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NEW EFFECTIVE BASIS SYSTEM FOR THE POD-SNAPSHOTS BASED REDUCTION MODELS

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Abstract. *The objective of this work is to improve the accuracy of the classical Proper Orthogonal Decomposition (POD) snapshots-based reduction model in the context of PDEs by coupling the POD with a new and appropriately built basis system. This will be done without contradicting the POD optimality theorem. The new basis-building criterion is discussed and mathematically expressed. This is based on the idea that the ideal scenario would be to have the snapshots already orthogonal so that the PDE solution is directly projected on the snapshots spanned space, the proposed criterion therefore aims to minimize the necessary transformation of the snapshots to turn them into orthonormal basis in a sense that will be defined. An algorithm to build such a basis is proposed. The efficiency of the proposed methods by comparison to the classical one is demonstrated on analytical solutions of steady convection equations.*

1 INTRODUCTION

Solving large-scale problems is one of the biggest challenges in computational science in general andin PDEs based problems in particular. Due to the limitation of the existing computational capacity comparing to the requirements to solve such problems and despite the huge progress in computers capability and parallel architectures, solving the original problems still unaffordable in almost complex cases. One of the most attracting methods to handle these problems is the so-called model reduction methods that reduces the original problem to a much low dimension one, which is much easy to solve. The Proper Orthogonal Decomposition [1, 2, 5, 11], know as well as Karhunen-Loeve's expansion (KLE) [6], is one of the methods that received a lot of attention due to its success in solving many problems in a wide range of fields. The principle of the technique is to represent a parametric family of functions, that could be solutions of PDEs, belonging to a given functional space, by their projections on a subspace of reduced dimension spanned by a reduced number of orthogonal basis functions called in some areas like in PDEs as modes. This reduces for instance solving Navier-Stokes equations by finite elements that requires a finite element subspace spanned by a basis of size in the order of millions to solve a small dynamical system of size smaller than hundred using the POD basis [3, 4, 7, 10]. The POD basis in PDEs is built from a set of solutions obtained with any classical numerical method like FE of FV, corresponding to a selected parameters, it is referred to these solutions by shots. It is clear that the accuracy of the projected solution for any parameters value depend on this selected set used to build the basis, many search works are dedicated to define a process of selecting the parameters or equivalently the shots in order to improve the accuracy of the method, see for instance [5]. In the context of PDEs, research oriented to improve the accuracy of the method is essentially focused on this aspect along with the impact of the scalar product of the considered functional space. This is due to a theorem based on Mercer theory [8] that proves the optimality of the POD basis [9] in a sense that we will recall later in the paper. In this paper we are proposing an improvement of the POD by a coupling with a new introduce basis without contradicting the optimality theorem. The new system is built based on a criterion that minimizes the transformation process, in a sense that will be defined later, of the original shots. The new method validated with comparison to exact solution of a convective equations and the result of POD technique.

2 THE POD TECHNIQUE

Let's summarize the POD method in the context of PDEs.
Let

$$\frac{\partial u}{\partial t} + L(u) = f \tag{1}$$

be an evolutionary PDE, where L any space differential operator and f a source term.
Let Λ be a space of parameters (design parameters, flying conditions, etc...) to be used for instance in the optimization process. For simplicity let's consider that of dimension 1. Then $u = u(t, x, \gamma) \quad \gamma \in \Lambda$. Let $U_i, 1 \leq i \leq N$ be a set of solutions (shots) of equation (1) for parameters i respectively. The goal of POD method is to reconstruct the solution of (1) for any parameter value (within certain range), without solving problem (1). To achieve this objective a discrete vector space with low dimension (as low as possible) is built from the shots, then the solution of (1) is projected into this space where and as a result, rather than solving (1), the approached POD solution is obtained by solving a simple ODE system.
To build the POD space we need to build a basis that spans the space. Let K be the correlation matrix given by $K_{i,j} = (U_i, U_j)$ where $(,)$ is any dot product, generally the one is used, then the basis functions are given by:

$$\Psi_i = \sum_{j=1}^{N} \lambda_{i,j} \, U_i \tag{2}$$

Where $\lambda_{i,j}$ are the components of the i-th eigenvector of K
Now by multiplying (1) by Ψ_i we obtain

$$(\frac{\partial u}{\partial t}, \Psi_i) + (L(u), \Psi_i) = (f, \Psi_i) \tag{3}$$

