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TOWARD GUARANTEED PGD-REDUCED MODELS

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Abstract. In this paper, a verification approach is introduced to build guaranteed PGD-reduced models for linear elliptic or parabolic problems depending on parameters. It is based on the concept of constitutive relation error and provides for strict bounds on both global error and error on outputs of interest defined with respect to the reference multi-parameter model. It also enables to assess contributions of various error sources, which helps driving adaptive strategies. Consequently, virtual charts associated with quantities of interest and computed from PGD models can satisfy a prescribed accuracy. Numerical experiments on transient thermal conduction illustrate the proposed verification approach and its performances.

Key words: Model Reduction, Verification, Error Estimation, Proper Generalized Decomposition, Separated Representation, Constitutive Relation Error.

1 INTRODUCTION

Nowadays, numerical simulation constitutes a common tool in science and engineering activities. It is especially used for prediction and decision making, or simply for a better understanding of physical phenomena. However, in order to give an accurate representation of the real world, a large set of parameters may need to be introduced in the mathematical models involved in the simulation, which leads to important (and often overwhelming) computational efforts. This is for example the case when dealing with models that aim at taking uncertainties into account, or in optimization problems. A drawback of such complex multi-parameter models is the fact that they usually lead to a huge number of degrees of freedom (due to the so-called *curse of dimensionality*)

so that they can not be tackled with classical brute force methods. Therefore, alternatives numerical approaches are necessary. For that purpose, model reduction methods exploit the fact that the response of complex models can often be approximated with a reasonable precision by the response of a surrogate model, seen as the projection of the initial model on a low-dimensional functional basis [1–4]. Model reduction methods distinguish themselves by the way of defining and constructing the reduced basis.

One of the promising model order reduction methods is the PGD which was introduced as radial loading approximation in [5]. It is nowadays named *Proper Generalized Decomposition* (PGD) [6] as it can be seen as a POD extension. The PGD approximation does not require any knowledge on the solution (it is thus referred as *a priori*) and does not use any orthogonality property. It operates in an iterative strategy in which a set of simple problems, that can be seen as pseudo eigenvalue problems, need to be solved. PGD has been developed during years for solving time-dependent nonlinear problems in Structural Mechanics [5, 7, 8] as a key-point of the so-called *LATIN method*. Extension to stochastic problems, initially under the name *Generalized Spectral Decomposition*, has been done in [9]. The PGD approach has also lead to major breakthroughs for real-time simulation [10], decision making tools [11], as well as multidimensional [12] or multiphysics [13] problems.

Even though PGD is usually very effective, a major question is to derive verification tools for controlling the calculation process. Basic results on a priori error estimation for representation using separation of variables can be found in [7], and a first work providing for strict bounds on global error in the PGD context is [14], in which specific error indicators are also given.

In this paper, after recalling the verification tools introduced in [14], we present a new approach for deriving guaranteed PGD-reduced models for linear elliptic or parabolic problems depending on parameters. The goal here is not to construct new numerical techniques to get the PGD approximation; the simplest greedy algorithm, i.e. the so-called *progressive Galerkin technique*, is used in the applications. We rather aim at controlling the PGD approximation by setting up robust global and goal-oriented error estimators, enabling to assess the quality of the global PGD solution as well as that of outputs of interest. Numerical experiments on transient thermal conduction illustrate the proposed verification approach and its performances.

2 REFERENCE PROBLEM AND NOTATIONS

We consider a transient diffusion problem defined on an open bounded domain $\Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3$), with boundary $\partial\Omega$, over a time interval $\mathcal{I} = [0, T]$. We assume that a prescribed zero temperature is applied on part $\partial_u\Omega \neq \emptyset$ of $\partial\Omega$ and that the domain is subjected to a time-dependent thermal loading that consists of: (i) a given thermal flux $r_d(\mathbf{x}, t)$ on $\partial_q\Omega \subset \partial\Omega$, with $\partial_u\Omega \cap \partial_q\Omega = \emptyset$ and $\overline{\partial_u\Omega} \cup \overline{\partial_q\Omega} = \partial\Omega$; (ii) a source term $f_d(\mathbf{x}, t)$ in Ω .

