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On the computation of intrinsic Proper Generalized Decomposition modes of parametric symmetric elliptic problems on Grassmann manifolds

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ABSTRACT

In this work, we introduce an iterative optimization algorithm to obtain the intrinsic Proper Generalized Decomposition modes of elliptic partial differential equations. The main idea behind this procedure is to adapt the general Gradient Descent algorithm to the algebraic version of the intrinsic Proper Generalized Decomposition framework, and then to couple a one-dimensional case of the algorithm with a deflation algorithm in order to keep enriching the solution by computing further intrinsic Proper Generalized Decomposition modes. For this novel iterative optimization procedure, we present some numerical tests based on physical parametric problems, in which we obtain very promising results in comparison with the ones already presented in the literature. This supports the use of this procedure in order to obtain the intrinsic PGD modes of parametric symmetric problems.

1. Introduction

Many engineering problems are modeled by Partial Differential Equations (PDEs) that depend on some parameters, and its numerical resolution could be very expensive in terms of computational time, or even in terms of storage, when dealing with multiphysics or large scale problems. Also, in many industrial applications, several resolutions of these problems for different values of the parameters are needed, or they should be done on-the-fly to help in the decision-making. Therefore, many techniques have been developed to overcome these problems [1–14]. The main idea behind these techniques is to build a numerical problem, which dimension is lower than the one of the original model, but whose solution reproduces truly the main qualitative and quantitative behaviors of the original solution. The models arising from these techniques are the so-called Reduced Order Models (ROMs).

One of the most widely used tools in mechanical computations is the so-called Proper Orthogonal Decomposition (POD) [3,15, 13,14], which is commonly used along with Galerkin projection strategies in order to reduce the dimensionality of the problems [4,9,10], and the use of Galerkin-POD strategies makes affordable the solution of many-query and on-the-fly simulations. However, the application of the POD technique requires some knowledge of the solution for a variety of parameters, large enough to capture the main behaviors of the real solution over a range of the parameters. This can be extremely expensive in terms of computational time or storage, as we have stated before.

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In order to overcome this problematic, a new approach was introduced in [2], the so-called Proper Generalized Decomposition (PGD). The idea behind this technique is to assume that the solution admits a decomposition into a sum of basis functions that do not need to be orthogonal between them, and to iteratively enrich the reduced solution by computing a tensorized representation of the parametric PDE that separates the problem into a parametric and a non-parametric part. The mathematical analysis and the application of the PGD has experienced an important development in the last years [1,2,5–7,11].

We would like to highlight an extension of the PGD presented in [16], that the authors call the intrinsic PGD. This technique is based on the construction of recursive approximations on finite-dimensional optimal subspaces. These approximations are obtained by means of the minimization of the mean parametric error of the residual, similar to the one introduced in [17]. In a latter work [18], this technique is applied along with a deflation algorithm and a Power Iterate (PI) method to compute the PGD modes for parametric elliptic partial differential equations both, symmetric and non-symmetric.

In this paper, we propose the resolution of the intrinsic PGD for parametric symmetric elliptic partial differential equations directly by means of the Gradient Descent (GD) algorithm in a matrix framework. This matrix framework can be identified with the Grassmann manifold [19], to obtain the optimal subspaces. Furthermore, we combine this method with a deflation algorithm in order to obtain one-dimensional subspaces and keep enriching the solution, simplifying the computations. In this contribution, we compare our results with the ones obtained in [18] as a validation of our method, and we also apply this novel technique to an elastostatics problem.

The article outline is as follows. In Section 2, we start by presenting the problem arising from the intrinsic PGD in the continuous and algebraic form. Additionally, we will provide an overview of numerous mathematical results and properties established in the article [16]. In Section 3, we present the general GD algorithm, and we explain the changes that are necessary to adapt the general GD algorithm to our framework. Then, we present the one-dimensional version of that adaptation to overcome some computational difficulties that may arise. In order to end this section, we present the deflation algorithm used in [18], which will allow us to obtain higher dimensional optimal subspaces by recursively obtaining one-dimensional optimal subspaces. Section 4 is devoted to the validation of our model and its comparison with the PI method proposed in [18]. We also provide some numerical results obtained for an elastostatics problem. Results for both problems are very promising, as we obtain very low errors with very few modes, reaching up to 3 more orders of error in comparison with the methods proposed in the literature. Finally, in Section 5 we present the main conclusions of the work as well, as some future research problems.

2. Statement of the problem

In this section, we will present the continuous version of the intrinsic PGD problem in Subsection 2.1, first presented in [16]. After that presentation, we will also present the algebraic form of the intrinsic PGD problem in Subsection 2.2.

In order to be consistent with previous works, we begin by introducing the notation that we are going to use in this article, and that we inherit from [16,18]. In the following, we assume that H represents a separable Hilbert space with an associated norm denoted by $\|\cdot\|$, $B_S(H)$ denotes the space of bilinear, symmetric and continuous forms in H, $\langle\cdot,\cdot\rangle$ is the duality pairing between H and its dual H', Γ is a specified parametric space, $(\Gamma,\mathcal{B},\mu)$ stands for a given measure space, a denotes a parametric coercive and continuous bilinear form defined over $H\times H$ and f represents the parametric data function belonging to H'.

We will denote by u the parametric solution of the problem,

$$\text{Find function } u(\gamma)\in H \text{ that satisfies } a(u(\gamma),v;\gamma)=\langle f(\gamma),v\rangle, \quad \forall v\in H, d\mu\text{-a.e. } \gamma\in\Gamma, \tag{1}$$

and by $u_{\mathcal{Z}}$ the parametric solution of the Galerkin approximation of problem (1) on a closed subspace $\mathcal{Z}$ of H, which can be expressed as,

$$\text{Find } u_{\mathcal{Z}}(\gamma)\in\mathcal{Z} \text{ such that } a(u_{\mathcal{Z}}(\gamma),z;\gamma)=\langle f(\gamma),z\rangle, \quad \forall z\in\mathcal{Z}, d\mu\text{-a.e. } \gamma\in\Gamma. \tag{2}$$

Also, we consider $\{H_n\}_{n\in\mathbb{N}}$ an internal approximation of H, which refers to a sequence of subspaces of finite dimension within H in such a way that $\lim_{n\to\infty}\inf_{\psi\in H_n}\|v-\psi\|=0, \forall v\in H$. This allows us to approximate the original infinite-dimensional space H by some finite dimensional space H_n, which can also be identified as $\mathbb{R}^n$.

2.1. Continuous version of the intrinsic PGD

We proceed now to state the continuous version of the intrinsic PGD. We are interested in obtaining the optimal subspace that approximates the solution of a parametric PDE by solving the following minimization problem for a given $k\in\mathbb{N}$.

$$\begin{cases}\text{Find the optimal subspace } \mathcal{W} \text{ of } H \text{ with a dimension less than or equal to } k, \text{ which solves}\\ \qquad\qquad \min_{\mathcal{Z}\in\mathbb{G}_{\leq k}} \overline{a}(u-u_{\mathcal{Z}},u-u_{\mathcal{Z}}),\end{cases} \tag{3}$$

where $\mathbb{G}_{\leq k}=\bigcup_{m\leq k}\mathbb{G}_m(H)$, is the family of subspaces of H of dimension less than or equal to k, and $\overline{a}\in B_S(L^2(\Gamma,H;d\mu))$ is a bilinear form given by

$$\overline{a}(v,w)=\int_\Gamma a(v(\gamma),w(\gamma);\gamma)d\mu(\gamma), \quad \forall v,w\in L^2(\Gamma,H;d\mu). \tag{4}$$

The following fundamental theorem for the intrinsic PGD was also presented in [16, Theorem 4.1], where the interested reader could find the proof.

Theorem 2.1. *For any fixed $k \geq 1$, the problem defined by (3) admits at least one solution.*

Furthermore, the authors stated that when $\overline{a}$ is symmetric, an equivalent formulation can be provided, for which problem (3) is independent on the knowledge of the solution u to (1), relying uniquely on the parametric data function f. The proof of this proposition can also be found in [16, Proposition 2.6].