The projection of problem (1) solution on the POD space gives

$$u(x,t) \approx \sum_{j=1}^{N} Y_j(t)\Psi_j(x) \tag{4}$$

Finally, building the POD solution reduces to solve for $Y_j(t)$.
Using equation (3) and the fact that Ψ_j are orthogonal (which is the case if the eigenvectors of K are so), we obtain a quadratic dynamical system of the form:

$$Y' = A + (BY) + (C_i Y, Y) = 0 \qquad 0 \leq i \leq N \tag{5}$$

3 MOTIVATION AND MAIN IDEA

Let's first recall the optimality theorem,

Theorem 1 *Let $V_N = Span\{\Psi_1, ..., \Psi_N\} \subset H = L^2(\Omega)$, then for a subspace $S_N = Span\{W_1, ..., W_N\} \subset H$ we have:*

$$\int_{\Lambda} d_H(u(.,.,\gamma), V_N)\mathrm{d}\gamma \leq \int_{\Lambda} d_H(u(.,.,\gamma), W_N)\mathrm{d}\gamma \tag{6}$$

where $d_H(u(.,.,\gamma), V_N)$ is a distance from $u(.,.,\gamma)$ to the subspace V_N

The POD optimality is guaranteed in the sense of average over the parameters space as it is shown in the theorem. This optimality is not satisfied pointwise as we will demonstrate later. The idea then is to build another basis under some criterion such that the POD results could be improved for some parts of the parameter space Λ without contradicting the optimality theorem and then couple both basis to get the best results. To illustrate the idea in a very sample example, let's consider 3 vectors in the $\mathbb{R}^3$, where two of them are orthogonal and span the horizontal plan as in Figure 1. The third one makes an angle of degrees with horizontal plan. Assume that these vectors are selected over a parametrized family of vectors and we want to build a reduction model of two dimensions (a plan) from the given vectors to approximate the parametrized family. Applying the POD method we will get two orthogonal vectors spanning the plan passing between the horizontal one and the third vector as in Figure 2. Now for vectors close or belonging to the horizontal plan the best approximations is to use this plan. The idea then is to build another basis that spans the horizontal plan and find a mechanism to choose this plan to approximate the vectors that are closer to it (and only those) rather than using the POD plan.

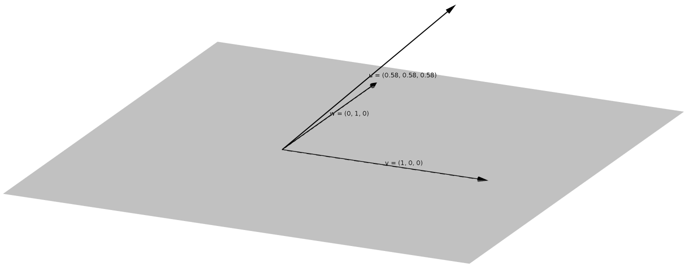

Figure 1: The three vectors

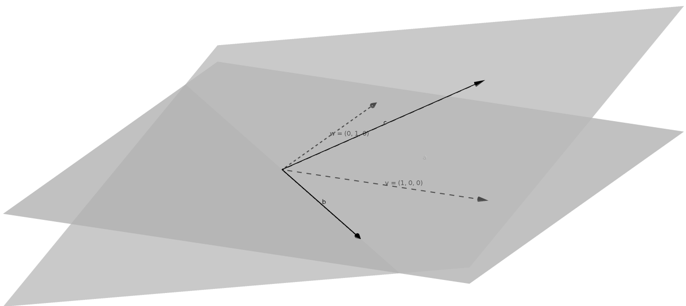

Figure 2: POD plan and horizontal plan

4 THE NEW BASIS SYSTEM

To build the basis described in the previous section, we need to put a criterion based on some observations. The first one is that the best scenario is to have the shots already orthogonal, we assume of course that the corresponding parameters location is optimal, and then there is nothing to do. The second observation is that we need to keep in mind that the shots are solutions of the PDE we want to solve with the model reduction, and then each shots contain valuable information. Combing these two observations we propose the following criterion that that requires building a basis with a minimum change of the original shots system. Mathematically we can express this criterion as:

