t_1$ it holds that

$$x_{min}^b - x_{min}^w \le w_i(t) \le x_{max}^w - x_{max}^b \quad \text{for all} \quad i = 1, .., m$$

Under this assumption, the function $\phi_{b,w}^{(i)}(x)$ is now defined everywhere on its domain. Using the inner product $(\cdot,\cdot)_{\mathbb{X}_b}$, we can now directly apply the method proposed in this Section on the bounded domain $\mathbb{X}_b$ for the time period $t_0 \le t \le t_1$.

5. SNAPSHOT ALIGNMENT

For this point on we assume that a single phase or wave is present. To identify the dominant modes of the wave profile from data, this data is first put into a frame of reference which negates the displacement from the single phase, so that the coherent structures of the wave can be identified. For a set of samples $\{y^{(1)}, \ldots, y^{(p)}\}$ this amounts to finding a set of offsets $\{w^{(1)}, \ldots, w^{(p-1)}\}$. The aligned samples can then be reconstructed by

$$y_w^{(i)}(x) = y^{(i)}(x - w^{(i)}) \quad (24)$$

Centering, Glavaski et al. (1998), and template fitting, Kirby and Armbruster (1992), are two methods to accomplish this, with and without prior knowledge of the dominant waveform, respectively. In the template fitting approach a wave template y_0 is translated to match each sample.

$$\hat{w}^{(i)} = \arg\max_w \langle y_0(x - w), y^{(i)}(x)\rangle \quad (25)$$

In practice the simulation data $y^{(i)}$ is obtained for the bounded domain $\mathbb{X}_b$. We propose an approach similar to template fitting, with the template being determined from data. First the intersample wave displacement is estimated on the bounded domain as

$$\hat{w}^{(i,j)} = \arg\max_w corr(y^{(i)}(x - w), y^{(j)}(x))_{\mathbb{X}_b} \quad (26)$$

Repeating this procedure for each pair of snapshots in the snapshot matrix a distance matrix $\hat{W}_{ij}$ can be estimated.

$$\hat{W}_{ij} = \begin{pmatrix} 0 & \hat{w}^{(1,2)} & \hat{w}^{(1,3)} & .. & \hat{w}^{(1,n)} \\ \hat{w}^{(2,1)} & 0 & \hat{w}^{(2,3)} & .. & \hat{w}^{(2,n)} \\ .. & .. & .. & .. & .. \\ \hat{w}^{(n,1)} & \hat{w}^{(n,2)} & .. & \hat{w}^{(n,n-1)} & 0 \end{pmatrix} \quad (27)$$

As w is a measure for the offset, for any triple i, j, k with $j > k > i$ it holds that

$$w^{(i,j)} = w^{(i,k)} + w^{(k,j)} \quad (28)$$

From these constraints and the estimates in the distance matrix (27) a vector $\hat{w}_a$ can be estimated that updates the estimates $\hat{w}^{(i,i+1)}$ for $i \in 1, \ldots, p-1$ to conform to (28). This can be accomplished by solving an over-determined linear equation system in the least square sense,

$$min_{\hat{w}_a} \|A\hat{w}_a - b\|_2, \quad (29)$$

where b contains the off-diagonal elements of the distance matrix (27) stacked in a single vector and the matrix A is determined from the distance constraints (28). The offsets $\{w^{(1)}, \ldots, w^{(p-1)}\}$ can be obtained from $\hat{w}_a$ as

$$\hat{w}(i) = \sum_{j=1}^{i} w_{a,j} \quad (30)$$

Using this set of offsets, the series of translated snapshots $\hat{y}_w^{(i)}(x)$ is determined .

To use the approach in the previous Section we have to generate a set of basisfunctions on $\mathbb{X}_w : x \in [x_{min}^w, .., x_{max}^w]$. As the data obtained on $\mathbb{X}_b$ and then translated, extrapolation is required. Furthermore, as simulation data is sampled at a finite number of spatial points, interpolation is also required to obtain samples of translated snapshots $y^{(i)}(x - w)$. Both these procedures will be formulated for the domain sampled at finite resolution. Let $\mathbb{X}_b$ and its bounded encompassing domain $\mathbb{X}_w$ be sampled at a finite number of equidistant points $x_1, .., x_{q_{max}}$. Using $1 \le q_1 \le q_2 \le q_{max}$ the following indexing for the samples is used:

$$x_{q_1+1},..,x_{q_2} \in \mathbb{X}_b, \mathbb{X}_w$$
$$x_1,..,x_{q_1},\ x_{q_2+1},..,x_{q_{max}} \in \mathbb{X}_w$$