Proposition 2.2. *Assuming that $\overline{a}$ is symmetric, the subspace $\mathcal{W} \in \mathbb{G}_{\leq k}$ solves problem (3) if and only if it is a solution of the problem,*

$$\begin{cases} \text{Find the optimal subspace } \mathcal{W} \text{ of } H \text{ with a dimension less than or equal to } k, \text{ which solves} \\ \max_{\mathcal{Z} \in \mathbb{G}_{\leq k}} \int_{\Gamma} \left\langle f(\gamma), u_{\mathcal{Z}}(\gamma) \right\rangle d\mu(\gamma). \end{cases} \tag{5}$$

Also, in order to simplify the notation, we can define a real-valued function on $\mathbb{G}_{\leq k}$, as

$$\begin{array}{rccl} F: & \mathbb{G}_{\leq k} & \longrightarrow & \mathbb{R} \\ & \mathcal{Z} & \longmapsto & -\displaystyle\int_{\Gamma} \left\langle f(\gamma), u_{\mathcal{Z}}(\gamma) \right\rangle d\mu(\gamma), \end{array} \tag{6}$$

where we have kept the formulation as a minimization problem, changing the sign of the function. This will allow us to express the continuous version of the intrinsic PGD for symmetric problems as,

$$\begin{cases} \text{Find the optimal subspace } \mathcal{W} \text{ of } H \text{ with a dimension less than or equal to } k, \text{ which solves} \\ \min_{\mathcal{Z} \in \mathbb{G}_{\leq k}} F(\mathcal{Z}). \end{cases} \tag{7}$$

Now, we can present the algebraic form of the intrinsic PGD, that will be the one used in the applications.

2.2. Algebraic form of the intrinsic PGD problem

In this section, we will present the algebraic version of the intrinsic PGD for symmetric PDEs (7).

In the previous subsection, we have stated that we can consider an internal approximation H_n of H, so, we first identify our original Hilbert space H with the finite dimensional subspace H_n, that can be also identified with $\mathbb{R}^n$. In this framework, the parametric symmetric bilinear form a in problem (1) can be identified as a parametric matrix $A(\gamma)$ in $\mathcal{M}_n$, the set of real square matrices of dimension n, for all $\gamma \in \Gamma$. Similarly, the parametric data function $f(\gamma)$ in problem (1) can be identified as a vector $b(\gamma) \in \mathbb{R}^n$ for all $\gamma \in \Gamma$, and the duality pairing $\langle \cdot, \cdot \rangle$ becomes the scalar product of two vectors in $\mathbb{R}^n$, thanks to the Riesz Representation Theorem.

Taking this into account, solving system (1) inside the finite dimensional space H_n is equivalent to solve the following linear system,

$$A(\gamma)u(\gamma) = b(\gamma), \quad d\mu\text{-a.e. } \gamma \in \Gamma. \tag{8}$$

Also, we can identify the k-dimensional subspace $\mathcal{Z}$, that is now a subspace of $\mathbb{R}^n$, as a matrix $Z \in St(n,k) = \{Z \in \mathbb{R}^{n \times k} : Z^T Z = I_k\}$, that is, belonging to the Stiefel manifold. More precisely, $\mathcal{Z}$ is spanned by the columns of Z, i.e. $\mathcal{Z} = \text{col}(Z)$. Taking this into consideration, the bilinear form $a(\cdot, \cdot; \gamma)$ and data function $f(\gamma)$ in problem (2) can be identified as $Z^T A(\gamma) Z \in \mathcal{M}_k$ and $Z^T b(\gamma) \in \mathbb{R}^k$, respectively. Therefore, if we consider the ansatz $u_Z(\gamma)$, defined as $u(\gamma) = Z u_Z(\gamma)$, solving problem (2) is equivalent to solve the following linear system

$$(Z^T A(\gamma) Z) u_Z(\gamma) = Z^T b(\gamma). \tag{9}$$

Now, we can present the algebraic version of the intrinsic PGD.

Proposition 2.3. *Let Z be a matrix identified with the subspace $\mathcal{Z}$. Then, the algebraic form of problem (7) is*

$$\begin{cases} \text{Find the matrix } Z_* \in St(n,k) \text{ that solves} \\ \min_{Z \in St(n,k)} F(Z), \end{cases} \tag{10}$$

where $F : St(n,k) \to \mathbb{R}$ is defined as

$$F(Z) = -\int_{\Gamma} (b(\gamma)^T Z)(Z^T A(\gamma) Z)^{-1}(Z^T b(\gamma)) d\mu(\gamma). \tag{11}$$

Proof. In order to obtain the algebraic form of problem (7), we work with F defined as (6) and we build its algebraic form.

Let Z be a matrix identified with the subspace $\mathcal{Z}$, then, from expression (9), the solution $u_Z(\gamma)$ can be expressed as

$$u_Z(\gamma) = (Z^T A(\gamma) Z)^{-1}(Z^T b(\gamma)).$$

Now, explicitly writing the inner product and integrating over Γ, we obtain the desired algebraic form.

We highlight now a property of this algebraic version of the intrinsic PGD that states the independence of function (11) with respect to the representative matrix of the subspace $\mathcal{Z}$.

Corollary 2.4. *It is easy to see that the algebraic form of F does not depend on the matrix identified with the subspace $\mathcal{Z}$, that is, $F(Z) = F(ZQ), \forall Q \in \mathcal{O}_k$, the set of orthonormal matrices of order k.*

Proof. $F(ZQ)$ can be expressed as

$$F(ZQ) = -\int_{\Gamma} (b(\gamma)^T ZQ)(Q^T Z^T A(\gamma) ZQ)^{-1}(Q^T Z^T b(\gamma)) d\mu(\gamma).$$

Noticing that $(Q^T Z^T A(\gamma) ZQ)^{-1} = Q^T (Z^T A(\gamma) Z)^{-1} Q$, injecting this in the previous expression and taking into account that $QQ^T = I_k$, we obtain

$$\begin{aligned} F(ZQ) = & -\int_{\Gamma} (b(\gamma)^T Z)(QQ^T)(Z^T A(\gamma) Z)^{-1}(QQ^T) Z^T b(\gamma)) d\mu(\gamma) = \\ = & -\int_{\Gamma} (b(\gamma)^T Z)(Z^T A(\gamma) Z)^{-1}(Z^T b(\gamma)) d\mu(\gamma) = F(Z). \end{aligned}$$

That is the desired result.

Since $F(Z) = F(ZQ)$ holds for all $Q \in \mathcal{O}_k$, then we could express function (11) as a function on the Grassmann manifold, as follows

$$F_{\mathbb{G}} : St(n,k)/\mathcal{O}_k \cong \mathbb{G}_k(\mathbb{R}^n) \to \mathbb{R}, \tag{12}$$

defined as $F_{\mathbb{G}}(Z\mathcal{O}_k) = F(Z)$, and where $\mathcal{Z} = \mathrm{col}(Z) = Z\mathcal{O}_k$.

However, for numerical computations, it is natural to consider the discretized version. So, in the following we will work in the matrix framework for the discrete version of the intrinsic PGD (10).

3. Computation of intrinsic PGD modes via the Gradient Descent Algorithm

In this section, we will develop a procedure to solve the intrinsic PGD in its algebraic form (10) through an adapted version of the GD Algorithm to our framework of matrix spaces. Then, we will present the one-dimensional version of it, and how it can be coupled with a deflation algorithm in order to obtain optimal subspaces of higher dimensions.

The general GD Algorithm can be roughly stated as presented in Algorithm 1. Note that the time step t can be adapted for each iterate to speed up the convergence of the Algorithm.

Algorithm 1: Gradient Descent Algorithm.

Require: Differentiable real-valued function $f : \mathbb{R}^n \to \mathbb{R}$, step size t.
Goal: Find a local minimum of f.
Input: Initial point x_0.
Output: Sequence of iterates $\{x_i\}_{i \geq 0}$.
for $i = 0, 1, 2, \ldots$ **do**
  Compute the gradient of f at x_i, $\nabla f(x_i)$.
  Solve the Gradient Descent equation to obtain the next iterate

$$x_{i+1} = x_i - t\nabla f(x_i). \tag{13}$$

end

However, the general GD Algorithm 1 is not suitable to solve the intrinsic PGD in our matrix framework. First, the computation of the gradient is not straightforward and, furthermore, we could leave the matrix space if we were to update the iterates directly by

the GD equation (13) in Algorithm 1. So, in the following, we will study the necessary changes in Algorithm 1 in order to adapt it to the algebraic form of the intrinsic PGD (10).

3.1. GD algorithm in the algebraic framework

As we have already commented in the introduction of this section, we have to adapt the general GD Algorithm 1 to the algebraic framework, that is, to a function defined on $St(n,k)$. Some of the adjustments are straightforward, but we need to focus on two main adaptations, the computation of the gradient of a function defined in a matrix subspace and the resolution of the GD equation (13) in the matrix subspace without leaving the space.