$$\{W_1, ..., W_d\} = Arg\left(\max_{U,\sigma} \sum_{k=1}^{d} \frac{|\langle U_k, \varphi_{\sigma(k)}\rangle_H|}{\|U_k\|_H \|\varphi_{\sigma(k)}\|_H}\right) \tag{7}$$

Where H is a functional space, in general $H = L^2$, and σ are all possible one to one functions from a natural numbers set of dimension d (the desirable dimension) onto a natural numbers set of dimension N (the initial shots set size).
It is very difficult to solve exactly the optimization problem (7), instead we will give an algorithm that reproduce the spirit of this criterion and do some validation.

4.1 The Sorted Gram Schmidt (SGS) algorithm

We propose to build the targeted basis using the classical Gram Schmidt process but after sorting the shots in the sense of problem (7). We refer to this procedure by sorted Gram Schmidt (SGS) algorithm. The algorithm is summarized as folow.

1. Find the less correlated two shots among the set of shots.
2. Do GS orthogonalization
3. Find the less correlated shot to the previous subspace spanned by the basis elements built so far.
4. Complete GS orthogonalization with the selected shot in 3.
5. Use the correlation computed in 3 as a test criterion. If it is bigger than a threshold stop, otherwise repeat from step 3.

5 APLICATION AND VALIDATION

To demonstrate the validity of the proposed idea and algorithm, we will apply the method to sample case of incompressible, steady state flow given by the following governing equations:

$$\begin{aligned} v\left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}\right) &= 0 \\ u\left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right) &= 0 \end{aligned} \tag{8}$$

Defined first on the whole plan $\mathbb{R}^2$

In this validation we will not focus of on physics but on the mathematical aspect, therefore and for the sake of comparison we built "artificial" exact solutions of problem (8). To do so, let?s consider the following functions

$$\begin{aligned} u &= \exp^{-\alpha[(a-a_0)^2+(b-b_0)^2)][x^2+y^2+\beta]} \\ v &= \exp^{-\alpha[(a-a_0)^2+(b-b_0)^2)][xy+\beta]} \end{aligned} \tag{9}$$

Where α and β are given values, and a and b are the parameters on which depend the solutions. To force the two functions to be solution of (8) with appropriate source term, we replace their expression in (8) and then we get the corresponding new equations:

$$\begin{aligned} v(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}) &= S_1 \\ u(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}) &= S_2 \end{aligned} \tag{10}$$

where

$$\begin{aligned} S_1 = \exp^{-\alpha[(a-a_0)^2+(b-b_0)^2)][x^2+y^2+\beta]}&(-2\alpha y[(a-a_0)^2+(b-b_0)^2] \\ &\exp^{-\alpha[(a-a_0)^2+(b-b_0)^2)][x^2+y^2+\beta]} + \\ \alpha y[(a-a_0)^2+(b-b_0)^2]&\exp^{-\alpha[(a-a_0)^2+(b-b_0)^2)][xy+\beta]}) \\ S_2 = \exp^{-\alpha[(a-a_0)^2+(b-b_0)^2)][x^2+y^2+\beta]}&(-\alpha y[(a-a_0)^2+(b-b_0)^2] \\ &\exp^{-\alpha[(a-a_0)^2+(b-b_0)^2)][xy+\beta]} + \\ 2\alpha y[(a-a_0)^2+(b-b_0)^2]&\exp^{-\alpha[(a-a_0)^2+(b-b_0)^2)][x^2+y^2+\beta]}) \end{aligned} \tag{11}$$