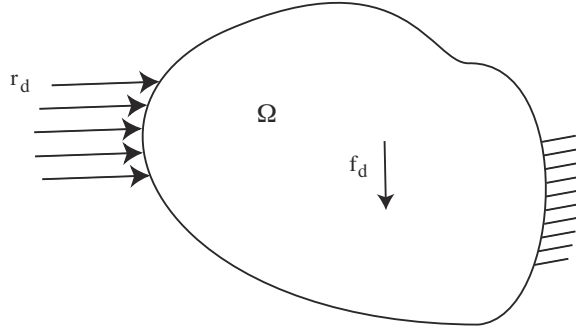


Figure 1. Representation of the reference problem.

The material that composes Ω is assumed to be isotropic. Furthermore, for the sake of simplicity, we consider that initial conditions are zero. The problem thus consists of finding the temperature-flux pair $(u(\mathbf{x}, t), \mathbf{q}(\mathbf{x}, t))$, with $(\mathbf{x}, t) \in \Omega \times \mathcal{I}$, that verifies:

- the thermal constraints:

$$u = 0 \quad \text{in } \partial_u \Omega \times \mathcal{I} \quad (1)$$

- the equilibrium equations:

$$\frac{\partial u}{\partial t} = -\nabla \cdot \mathbf{q} + f_d \quad \text{in } \Omega \times \mathcal{I} \quad ; \quad \mathbf{q} \cdot \mathbf{n} = r_d \quad \text{in } \partial_q \Omega \times \mathcal{I} \quad (2)$$

- the constitutive relation:

$$\mathbf{q} = -k \nabla u \quad \text{in } \Omega \times \mathcal{I} \quad (3)$$

- the initial conditions:

$$u(\mathbf{x}, 0^+) = 0 \quad \forall \mathbf{x} \in \Omega \quad (4)$$

where \mathbf{n} denotes the outgoing normal to Ω , and k is a positive material parameter. In the following, in order to be consistent with other linear problems encountered in Mechanics (linear elasticity for instance), we carry out the change of variable $\mathbf{q} \rightarrow -\mathbf{q}$ which leads, in particular, to the new constitutive relation $\mathbf{q} = k \nabla u$.

Defining $\mathcal{V} = H_0^1(\Omega) = \{v \in H^1(\Omega), v|_{\partial_u \Omega} = 0\}$, the weak formulation in space of the diffusion problem consists of finding $u(\mathbf{x}, t)$, with $u(\cdot, t) \in \mathcal{V}$ for all $t \in \mathcal{I}$, such that:

$$\begin{aligned} b(u, v) &= l(v) \quad \forall v \in \mathcal{V}, \forall t \in \mathcal{I} \\ u|_{t=0^+} &= 0 \end{aligned} \quad (5)$$

where bilinear form $b(\bullet, \bullet)$ and linear form $l(\bullet)$ are defined as:

$$b(u, v) = \int_{\Omega} \left\{ \frac{\partial u}{\partial t} v + k \nabla u \cdot \nabla v \right\} d\Omega \quad ; \quad l(v) = \int_{\Omega} f_d v d\Omega - \int_{\partial_q \Omega} r_d v dS \quad (6)$$

As regards the space-time weak formulation, we introduce functional spaces $\mathcal{T} = L^2(\mathcal{I})$ and $L^2(\mathcal{I}; \mathcal{V}) = \mathcal{V} \otimes \mathcal{T}$. We therefore search the solution $u \in L^2(\mathcal{I}; \mathcal{V})$ such that $\dot{u} \in L^2(\mathcal{I}; L^2(\Omega))$ and

$$B(u, v) = L(v) \quad \forall v \in L^2(\mathcal{I}; \mathcal{V}) \quad (7)$$

with

$$B(u, v) = \int_0^T b(u, v) dt + \int_{\Omega} u(\mathbf{x}, 0^+) v(\mathbf{x}, 0^+) d\Omega \quad ; \quad L(v) = \int_0^T l(v) dt \quad (8)$$

Problem (7) is classically solved using the FEM in space associated with a time integration scheme, or a (discontinuous) Galerkin approximation in time. The exact solution of (7), which is usually out of reach, is denoted $(u_{ex}, \mathbf{q}_{ex})$.