3.1.1. Gradient of a function on a matrix space

The gradient of the function on $St(n,k)$ belongs to the tangent space of $St(n,k)$ and it is known [19] that the tangent space of $St(n,k)$ at the point Z can be expressed as,

$$T_Z St(n,k) = \{\Delta \in \mathbb{R}^{n\times k} \mid Z^T\Delta = -\Delta^T Z\} = \{\Delta \in \mathbb{R}^{n\times k} \mid \mathrm{sym}(Z^T\Delta) = 0_k\},$$

that is, the matrices in $\mathbb{R}^{n\times k}$ such that after a left-multiplication by the transpose of matrix Z give an antisymmetric square matrix of dimension k. Note that if $Z^T\Delta = 0_k$, then $Z^T\Delta = -\Delta^T Z$, so it would be enough to prove that $Z^T\Delta = 0_k$, to check that Δ belongs to $T_Z St(n,k)$.

Furthermore, following [19], for a function F defined on $St(n,k)$, the gradient of F at Z can be expressed as

$$\nabla F(Z) = dF(Z) - Z Z^T dF(Z), \tag{14}$$

where $dF : St(n,k) \to \mathbb{R}^{n\times k}$ is the matrix derivative of function F with respect to Z. Therefore, it is clear that, for a fixed $Z \in St(n,k)$, $\nabla F(Z)$ belongs to the tangent space $T_Z St(n,k)$, and that, in order to obtain the gradient of F, first, we need to compute the matrix derivative of function F.

In the following proposition, whose proof has been relegated to Appendix A.1, we give the algebraic form for the derivative of the intrinsic PGD function (11) with respect to the point Z in our case of study.

Proposition 3.1. *The algebraic form of the matrix derivative of the intrinsic PGD function F given in (11) can be expressed as*

$$dF(Z) = -2\int_\Gamma \left(I_n - A(\gamma)Z(Z^TA(\gamma)Z)^{-1}Z^T\right) b(\gamma)b(\gamma)^T Z(Z^TA(\gamma)Z)^{-1} d\mu(\gamma). \tag{15}$$

Now, according to (14) we can compute the gradient of the intrinsic PGD function (11) in the matrix framework. Nevertheless, in the following remark, we state that, actually, the derivative of the intrinsic PGD function (15) belongs to the tangent space $T_Z St(n,k)$. So, the derivative of the intrinsic PGD function (15) is the gradient of the intrinsic PGD function (11).

Corollary 3.2. *Given $dF(Z)$ computed as in Proposition 3.1. Then, $Z^T dF(Z) = 0_k$, thus, $\nabla F(Z) = dF(Z)$ and $dF(Z) \in T_Z St(n,k)$.*

Proof. We focus on the first term inside the parenthesis in the integral of the intrinsic PGD function derivative (15) and we left-multiply it by Z^T.

$$\begin{aligned} &Z^T(I_n - A(\gamma)Z(Z^TA(\gamma)Z)^{-1}Z^T) = \\ &\quad = Z^T - (Z^TA(\gamma)Z)(Z^TA(\gamma)Z)^{-1}Z^T = Z^T - Z^T = 0_{k\times n}, \quad \forall\gamma\in\Gamma. \end{aligned}$$

Now, taking into account (14), the right term vanishes and we obtain the desired result.

In addition, we keep the independence with respect to the matrix representative of the subspace $\mathcal{Z}$. The proof is straightforward, as we can follow the same procedure as for the proof of Corollary 2.4.

Corollary 3.3. *The derivative (15), and therefore the gradient, of the intrinsic PGD function (15) is also invariant under right multiplication of matrix Z by k-dimensional orthonormal matrices, that is,*

$$dF(Z) = dF(ZQ), \quad \forall Q \in \mathcal{O}_k.$$

Taking this into account, we could consider a map in the Grassmann manifold $\mathbb{G}_k(\mathbb{R}^n)$ in the same way as we did in (12).

Finally, we have an explicit expression for the matrix derivative of the intrinsic PGD function (15). We can move to the next necessary adaptation, the GD equation (13).

3.1.2. GD equation on a matrix space

In this section, we focus on the fact that if we try to update the matrix representative Z directly through the GD equation (13), we almost surely leave the matrix space $St(n,k)$. In order to overcome this issue, we need to consider a tool to update the matrix representative Z similarly as the GD equation (13), while remaining in $St(n,k)$.

In this work, we will consider a retraction on the matrix space, that is, a continuous mapping from a topological space into a subspace that preserves the position of all points in that subspace.

More precisely, in the following and in the applications, we consider a map that transforms a tangent vector $\Delta \in T_Z St(n,k)$ to the endpoint $g_Z(t,\Delta) \in St(n,k)$ for a given step t of the unique geodesic g that emanates from Z in the direction Δ. Therefore, this geodesic allows us to update the matrix representative Z as done with the GD equation (13), while obtaining a result that belongs to the matrix space $St(n,k)$.

In the next proposition, we state how the geodesic in the matrix space can be expressed. This proposition is a modification of [20, Theorem 2.3], where the proof can be consulted.

Proposition 3.4. *Let $Z \in St(n,k)$, $t \in (0,1]$, and $\Delta \in T_Z St(n,k)$, that is, $Z^T\Delta = 0$. Then,*

$$g_Z(t,\Delta) = (ZV\cos(t\Sigma) + U\sin(t\Sigma))V^T, \tag{16}$$

where $U\Sigma V^T$ is the compact Singular Value Decomposition (SVD) of Δ, so $U \in \mathbb{R}^{n\times r}$, Σ is a diagonal nonsingular matrix in $\mathbb{R}^{r\times r}$, and $V \in \mathbb{R}^{r\times k}$, with r the number of non-zero singular values. Here, $\cos(X)(resp.\sin(X))$ denotes the matrix whose entries are the cosine (sine) of the entries of matrix X.

We state in the next proposition, whose proof has been relegated to Appendix A.2, that the orthonormality is conserved.

Proposition 3.5. *Let $Z \in St(n,k)$, and $\tilde{Z}$ such that, $\tilde{Z} = g_Z(t,-\nabla F(Z))$. Then, $\tilde{Z}^T\tilde{Z} = I_k$, that is, $\tilde{Z} \in St(n,k)$.*

It is clear now that we can use the retraction (16) as a substitute of the gradient equation (13) in Algorithm 1, as it updates the matrix representative Z and the result belongs to $St(n,k)$.

3.1.3. Adapted GD algorithm to the matrix framework

At this point, we have all the necessary ingredients to adapt the general GD Algorithm 1 to our algebraic framework.

As discussed in the previous sections, we need to compute the gradient of the function F as stated in equation (15) and then, instead of solving the GD equation (13) directly, we would need to compute retraction (16) in order to conserve the orthonormality of the matrices.

Taking Propositions 3.1 and 3.4 into account, the GD Algorithm adapted to the general matrix framework can be stated as in Algorithm 2.

Algorithm 2: Gradient Descent Algorithm on the matrix framework.

Require: Differentiable real-valued function F, step size t.
Goal: Find a local minimum of F.
Input: Initial point $Z_0 \in St(n,k)$.
Output: Sequence of iterates $\{Z_i\}_{i\geq 0} \subset St(n,k)$.
for $i = 0,1,2,\dots$ **do**
  Compute the gradient of F at Z_i, $\nabla F(Z_i)$, via equation (15).
  Compute the compact SVD of $-\nabla F(Z_i)$ to obtain the matrices U,Σ and V.
  Compute the retraction (16)

$$Z_{i+1} = g_Z(t,-\nabla F(Z_i)) = (Z_iV\cos(t\Sigma) + U\sin(t\Sigma))V^T. \tag{17}$$

end

A reader familiar with the Stiefel manifold will note that Algorithm 2 is just the one expected when considering minimization in Stiefel manifold. This adapted GD Algorithm to the matrix framework is suitable to compute the intrinsic PGD modes. However, the computation of the SVD of a matrix, even in the compact version, can be very demanding in terms of computational effort. In order to overcome this issue, in the following section, we will present the particular case where the dimension of the desired subspace is 1. In this particular case, we will be allowed to simplify the computation of the gradient (15), as well as the computation of the retraction (16), as we will not need to perform the compact SVD at each step of the Algorithm 2. Furthermore, we will present this particular case along with a deflation algorithm in order to use the one-dimensional tools to obtain optimal subspaces of higher dimensions, by enriching the solution.

3.2. One-dimensional case

A particularly interesting scenario in terms of applications and computational simplification arises when the subspace $\mathcal{Z} \in H$ is one-dimensional, indicating that $\mathcal{Z} \in \mathbb{G}_1$. This implies the existence of a basis function $\phi \in H\backslash\{0\}$ such that $\mathcal{Z} = \text{span}\{\phi\}$. Conse-

quently, the solution $u_{\mathcal{Z}}(\gamma)$ of problem (2) can be expressed as a parameter-dependent scalar multiplied by that basis function, that is, $u_{\mathcal{Z}}(\gamma) = \alpha(\gamma)\phi$, $d\mu - a.e.\gamma \in \Gamma$.