We consider know the problem (10) in a rectangular domain and add boundary conditions extracted from the exact solution. The classical POD and the proposed SGS model reduction process are applied to solve problem (10). The Figure 3 below shows the error distribution of the approximated solutions by comparison to the exact one for both methods. First we can see that SGS results are competitive compared to the classical POD. Second the result demonstrates our statement that the POD optimality is not satisfied pointwise. Finally we can see that SGS is better than POD for some parameter intervals while keeping reasonable accuracy elsewhere. This answers the main objective of this work. The next step is to set up a mechanism allowing switching to SGS in the intervals where SGS provide better results within a POD process.

6 CONCLUSIONS

We presented in this paper a new method to build a basis for the reduction model approach in the context of PDEs. The basis is built based on an optimality criterion that

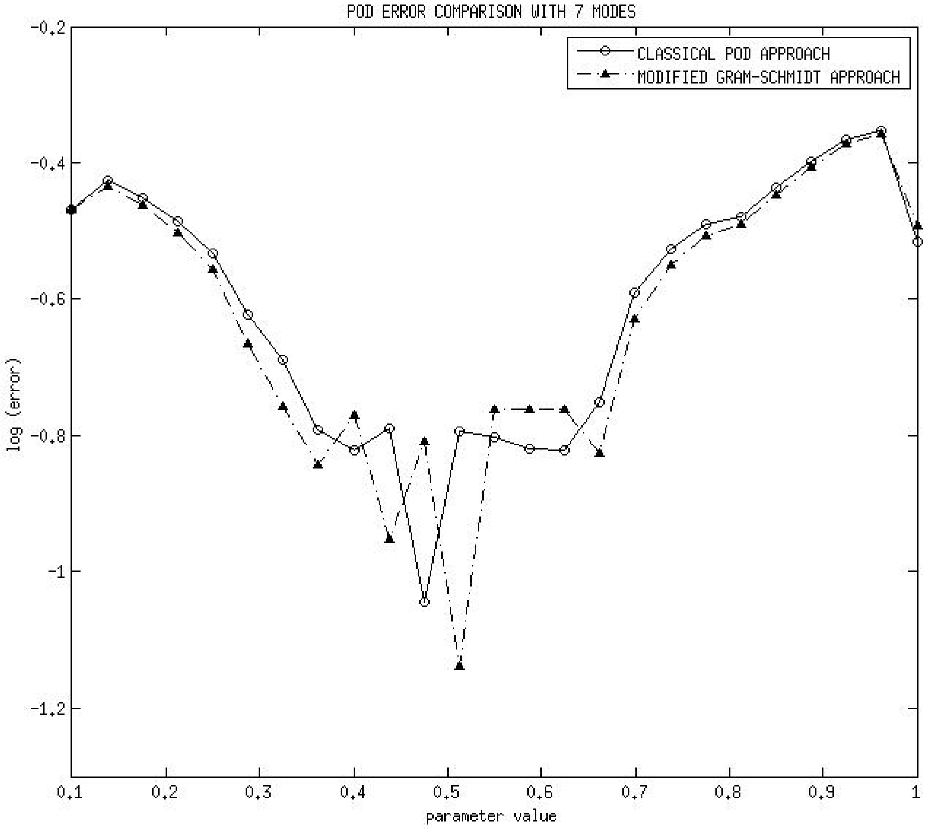

Figure 3: Error of POD and SGS results by comparison to exact solution.

minimizes the transformation of the initial set of shots. The method is applied to a 2D Euler type problem with a source term added in order to get an exact solution. The results of both POD and the new method are compared to the exact solution. As a conclusion the new method demonstrate it effectiveness, and the fact that the POD optimality theorem is not satisfied pointwise only in the average sense. Indeed, the new method shows better results for parts of the parameters space. This bring as and as a future work to build a hybrid method and set up a mechanism to select the new method where results are better than those of POD.

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