Eventually, we also assume that the material may be heterogeneous and partially unknown, so that k depends on a set of parameters $\boldsymbol{\theta} \in \Theta$. We thus define:

$$\tilde{B}(\bullet, \bullet) = \int_{\Theta} B(\bullet, \bullet) d\theta \quad ; \quad \tilde{L}(\bullet) = \int_{\Theta} L(\bullet) d\theta \quad (9)$$

and the solution of the problem reads $u(\mathbf{x}, t, \boldsymbol{\theta})$.

3 CONSTRUCTION OF THE PGD APPROXIMATION

We now introduce the recently called *Proper Generalized Decomposition* (PGD) technique [6, 12, 15, 16] which constitutes an *a priori* construction of a separated representation of the solution u , under the form:

$$u(\mathbf{x}, t, \boldsymbol{\theta}) \approx u_m(\mathbf{x}, t, \boldsymbol{\theta}) \equiv \sum_{i=1}^m \psi_i(\mathbf{x}) \lambda_i(t) \mu_i(\boldsymbol{\theta}) \quad (10)$$

An attractive feature of this technique is that it does not require any knowledge on u ; neither functions $\psi_i(\mathbf{x})$ nor functions $\lambda_i(t)$ and $\mu_i(\boldsymbol{\theta})$ are initially given; these are computed on the fly. In this section, we give a classical version of the PGD technique, called *progressive Galerkin-based PGD*.

We assume that a PGD approximation of order $m - 1$ has been computed. The PGD approximation of order m is then defined as

$$u_m(\mathbf{x}, t, \boldsymbol{\theta}) = u_{m-1}(\mathbf{x}, t, \boldsymbol{\theta}) + \psi(\mathbf{x}) \lambda(t) \mu(\boldsymbol{\theta}) \quad (11)$$

where ψ , λ , and μ are a priori unknown functions belonging respectively to the discretized subsets \mathcal{V}_h , \mathcal{T}_h , and \mathcal{P}_h ; \mathcal{V}_h and \mathcal{T}_h respect kinematic constraints and initial conditions, respectively. Starting from an initialization $\psi \lambda \mu$, one builds a new triplet $\bar{\psi} \bar{\lambda} \bar{\mu}$ thanks to the following sub-iteration:

- determine $\bar{\lambda} \in \mathcal{T}_h$ such that:

$$\tilde{B}(u_{m-1} + \bar{\lambda}\psi\mu, \lambda^*\psi\mu) = \tilde{L}(\lambda^*\psi\mu) \quad \forall \lambda^* \in \mathcal{T}_h \quad (12)$$

- determine $\bar{\mu} \in \Theta_h$ such that:

$$\tilde{B}(u_{m-1} + \bar{\lambda}\psi\bar{\mu}, \bar{\lambda}\psi\mu^*) = \tilde{L}(\bar{\lambda}\psi\mu^*) \quad \forall \mu^* \in \mathcal{P}_h \quad (13)$$

- determine $\bar{\psi} \in \mathcal{V}_h$ such that:

$$\tilde{B}(u_{m-1} + \bar{\lambda}\bar{\psi}\bar{\mu}, \bar{\lambda}\psi^*\bar{\mu}) = \tilde{L}(\bar{\lambda}\psi^*\bar{\mu}) \quad \forall \psi^* \in \mathcal{V}_h \quad (14)$$

Few sub-iterations are performed in practice; in the following examples, the process has been stopped after 4 sub-iterations. It is shown in [16] that the best PGD approximation could be interpreted in terms of eigenfunctions of a pseudo eigenvalue problem. This interpretation is fruitful in the sense that it allows to propose dedicated algorithms inspired from classical algorithms for eigenvalue problems.