On the domain $\mathbb{X}_b$ the sampled snapshot is given by

$$y^{(i)} : \{y^{(i)}(x_j)\}_{j=q_1+1,..,q_2}$$

The translation of a snapshot $y^{(i)}$ is formed on $\mathbb{X}_w$ in the following manner. Consider the following two sets of extrapolated samples:

$$\hat{y}_L^{(i)} : \{y^{(i)}(x_j)\}_{j=1,..,q_1-(w-1)}$$
$$\hat{y}_R^{(i)} : \{y^{(i)}(x_j)\}_{j=q_2-(w-1),..,q_{max}}$$

The translated snapshot $y^{(i)}(x-w)$ is obtained by padding the original snapshot $y^{(i)}$ on the left and right with $\hat{y}_L^{(i)}$ and $\hat{y}_R^{(i)}$ respectively. For displacements w that are exact multiples of the resolution the translated snapshot is given by

$$y^{(i)}(x-w) : (\hat{y}_L^{(i)}, y^{(i)}, \hat{y}_R^{(i)})$$

where $(,)$ denotes set concatenation. If w is not an exact multiple of the resolution, linear interpolation is used:

$$y^{(i)}(x-w) = (\overline{w}-w)y^{(i)}(x-\underline{w}) + (w-\underline{w})y^{(i)}(x-\overline{w})$$

where $\underline{w}, \overline{w} \in \mathbb{Z}$ represent w rounded down respectively up to the nearest integer.

To obtain $\hat{y}_L^{(i)}, \hat{y}_R^{(i)}$ by extrapolation from $y^{(i)}$ a number of methods can be used. The simplest approach is to use zero-padding. Alternatively, the samples of $\hat{y}_L^{(i)}, \hat{y}_R^{(i)}$ are obtained by replicating the nearest sample in $\mathbb{X}_b$. Thirdly, if the waveform is approximatively constant over time, the missing samples of the waveform at one time instant can be inferred from the samples of the waveform at other time instants. As is it assumed that changes in the waveform are continuous, the missing samples for a waveform are padded with the samples from the snapshot with the smallest time offset which includes the desired samples. The translation procedure that uses this type of padding for the finite domain and a finite number of samples is illustrated graphically in Figure 1. A final extrapolation method is to determine missing samples by assuming that the translated snapshot matrix is of low rank, and using an iterative method to update the missing samples such that the resulting snapshot matrix converges to a matrix of chosen (low) rank. First, the missing samples are initialized using another extrapolation method. Next, a singular value decomposition (SVD) is calculated, and a low order approximation to the snapshot matrix is formed using a small number of singular values and vectors. The values of the missing samples in the original snapshot matrix are padded from this low order approximation. In the next iteration, the singular value decomposition is applied to this updated snapshot matrix. This approach has been used to deal with missing data Troyanskaya (2001). However, this requires the determination of an SVD at each iteration. In addition poor convergence was observed.

A further issue with the finite resolution is that maximization of the correlation between a pair of snapshots (26) has to be implemented in the discrete domain. This maximization procedure can be carried out in two stages. First the pair of integer offsets $\hat{w}_1^{(i,j)}, \hat{w}_2^{(i,j)} \in \mathbb{Z}$ for which

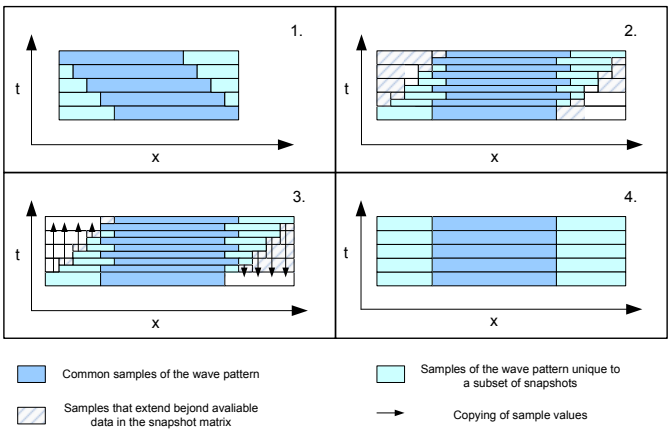


Fig. 1. Alignment of snapshots with finite resolution over a finite domain

the correlation is highest are determined by calculating the correlation over all possible integer offsets $w = 1,..,n$. To obtain a sub-sample resolution for the estimated offset $\hat{w}^{(i,j)}$, the derivatives of the correlation function are calculated at $\hat{w}_1^{(i,j)}, \hat{w}_2^{(i,j)}$. This information is used to fit a cubic spline function of which the extremal value is used to determine $\hat{w}^{(i,j)}$.