In this section, we will present a particular case of the adapted GD Algorithm 2 in which we are looking to solve the intrinsic PGD problem (10) when $k = 1$, that is, we are looking for the optimal one-dimensional space. We will start from the changes that occur at the level of the continuous formulation when $k = 1$, as it will help us to introduce naturally some concepts that will be used subsequently. Then, we present the particular case of the adapted GD Algorithm 2 with the one-dimensional adaptations of the gradient (15) and the retraction (16).

Letting $z = \phi$ in equation (2), after a short calculation using the bilinearity of a, we can see that,

$$\alpha(\gamma) = \frac{\langle f(\gamma), \phi\rangle}{a(\phi, \phi; \gamma)} \; d\mu\text{-a.e.}\gamma \in \Gamma, \tag{18}$$

so, thanks to problem (7), ϕ can be characterized by the solution of the following minimization problem,

$$\begin{cases} \text{Find the optimal one-dimensional subspace of } H, \text{ whose generating vector solves} \\ \min\limits_{\phi \in H\setminus\{0\}} F(\phi) \end{cases} \tag{19}$$

where F is a real-valued function on $H\setminus\{0\}$ defined as

$$F(\phi) = -\int_\Gamma \alpha(\gamma)\,\langle f(\gamma), \phi\rangle \, d\mu(\gamma) = -\int_\Gamma \frac{\langle f(\gamma), \phi\rangle^2}{a(\phi, \phi; \gamma)} d\mu(\gamma). \tag{20}$$

Now that we have stated the particular one-dimensional case for the continuous intrinsic PGD function (6), we can start to develop its algebraic version. The first remark that we need to take into account in this particular algebraic framework is that when $k = 1$, then the matrix representative Z identified with the subspace $\mathcal{Z}$ becomes the column matrix $\phi \in \mathbb{R}^{n\times 1} \cong \mathbb{R}^n$, that will allow us to identify the Galerkin discrete representatives by two scalars, as stated in the following remark.

Remark 3.1. The Galerkin discrete representatives of the bilinear form $Z^T A(\gamma) Z$ and the data $Z^T b(\gamma)$, become the scalars $\phi^T A(\gamma)\phi$, and $\phi^T b(\gamma)$, respectively.

The identification of the Galerkin representatives with scalar instead of matrices and vectors will allow us to simplify various steps in the calculation of the gradient and the retraction presented in the multidimensional framework, and that will lead to a subsequent reduction in the computational effort required to obtain the intrinsic PGD modes. Therefore, if we consider the one-dimensional version, we can define an algebraic form of problem (19), presented in the following Proposition.

Proposition 3.6. *In the one-dimensional case, subspace $\mathcal{Z}$ can be identified with the basis vector $\phi \in \mathbb{R}^n$. So, the coefficient $\alpha(\mu)$ can be computed as*

$$\alpha(\gamma) = \frac{\phi^T b(\gamma)}{\phi^T A(\gamma)\phi} \; d\mu\text{-a.e.}\gamma \in \Gamma. \tag{21}$$

As a consequence, problem (19) becomes:

$$\begin{cases} \textit{Find the best one-dimensional subspace of } H_n, \textit{ whose generating vector solves} \\ \min\limits_{\phi \in \mathbb{R}^n} F(\phi), \end{cases} \tag{22}$$

where

$$F(\phi) = -\int_\Gamma \frac{(\phi^T b(\gamma))^2}{\phi^T A(\gamma)\phi} d\mu(\gamma). \tag{23}$$

The proof of this proposition is straightforward, as it is a particular case of Proposition 2.3 and equation (18) with $k = 1$ in the matrix setting. One of the main advantages that we want to remark in this one-dimensional particular case, is that, as we have to work with scalars instead of matrices and vectors, we will avoid the computation of the inverses of matrices as we can just divide by the corresponding scalar.

We study now the particular one-dimensional version of the intrinsic PGD function derivative (15). Noticing that the matrix inverses can be substituted by a division by the respective scalar, we get to the following remark

Remark 3.2. For $St(n, 1)$, the algebraic form of the partial derivative of F in Proposition 3.1 takes the form

$$dF(\phi) = -2\int_\Gamma \left[I_n - \frac{A(\gamma)\phi\phi^T}{\phi^T A(\gamma)\phi}\right] \frac{b(\gamma)b(\gamma)^T\phi}{\phi^T A(\gamma)\phi} d\mu(\gamma). \tag{24}$$

As for the multidimensional version (see Corollary 3.2), we are able to identify the gradient of the one-dimensional intrinsic PGD function (23) with the one-dimensional intrinsic PGD function derivative (24), that is, $\nabla F(\phi) = dF(\phi)$. As after a left-multiplication by the transpose of the basis vector ϕ, we obtain the null vector,

$$\phi^T - \frac{\phi^T A(\gamma)\phi\phi^T}{\phi^T A(\gamma)\phi} = 0.$$

The main advantage that we obtain if we consider the one-dimensional particular case arrives at the computation of the retraction, as we will be able to avoid the computation of the compact SVD at each step of Algorithm 2. In the following Remark, we state the form of the retraction in the particular one-dimensional case.

Proposition 3.7. *For $St(n,1)$, the geodesic that emanates from ϕ in the direction Δ of Proposition 3.4 takes the form*

$$g_\phi(t,\Delta) = \cos(t\|\Delta\|_2)\phi + \sin(t\|\Delta\|_2)\frac{\Delta}{\|\Delta\|_2}. \tag{25}$$

Proof. When computing the compact SVD of a non-zero vector $v \in \mathbb{R}^n$, we can easily check that, $v = \frac{v}{\|v\|_2}\|v\|_2 1 = U\Sigma V^T$, that is,

- Diagonal matrix Σ becomes a scalar equal to the l_2-norm of the vector v, $\|v\|_2$.
- Left-singular matrix U becomes the normalized vector $v/\|v\|_2$.
- Right-singular matrix V becomes the scalar 1.

Substituting this changes in Equation (16) and rearranging the terms, we obtain the desired result.

Hence, we have all the ingredients to state the one-dimensional particular case of the adapted GD Algorithm 2. Taking Remark 3.2 and Proposition 3.7 into account, in the particular case of $St(n,1)$, the adapted GD Algorithm 2 is reduced to Algorithm 3.

Algorithm 3: Gradient Descent Algorithm on $St(n,1)$.

Require: Differentiable real-valued function F, step size t.
Goal: Find a local minimum of F.
Input: Initial point $\phi_0 \in St(n,1)$.
Output: Sequence of iterates $\{\phi_i\}_{i\geq 0} \subset St(n,1)$.
for $i = 0, 1, 2, \ldots$ **do**
  Compute the gradient of F at ϕ_i, $\nabla F(\phi_i)$ via equation (24).
  Compute $s = \|\nabla F(\phi_i)\|_2$ and $\delta = -\nabla F(\phi_i)/s$.
  Solve the Geodesic Descent equation via the retraction (25)

$$\phi_{i+1} = g_\phi(t, -\nabla F(\phi_i)) = \cos(ts)\phi_i + \sin(ts)\delta.$$

end

The algorithm cost of each step of the proposed technique goes like $O(mn^2)$, where m is the number of operations considered for evaluating the integral in equation (24) numerically by means of a suitable quadrature formula. One of the main drawback of this technique is that it only allows us to compute the optimal one-dimensional subspace, while in most applications it is more interesting to obtain optimal subspaces of higher dimension. With that objective in mind, we will present a deflation algorithm, in the same sense as in [18], that we can couple with the one-dimensional tools presented in Algorithm 3, in order to obtain optimal subspaces of increasing dimension in an iterative manner by an enrichment procedure.

The main idea behind the deflation algorithm is to express the solution of (1) as a series,

$$u(\gamma) = \sum_{i\geq 1} \alpha_i(\gamma)\phi_i,$$

where $\alpha_i \in L^2(\Gamma, d\mu)$ and $\phi_i \in H\backslash\{0\}$. Then, in the case in which we have computed $p-1$ basis functions, we can approximate the solution u as a sum of a known part and an unknown part, as

$$u(\gamma) \approx u_p(\gamma) = \sum_{i=1}^{p} \alpha_i(\gamma)\phi_i = \alpha_p(\gamma)\phi_p + \sum_{i=1}^{p-1} \alpha_i(\gamma)\phi_i = \alpha_p(\gamma)\phi_p + u_{p-1}(\gamma),$$

with

$$u_{p-1}(\gamma) = \sum_{j=1}^{p-1} \alpha_j(\gamma)\phi_j, \quad \text{for } p \geq 2, \tag{26}$$

this latter, is the known part of the solution. $u_k(\gamma)$ for $k \geq 1$ it is the so-called PGD expansion. Injecting this PGD expansion for $k = p-1$ along with the unknown part $\alpha_p(\gamma)\phi_p$ into equation (4), we obtain the following decomposition,

$$\overline{a}(\tilde{u},\tilde{v}) = \overline{a}(\alpha_p\phi_p,\tilde{v}) + \overline{a}(u_{p-1},\tilde{v}),$$

where the latter term is known and can be treated as a variation of the right term of the PDE.