As the domain is bounded, waves or shock fronts may enter and leave the domain at certain time instant. If this occurs during the time period when the snapshots are sampled, only a subset of the snapshots might exhibit high correlation for spatial shifted solutions. A practical method to decide whether for each pair of snapshots $y^{(i)}, y^{(j)}$ wave phenomena dominate the dynamics is to employ the following criteria:

- Sufficient correlation exists for an optimal choice of w :

$$\max_w corr(y^{(i)}(x), y^{(i)}(x-w^{(i)}))_{\mathbb{X}_b} > 1-\delta_1 \quad (31)$$

- Sufficient differentiation in the correlation exists:

$$\min_w corr(y^{(i)}(x), y^{(i)}(x-w^{(i)}))_{\mathbb{X}_b} < \delta_2 \quad (32)$$

- There is a single maximum:

$$\max_{w \in \mathcal{S}} corr(y^{(i)}(x), y^{(i)}(x-w^{(i)}))_{\mathbb{X}_b} < 1-\delta_4$$
$$\text{with} \quad \mathcal{S} : (w | w < w_{max} - \delta_3 \ \wedge \ w > w_{max} + \delta_3) \quad (33)$$

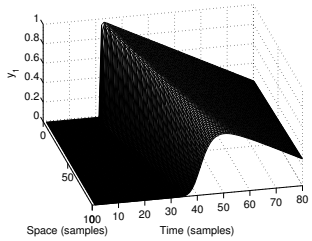
where $\delta_1,..,\delta_4$ are tuning parameters. If there is not sufficient differentiation in the correlation when varying w or the correlation is not sufficiently high for an optimal choice of w, the advantage of including basisfunctions that are translated by w is negligible and standard POD is the preferred method.

6. EXAMPLE

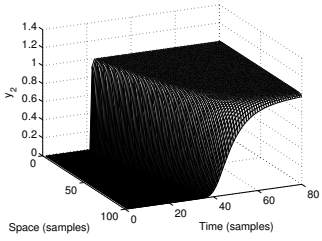
The proposed approach is illustrated using an example that is based on a reactor with a single absorbtion reaction.

$$A \xrightarrow{k} A* \quad (34)$$

With $\{y_1, y_2\} = \{[A], A*\}$ and $u = [A]_{in}$, the PDE for this example is given by



(a) Snapshot matrix for y_1



(b) Snapshot matrix for y_2

Fig. 2. Original snapshot matrices for y_1 and y_2

$$\epsilon_1 \frac{\partial y_1}{\partial t} = F\frac{\partial y_1}{\partial x} - k y_1 \max(0, 1 - y_2)$$
$$\epsilon_2 \frac{\partial y_2}{\partial t} = k y_1 \max(0, 1 - y_2)$$
$$\text{with BC} \quad y_1(0, x) = 0, \quad y_2(0, x) = 0, \quad y_1(t, 0) = u$$

The $\max(\cdot, 0)$ is used to prevent instability and divergence when approximation errors are incurred. The reaction rate is dependent on the spatial position. This situation might occur if the temperature is non-uniform throughout the reactor. The dependence of the reaction rate on the spatial position is given by

$$k(x) = k_0(1 + vx) \tag{35}$$

For $v > 0$ the rate is increasing and for $v < 0$ rate is decreasing along the reactor axis. Initially, the following values are chosen for the model parameters:

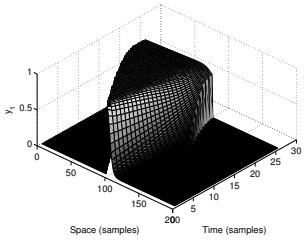
$$\epsilon_1 = 0.01, \quad \epsilon_2 = 1, \quad F = 1, \quad k_0 = 50, \quad v = -0.95$$

The inflow is given by

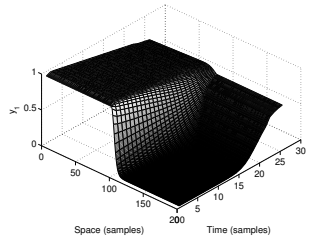
$$u = \begin{cases} 0 & \text{if } 0 < t < 1 \\ 1 - 0.5\min(2, \dfrac{1}{1.9}(t-1)) & \text{if } t \geq 1 \end{cases} \tag{36}$$

The system is simulated for the time interval $t \in [0, 4]$ and snapshots of y_1, y_2 are collected on a uniform time grid $t_s : \{0, 0.1, .., 1\}$. The snapshot matrices for y_1, y_2 are shown in Figure 2. From these snapshot matrices the snapshots that show sufficient correlation in time are selected. From the snapshots it can be observed that as the reaction constant decreases along the reactor axis, the shape of the reaction front becomes more gradual when it progresses through the reactor.

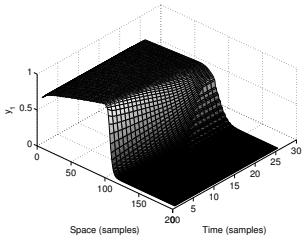
Using the alignment procedure that snapshots the show sufficient correlation are aligned. The resulting aligned snapshot matrices for four different padding methods are shown in Figure 3. It is clear that for this type of data zero-padding and, to a lesser extent, identical padding distort the wave shape. This is reflected by the singular value spectra for the matrices obtained using these padding methods, shown in Figure 4 (a) and Figure 4 (b). The ratios between the first and subsequent singular values are limited, in particular for zero-padding. If other samples are used for padding this ratio improves as shown in Figure 4 (c). Further improvement can be accomplished by iteratively adapting the padded samples from based on a low rank SVD approximation, employing for example the method proposed in Brand (2006). For this iterative procedure the snapshot matrix is shown in Figure 3 (d). The singular value spectrum, see Figure 4 (d), does indeed show an improvement between the first and subsequent singular values compared to padding from other samples.



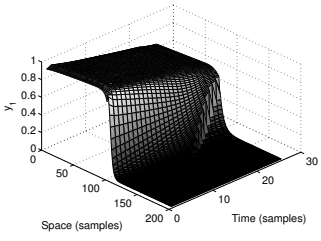
(a) Zero-padding



(b) Identical padding

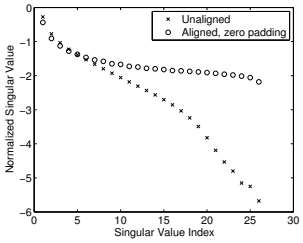


(c) Padding from other samples

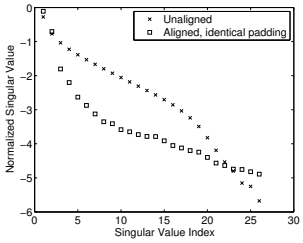


(d) Padding using SVD-iteration

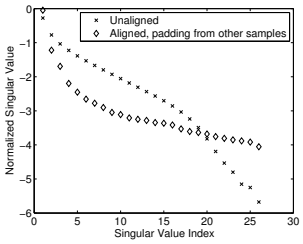
Fig. 3. Original and aligned snapshot matrices for different padding methods



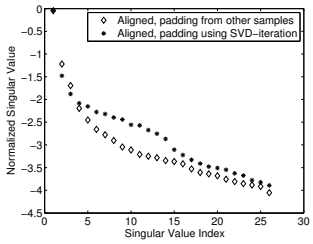
(a) Original - Zero padding.



(b) Original - Identical padding.



(c) Original - Padding from other samples.

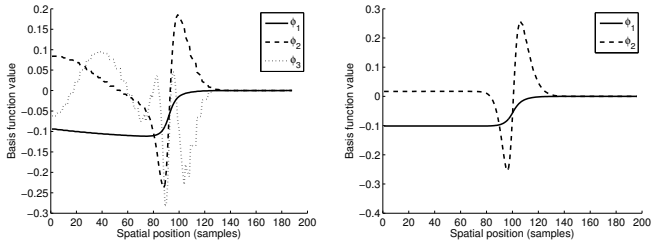


(d) Padding from other samples - Rank-1 SVD-iteration.

Fig. 4. Comparison between singular value spectra of the aligned snapshot matrices for different padding methods.