That is, we will solve functions of the same kind as (6), replacing the parametric data function f by a parametric data function f_p that will change with the dimension, defined by $f_1 = f$ and f_p, for $p \geq 2$ such that

$$\int_\Gamma \left\langle f_p(\gamma), v(\gamma)\right\rangle d\mu(\gamma) = \int_\Gamma \langle f(\gamma), v(\gamma)\rangle\, d\mu(\gamma) - \overline{a}(u_{p-1}, v),\ \forall v \in L^2(\Gamma, H, d\mu). \tag{27}$$

The following theorem ensures the convergence of the deflation algorithm, the proof can be consulted in [16, Theorem 5.3].

Theorem 3.8. *The sequence provided by the iterative deflation algorithm* (26) *strongly converges in* $L^2(\gamma, H; d\mu)$ *to the parametrized solution* $\gamma \in \Gamma \mapsto u(\gamma) \in H$ *of problem* (1).

Bearing this in mind, we can develop an iterative algorithm, that enriches the PGD expansion of the solution by means of the one-dimensional tools and the deflation algorithm. In Algorithm 4, we present the procedure to obtain a multidimensional subspace using this deflation method and the one-dimensional tools present in Algorithm 3.

Algorithm 4: Iterative Gradient Descent Algorithm by deflation.

Require: Matrices $A(\gamma)$, vectors $b(\gamma)$, associated to the parametrized PDE, objective dimension k, step size t.
Goal: Find optimal matrix $Z \in St(n,k)$ that solves problem (11).
Input: Initial point $\phi_0 \in St(n,1)$.
Output: Sequence of matrices $\{Z_i\}_{i=1,\dots,k}$ with $Z_i \in \mathcal{M}_i(\mathbb{R}^{n\times i})$, $\forall i = 1,\dots,k$.
Set $b_1(\gamma) = b(\gamma)$ and $Z_0 = [\,]$.
for $i = 1,\dots,k$ **do**
  Define real-valued function F_i with matrices $A(\gamma)$ and vectors $b_i(\gamma)$.
  Apply Algorithm 3 to obtain ϕ_i.
  Make ϕ_i orthonormal to the subset Z_{i-1}.
  Compute $\alpha_i(\gamma) = \dfrac{\phi_i^T b_i(\gamma)}{\phi_i^T A(\gamma)\phi_i}\ d\mu$-a.e.$\gamma \in \Gamma$.
  Update $b_{i+1}(\gamma) = b_i(\gamma) - \sum_{j=1}^{i} \alpha_j A(\gamma)\phi_j$.
  Set $Z_i = [Z_{i-1}|\phi_i]$.
end

4. Numerical experiments

This section is devoted to the validation and numerical study of the procedure presented in Algorithm 4. We will apply the procedure to two different parametric symmetric problems:

1. A problem of parametric diffusion, where two different materials coexist in a domain. Here, the parameter will be the relationship between the diffusion of both materials.
2. A classic elastostatics problem of a block of material fixed on one side, and which is under the action of gravity. Here, the parameter will be the relationship between the Lamé parameters of the material.

In both cases, we will present the modes obtained by means of Algorithm 4 and the error decay of the reduced solutions. Here, $u(\gamma)$ stands for the reference numerical solutions obtained by means of the Finite Element Method with a fine mesh, and $u_p(\gamma)$ denotes the intrinsic PGD expansion up to mode p as in (26).

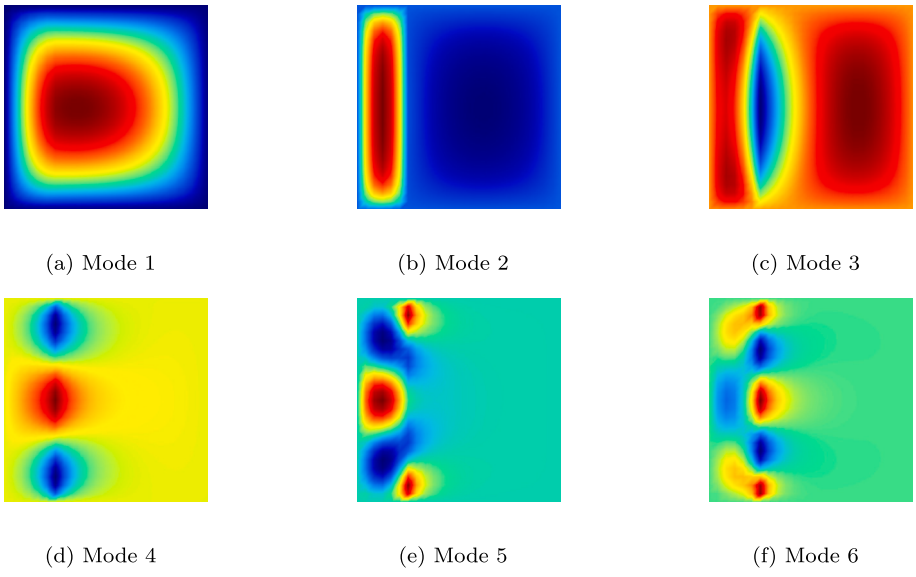
4.1. Diffusion problem

In this section, we will test Algorithm 4 in a diffusion problem previously treated in [18], and we will compare the results obtained with the ones obtained by means of the Power Iterate (PI) algorithm proposed in that paper. This test will serve as a validation of our procedure.

The diffusion problem that we are treating in this section, is related to a parametric second-order elliptic partial differential equation, in which the diffusion varies in space, and shows a dependence on the parameter. This problem could model a certain block composed by two materials with different diffusion parameters. The problem, as presented in [18], reads

$$\begin{cases} -\nabla\cdot(\nu(\gamma)\nabla u) = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases} \tag{28}$$

where $\Omega = (0,1)^2$, $f(x,y) = 1$ and



(a) Mode 1 (b) Mode 2 (c) Mode 3

(d) Mode 4 (e) Mode 5 (f) Mode 6

Fig. 1. First 6 intrinsic PGD modes of problem (28) obtained by means of the iterative Algorithm 4.

$$\nu(\gamma)(x,y) = \begin{cases} \gamma & \text{if } 0 \le x < 1/4, \\ 1 & \text{if } 1/4 \le x \le 1, \end{cases} \quad \text{for all } (x,y) \in \overline{\Omega}.$$

Problem (28) admits the following weak formulation

$$\begin{cases} \text{Find } u(\gamma) \in H_0^1(\Omega) \text{ such that} \\ \displaystyle\int_\Omega \nu(\gamma)\nabla u(\gamma)\cdot\nabla v = \int_\Omega f v, \quad \forall v \in H_0^1(\Omega). \end{cases} \tag{29}$$

In the following, as done in [18], we set $\gamma \in \Gamma = [0.01, 1]$, and μ denotes the Lebesgue measure on Γ. Thanks to the properties of ν and f and Lax-Milgram Theorem, there exists a unique solution of problem (29). The integrals on Γ that appear in the function (23), as well as its gradient (24), need to be addressed by means of a quadrature formula constructed on a subdivision of Γ in N subintervals, for instance, the midpoint, trapezoid or Simpson's rule, among others. In every case, we substitute Γ with the set comprising the quadrature formula nodes $\Gamma_N = \{\gamma_i\}_{i=1}^N$, and the Lebesgue measure is replaced by a discrete measure μ_N concentrated at these nodes. The weights associated with the quadrature formula, denoted as w_i, serve as the weights for the discrete measure. Then, we can rewrite the integrals on Γ as a sum

$$\begin{aligned} &\int_\Gamma v(\gamma)d\mu(\gamma) \approx \hat{I}_N(v) = \sum_{i=1}^N w_i v(\gamma_i), \\ &\int_\Gamma v_1(\gamma)v_2(\gamma)d\mu(\gamma) \approx I_N(v_1,v_2) = \sum_{i=1}^N w_i v_1(\gamma_i)v_2(\gamma_i). \end{aligned} \tag{30}$$

It is important to note that Algorithms 2 and 3, as well as the iterative procedure presented in Algorithm 4 do not change when replacing Γ by Γ_N and μ by μ_N.