From the aligned snapshot matrix, for which the padding is done based on other time samples, a POD basis is determined. A separate basis was be determined for each component y_1, y_2. The first basisfunctions for aligned snapshot matrix are shown in 5. For y_2, the first basisfunction captures the wave shape and the second is used to change the slope of the wave. For y_1 the basisfunctions also reflect the effect of the padding.

For both the standard POD approach and the approach using the moving basis functions, simulations for the time interval $t \in [1.15, 1.9]$, in which the front travels through



(a) Basisfunctions for y_1 (b) Basisfunctions for y_2

Fig. 5. Basisfunctions obtained from the aligned snapshot matrix for y_1 and y_2.

the reactor, are shown in Figure 6. The error for the standard POD approach is more oscillatory, while the error for the approach using the moving basis functions manifests itself as an offset in amplitude and phase of the wave. A more extensive comparison between both approaches is given in Table 8. As can be expected, the approach using moving basis functions permits lower model orders with errors comparable to POD. If a high accuracy is required, this advantage diminishes. This is due the fact that errors which are incurred during the alignment procedure and the projection onto the moving basis functions become significant relative to the error that results from truncating the POD basis. These alignment and projection errors can be characterized as:

- Linear interpolation errors incurred when translating over non-integer intervals.
- The error due to the fact that the padded samples are obtained using an extrapolation of observed samples.

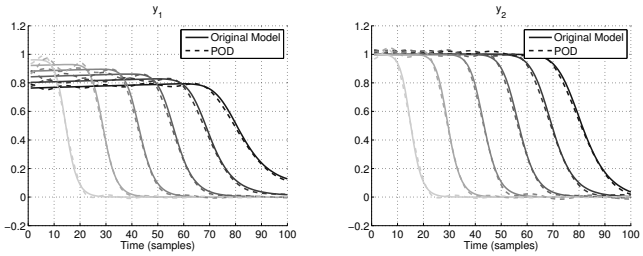
The diminishing advantage at higher accuracies is also related to the fact that for higher accuracies an increasing fraction of the basisfunctions capture the changing shape of the wave. The extent to which this is possible in terms of the number of basisfunctions required is the same as for standard POD. Therefore, at higher accuracies, the number of basisfunction required by the moving wave POD approach tends to that of the standard POD approach.

	POD		Translated POD	
Accuracy	Modes	MSE	Modes	MSE
0.95	16	2.0311	6 (4 + 2)	0.5257
0.99	26	0.4694	7 (5 + 2)	0.3300
0.999	34	0.0775	16 (13 + 3)	0.1783

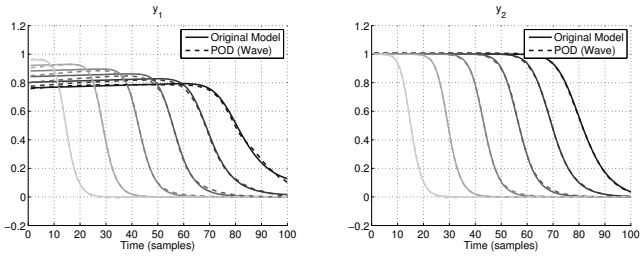
Table 8 : Comparison of standard and translated POD method.

7. CONCLUSIONS AND FURTHER WORK

The use of translating basisfunctions allows a significant reduction in the number of modes required to approximate systems of which the responses are characterized by traveling waves or shock fronts. When multiple waves are present simultaneously or when the spatial domain is finite, a dual basis is used to project the reduced domain. This dual basis requires updating during simulation. The alignment of snapshot data is required as a pre-processing step to eigenmode decomposition. On the finite domain both interpolation and extrapolation are required to perform this alignment. The extrapolation method used has a large effect on the basisfunctions that are obtained. Several choices are possible for extrapolation, and the optimal choice in general depends on the application and the a-priori knowledge that is available. When the wave shape remains relatively constant in time, in many cases the most practical choice is to extrapolate spatial samples of a snapshot based on snapshots at earlier or later time instances. The example shows that in particular for lower accuracy requirements a relatively low number of modes are needed for the approach with translating basisfunctions as opposed to standard POD. As accuracy requirements increase, this relative difference diminishes. A major disadvantage of this method is the requirement to update the dual basis during simulation.



(a) Comparison of the original model and the standard POD approximation.



(b) Comparison of the original model and the projected model with translating basisfunctions.

Fig. 6. Comparisons of the standard POD approximation (POD) to the projected model with translating basisfunctions (Wave POD).

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