Subsequently, the PGD expansions, as defined in equation (26), will converge to the original solution $u(\gamma)$ to problem (28), in the following sense

$$\lim_{i\to\infty} I_N(u-u_i, u-u_i) = 0. \tag{31}$$

For this first test, in order to be consistent with the previous works, we have employed the midpoint quadrature formula with $N = 10$ subintervals. This can be expressed as

$$\gamma_i = \frac{1}{N}(i - 1/2), \quad w_i = \frac{1}{N}, \quad i = 1, \dots, N.$$

After applying the iterative Algorithm 4, we obtain the intrinsic PGD modes that can be seen in Fig. 1. It is clear that the first modes keep the most important information about the solutions, and that the higher modes try to correct the differences that arise in the interface of the materials where the diffusion presents a discontinuity. A simple comparison with the intrinsic PGD modes,

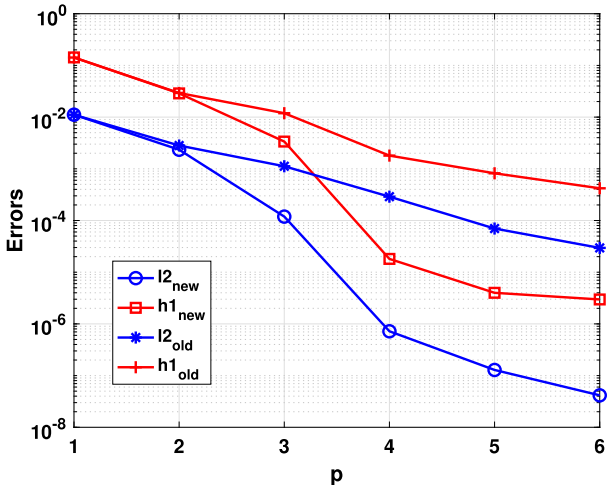


Fig. 2. Convergence of the PGD expansions u_i to $u(\gamma)$ as specified in (31). Comparison with the convergence history in [18]. Blue circles and red squares represent, respectively, the L^2 and H_0^1 norms of our methods, and blue asterisks and red crosses represent, respectively, the L^2 and H_0^1 norms of the PI method.

obtained in [18], shows that there are some qualitative differences between them, and they become more visible after the second mode.

Now, we are going to examine the convergence of the PGD expansions u_i given by formula (26) towards the original solution $u(\gamma)$, as specified in expression (31). In Fig. 2, we show the obtained truncation errors, measured in $L^2(\Gamma, L^2(\Omega), d\mu)$ and $L^2(\Gamma, H_0^1(\Omega), d\mu)$ norms and presented in logarithm scale, versus the dimension of the reduced subspace. We also compare the error decay with the one obtained in [18] for the PI algorithm. We can easily see that the decay is pretty similar for the two methods until the third PGD mode, where the new procedure gives a much faster decay of the error, achieving up to four less orders of magnitude.

Finally, in order to present a better comparison of the results with those obtained in [18], we show in Figs. 3-4, for each subspace dimension, a comparison of the true errors obtained in the whole domain obtained between the reduced solutions and the parametric solution $u(\gamma)$ of problem (28) for a fixed instance of the parameter $\gamma = 0.3$. In the left panels, we show the errors obtained by means of Algorithm 4, and the errors represented on the right panels are the ones obtained by means of the PI Algorithm presented in [18]. We can see that the errors are comparable in magnitude up to the second PGD mode, and that after the third mode the errors given by the iterative Algorithm 4 are much better in the whole domain than the ones obtained in [18] by means of the PI method.

As presented before, our new procedure based on the GD to obtain the intrinsic PGD modes and a deflation algorithm to keep enriching the PGD expansion seems to perform better in terms of error decay than the procedure presented in [18] based on the PI algorithm, achieving up to three more order of magnitude for the error. This clearly support the use of this procedure in order to obtain the intrinsic PGD modes of parametric symmetric problems.

This test concludes the validation of the procedure presented in Algorithm 4.

4.2. Elastostatics problem

In this section, we will test Algorithm 4 in a linear and parametric elasticity problem, where the parameter is the relationship between the Lamé parameters. The main difference between this problem and the previous one, besides the governing PDE, is that, in this problem, the solution is a vector, as the deformation of the blocks has two components, horizontal and vertical. The problem reads,

$$\begin{cases} -\nabla\sigma(u) = f & \text{on } \Omega, \\ \sigma(u)\cdot n = 0 & \text{on } \partial\Omega_1, \\ u = 0 & \text{in } \partial\Omega_2, \end{cases} \tag{32}$$

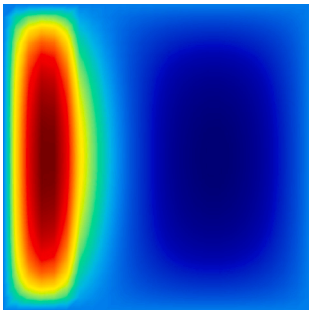
where f is the external force, $u = (u_1, u_2)^T$ is the displacement vector, $\sigma(u)$ is the stress tensor defined as

$$\sigma_{ij}(u) = \delta_{ij}\nabla\cdot u + \gamma\epsilon_{ij}(u), \tag{33}$$

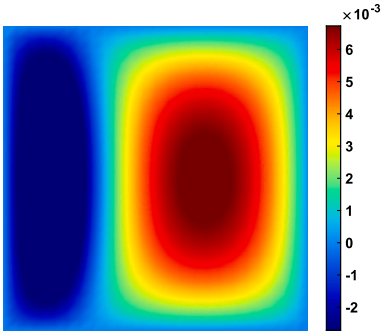
with δ_{ij} the Kronecker delta, γ the parameter of our problem and $\epsilon(u)$ the strain tensor, defined as,

$$\epsilon_{ij}(u) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right). \tag{34}$$

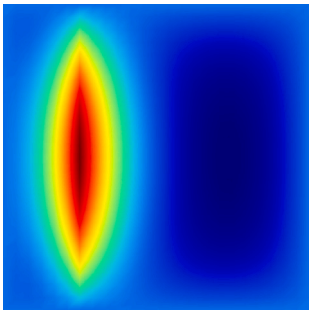
This problem could model blocks of different materials fixed on one side and under the action of gravity. It admits the following weak formulation



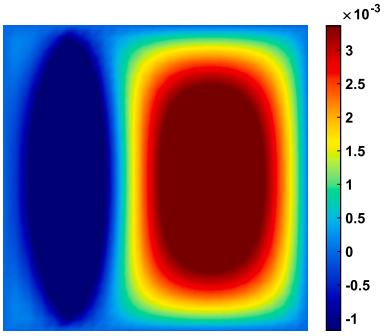
(a) Error for subspace of dimension equal to 1.



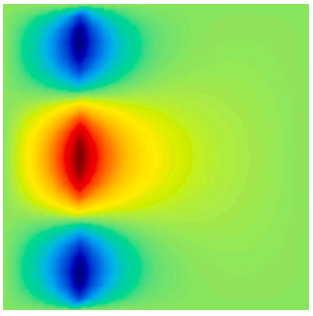
(b) Error for subspace of dimension equal to 1.



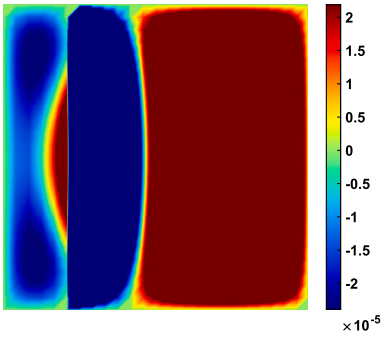
(c) Error for subspace of dimension equal to 2.



(d) Error for subspace of dimension equal to 2.



(e) Error for subspace of dimension equal to 3.



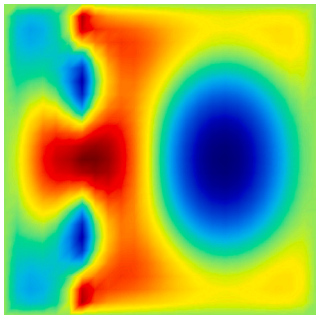
(f) Error for subspace of dimension equal to 3.

Fig. 3. Comparison of the errors obtained between the reduced solutions and the parametric solution $u(\gamma)$ for $\gamma = 0.3$. Errors in the left panels are the ones obtained by means of Algorithm 4 and the ones on the right panels are the ones obtained by means of the PI Algorithm presented in [18]. (Part 1: Dimensions 1 (top), 2 (middle), 3 (bottom)).

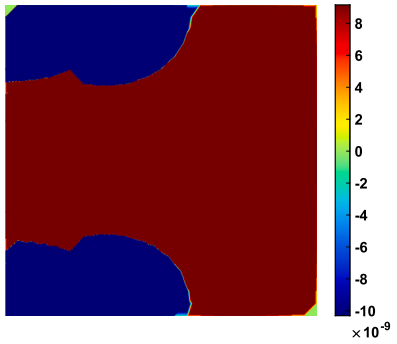
$$\begin{cases} \text{Find } u(\gamma) \in H^1_{\partial\Omega_2}(\Omega) \text{ such that} \\ \displaystyle\int_\Omega \sigma(u) : \epsilon(v) = \int_\Omega f \cdot v, \quad \forall v \in H^1_{\partial\Omega_2}(\Omega), \end{cases} \tag{35}$$

where $H^1_{\partial\Omega_2}(\Omega) := \{v \in H^1(\Omega) \text{ such that } v|_{\partial\Omega_2} = 0\}$.

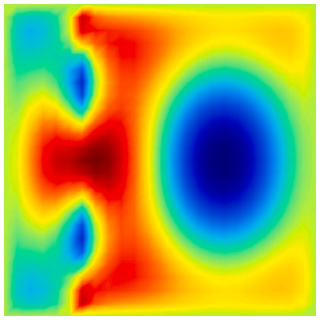
Once again, thanks to the properties of σ, ϵ and f, Lax-Milgram Theorem assures the existence and uniqueness of a solution of problem (35). For this test case, we will set the domain as a rectangle, $\Omega = (0, 10) \times (0, 2)$, the only external force will be a normalized gravity $f(x, y) = (0, -10^{-3})$, and the parameter $\gamma \in \Gamma = [0.5, 5]$, represents a relationship between the Lamé parameters. Boundary conditions impose that the rectangle is fixed on the left. The integrals on Γ are addressed as done in the previous test.



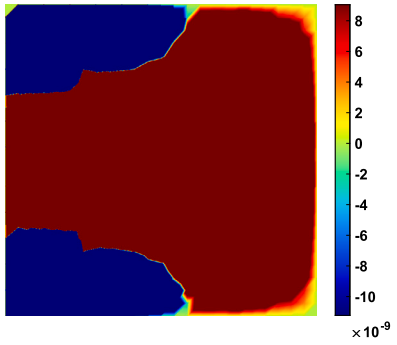
(a) Error for subspace of dimension equal to 4.



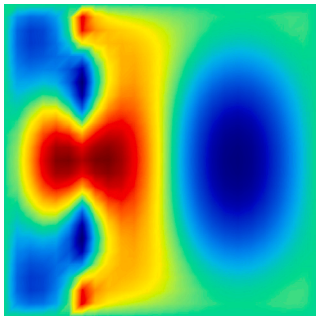
(b) Error for subspace of dimension equal to 4.



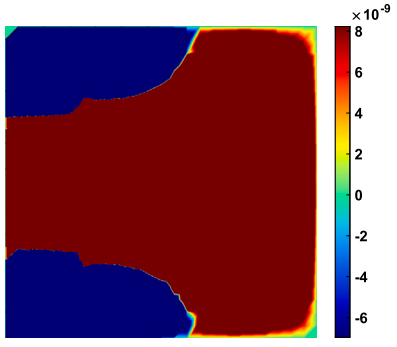
(c) Error for subspace of dimension equal to 5.



(d) Error for subspace of dimension equal to 5.



(e) Error for subspace of dimension equal to 6.



(f) Error for subspace of dimension equal to 6.

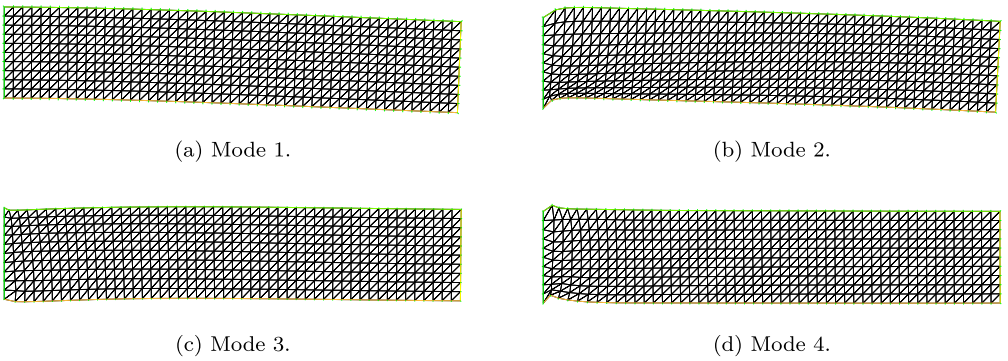
Fig. 4. Comparison of the errors obtained between the reduced solutions and the parametric solution $u(\gamma)$ for $\gamma = 0.3$. Errors in the left panels are the ones obtained by means of Algorithm 4 and the ones on the right panels the ones obtained by means of the PI Algorithm presented in [18]. (Part 2: Dimensions 4 (top), 5 (middle), 6 (bottom)).

After applying Algorithm 3, we obtain the intrinsic PGD modes that can be seen in Fig. 5. We can see that the first mode represents the main deformation of the block, the second mode represents some corrections in the borders of the block near the fixed side and modes three and four represent further corrections more localized.

As done in the previous test, we also examine the convergence of the PGD expansion u_i given by formula (26) to the original solution $u(\gamma)$ in both $L^2(\Gamma, L^2(\Omega)^2, d\mu)$ and $L^2(\Gamma, H^1(\Omega)^2, d\mu)$ norms. We show in Fig. 6 the truncation errors measured in those two norms in logarithm scale versus the dimension of the reduced space. As in the previous test, we can see that the error decay is very sharp and that we obtain a very good error in both norms after just a few modes.

We also present the same convergence of the truncated series for each component of the displacement vector in Fig. 7 in both $L^2(\Gamma, L^2(\Omega), d\mu)$ and $L^2(\Gamma, H^1(\Omega), d\mu)$ norms. We can see that we seem to obtain a slightly better approximation of the x component than of the y component. Nevertheless, both components show a very efficient error decay in both norms.

As well as done for the diffusion problem, we present in Fig. 8, for each dimension of the subspace, the modulus of the truncation error between the reduced solution and the parametric solution of problem (32) obtained by means of Algorithm 4 in the whole



(a) Mode 1. (b) Mode 2.

(c) Mode 3. (d) Mode 4.

Fig. 5. Intrinsic PGD modes of problem (32) obtained by means of Algorithm 4. Deformations are presented in scale with respect to the modulus of the deformation.

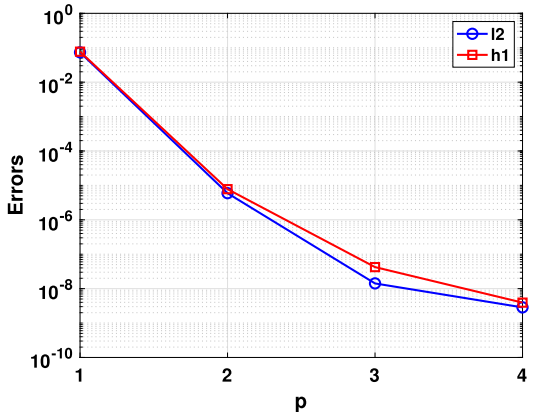


Fig. 6. Convergence of the PGD expansions u_i to $u(\gamma)$ as specified in (31). Blue circles represent the L^2 norm, while red squares represent the H^1 norm.

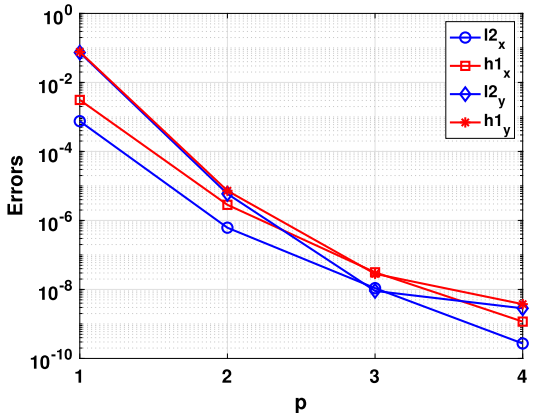
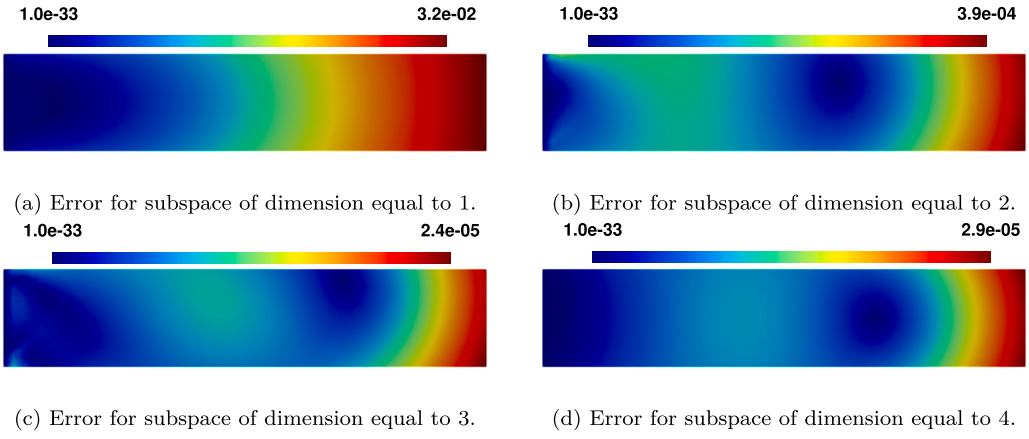


Fig. 7. Convergence history of the x and y components of the PGD expansion u_i to the x and y components of $u(\gamma)$ as specified in (31). Blue circles and red squares represent respectively the L^2 and H^1 norm of the x component of the PGD expansion, and blue diamonds and red asterisks represent respectively the L^2 and H^1 norm of the y component.

domain for a fixed instance of the parameter $\gamma = 1$. We can clearly see that the errors are accumulated on the right part of the block, as it is the part under the most influence of the gravity. We can see that in the fourth iteration the numerical artifacts that appeared in the left part of the block after the second iteration disappear and that the maximum of the error is of order 10^{-5} after the third iteration.

These results support the use of this novel procedure presented in Algorithm 4 to obtain the intrinsic PGD modes of parametric symmetric problems.



(a) Error for subspace of dimension equal to 1.

(b) Error for subspace of dimension equal to 2.

(c) Error for subspace of dimension equal to 3.

(d) Error for subspace of dimension equal to 4.

Fig. 8. Modulus of the errors obtained by means of Algorithm 4 for problem (32) for different optimal subspace dimensions between the reduced solution and the parametric solution for $\gamma = 1$. From left to right and from top to bottom, dimensions of the subspace are a) Dimension 1, b) Dimension 2, c) Dimension 3, d) Dimension 4.

5. Conclusions and further development

In this work, we have developed a novel technique based on the GD on matrix spaces (Algorithm 2) to obtain the intrinsic PGD modes of parametric symmetric problems. Furthermore, we have also presented the one-dimensional variants of this technique (Algorithm 3) and coupled them with a deflation algorithm in order to obtain higher-dimensional optimal subspaces avoiding some numerical computations whose cost would be excessive (Algorithm 4).

We have also tested Algorithm 4 in two physical parametric symmetric problems, a diffusion problem that had been tested with the intrinsic PGD method before in the literature and that allowed us to validate our procedure, and a classical elastostatics problem in which the solution has two components. This method has been proven to produce very accurate approximations of the original parametric solutions of both problems, reaching relative errors of order 10^{-8} after just few intrinsic PGD modes, and improving the error decay obtained by the procedures already present in the literature for the intrinsic PGD.

Therefore, this novel technique based on the GD on matrix spaces is a very promising tool in the obtention of the intrinsic PGD modes of parametric symmetric problems.

In future works, we intend to apply these techniques to higher-dimensional problems, and we also aim to develop similar techniques also based on the GD on matrix spaces suitable to parametric nonsymmetric problems. Another perspective is to develop accelerated GD procedures, like Nesterov algorithm and other optimization techniques, such as the Newton method in the intrinsic PGD framework. Furthermore, we aim to couple the presented technique with a tensor decomposition by variables in order to calculate high-dimensional solutions from a sequence of 1D problems. Moreover, we could perform a comparison between this technique with other Reduced Order Model approaches.

Data availability

No data was used for the research described in the article.

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Appendix A. Proofs of technical results

In this Appendix, we collect the proofs of some results introduced along the article.

A.1. Proof of Proposition 3.1

In order to simplify some calculations, we need to state two technical lemmas from [21,22], where their proofs can be found. The first one is related to the derivative of an inverse matrix.

Lemma A.1. *Let A be a nonsingular matrix, then its derivative can be expressed as follows,*

$$d(A^{-1}) = -A^{-1}d(A)A^{-1}.$$

And the other one is related to a multiplication property of the matrix derivative.

Lemma A.2. *Let a and b be two vectors and A a matrix, then the following equality follows,*

$$a^T d(A)b = a \otimes b = ab^T,$$

where $\otimes$ denotes the external product.

Now that the two technical lemmas have been presented, we can start the proof of Proposition 3.1. For the sake of brevity, we name $h(Z) = -F(Z)$ and we omit the dependence of matrix A and vector b on the parameter γ and the integral on Γ, as it does not affect the following computations.

First, we know the dependence of h on the matrix Z explicitly,

$$h(Z) = b^T Z (Z^T A Z)^{-1} Z^T b, \tag{A.1}$$

so, using the product rule, the derivative can be expressed as follows,

$$dh(Z) = b^T dZ (Z^T A Z)^{-1} Z^T b + b^T Z d((Z^T A Z)^{-1}) Z^T b + b^T Z (Z^T A Z)^{-1} dZ^T b. \tag{A.2}$$

Now, taking into account Lemma A.1 and regrouping, we obtain,

$$\begin{aligned} dh(Z) = \; & b^T dZ (Z^T A Z)^{-1} Z^T b + b^T Z (Z^T A Z)^{-1} dZ^T b \\ & - b^T Z [(Z^T A Z)^{-1} (dZ^T A Z + Z^T A dZ)(Z^T A Z)^{-1}] Z^T b. \end{aligned} \tag{A.3}$$

Noticing that A is symmetric, we can express (A.3) as,

$$dh(Z) = 2[b^T dZ (Z^T A Z)^{-1} Z^T b - b^T Z (Z^T A Z)^{-1} Z^T A dZ (Z^T A Z)^{-1} Z^T b], \tag{A.4}$$

and applying Lemma A.2 we can express it as,

$$\begin{aligned} dh(Z) = \; & 2[bb^T Z (Z^T A Z)^{-1} - AZ (Z^T A Z)^{-1} Z^T bb^T Z (Z^T A Z)^{-1}] \\ = \; & 2[I_n - AZ (Z^T A Z)^{-1} Z^T] bb^T Z (Z^T A Z)^{-1}. \end{aligned} \tag{A.5}$$

And that is the desired result.

A.2. Proof of Proposition 3.5

First, we know that $Z^T \nabla F(Z) = 0_k$ as $\nabla F(Z) \in T_Z St(n,k)$. So let $U \Sigma V^T$, be the compact singular value decomposition of $\nabla F(Z)$, so $U \in \mathbb{R}^{n \times r}$ is a semi-unitary, Σ is a diagonal nonsingular matrix in $\mathbb{R}^{r \times r}$, and $V \in \mathbb{R}^{k \times r}$ is a semi-unitary, where r is the number of non-zero singular values.

It follows that, $Z^T U \Sigma V^T = 0_k$ implies $Z^T U = 0_k$, after two right-multiplications, one by V, so $V^T V = I_r$ as V is semi-unitary, and another one by Σ^{-1}, leading us to the previous result. Then, if we left-multiply $\tilde{Z}$ by its transpose, we obtain the following

$$\begin{aligned} \tilde{Z}^T \tilde{Z} = \; & V(\cos(t\Sigma)^T V^T Z^T + \sin(t\Sigma) U^T)(ZV \cos(t\Sigma) + U \sin(t\Sigma)) V^T \\ = \; & V(\cos(t\Sigma)^T \cos(t\Sigma) + \sin(t\Sigma)^T \sin(t\Sigma) + \\ & + \cos(t\Sigma)^T V^T Z^T U \sin(t\Sigma) + \sin(t\Sigma)^T U^T Z V \cos(t\Sigma)) V^T, \end{aligned}$$

where the last two terms cancel because $Z^T U = 0_k$, and we obtain

$$\tilde{Z}^T \tilde{Z} = V(\cos(t\Sigma)^T \cos(t\Sigma) + \sin(t\Sigma)^T \sin(t\Sigma)) V^T = I_k.$$

So, matrix $\tilde{Z}$ arising from the retraction (16) is orthonormal, and therefore $\tilde{Z} \in St(n,k)$, which is the desired result.

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