4 GLOBAL ERROR ESTIMATION IN THE PGD FRAMEWORK

4.1 The Constitutive Relation Error method – Principle

Let $(\hat{u}, \hat{\mathbf{q}})$ be an admissible solution of the problem, i.e. verifying (1), (2), and (4). The Constitutive Relation Error (CRE) reads:

$$E_{CRE}^2(\hat{u}, \hat{\mathbf{q}}) = \frac{1}{2} \int_0^T \int_{\Omega} \frac{1}{k} [\hat{\mathbf{q}} - k\nabla\hat{u}] \cdot [\hat{\mathbf{q}} - k\nabla\hat{u}] d\Omega dt \equiv \frac{1}{2} ||| \hat{\mathbf{q}} - k\nabla\hat{u} |||_q^2 \quad (15)$$

and one has the equivalent of the Prager–Synge theorem:

$$||| \mathbf{q}_{ex} - \mathbf{q}^* |||_q^2 + \frac{1}{2} \int_{\Omega} (u_{ex} - \hat{u})_T^2 d\Omega = \frac{1}{2} E_{CRE}^2(\hat{u}, \hat{\mathbf{q}}) \quad (16)$$

with $\mathbf{q}^* = \frac{1}{2}[\hat{\mathbf{q}} + k\nabla\hat{u}]$. All these quantities depend on $\boldsymbol{\theta} \in \Theta$.

4.2 Construction of an admissible solution

For the construction of the kinematically admissible field $\hat{u}(\mathbf{x}, t, \boldsymbol{\theta})$, one takes as usual:

$$\hat{u} = u_m = \sum_{i=1}^m \psi_i \lambda_i \mu_i \quad (17)$$

Getting $\hat{\mathbf{q}}(\mathbf{x}, t, \boldsymbol{\theta})$ is more difficult and technical. First, one constructs $\mathbf{q}_m(\mathbf{x}, t, \boldsymbol{\theta})$ which should satisfy the following FE equilibrium for all $(t, \boldsymbol{\theta}) \in [0, T] \times \Theta$:

$$\int_{\Omega} \mathbf{q}_m \cdot \nabla u^* d\Omega = \int_{\Omega} (f_d - \frac{\partial \hat{u}}{\partial t}) u^* d\Omega - \int_{\partial_q \Omega} r_d u^* dS \quad \forall u^* \in \mathcal{V}_h \quad (18)$$

For the sake of simplicity, let us suppose that the loading can be written:

$$(f_d, r_d) = \sum_{j=1}^J \alpha_j(t) \left(f_d^j(\mathbf{x}), r_d^j(\mathbf{x}) \right) \quad (19)$$

and that we compute a FE approximation of:

$$\begin{aligned} -\operatorname{div} k \nabla v^j &= f_d^j \\ -k \nabla v^j \cdot \mathbf{n} &= r_d^j \quad \text{on } \partial_q \Omega \\ v^j &= 0 \quad \text{on } \partial_u \Omega \end{aligned} \quad (20)$$

It follows that $\mathbf{q}_d = \sum_{j=1}^J \alpha_j(t) k \nabla v^j$ can be introduced in the calculation of \mathbf{q}_m , which should then verify for all $(t, \theta) \in [0, T] \times \Theta$:

$$\int_{\Omega} (\mathbf{q}_m - \mathbf{q}_d) \cdot \nabla u^* \, d\Omega = - \int_{\Omega} \frac{\partial \hat{u}}{\partial t} u^* \, d\Omega = - \sum_{i=1}^m \dot{\lambda}_i \mu_i \int_{\Omega} \psi_i u^* \, d\Omega \quad \forall u^* \in \mathcal{V}_h \quad (21)$$

Noticing that at the end of sub-iterations to compute each PGD mode $m_0 \in [1, m]$, condition (14) yields:

$$\tilde{B}(u_{m_0}, \lambda_{m_0} \mu_{m_0} \psi^*) = \tilde{L}(\lambda_{m_0} \mu_{m_0} \psi^*) \quad \forall \psi^* \in \mathcal{V}_h \quad (22)$$

we thus get:

$$\begin{aligned} & \int_{\Omega} \left[\int_{\Theta} \int_0^T \lambda_{m_0} \mu_{m_0} (k \nabla u_{m_0} - \mathbf{q}_d) \, dt \, d\theta \right] \nabla \psi^* \, d\Omega = \\ & - \int_{\Omega} \left[\int_{\Theta} \int_0^T \lambda_{m_0} \mu_{m_0} \frac{\partial u_{m_0}}{\partial t} \, dt \, d\theta \right] \psi^* \, d\Omega \quad \forall \psi^* \in \mathcal{V}_h = \\ & - \int_{\Omega} \sum_{k=1}^{m_0} \left[\int_{\Theta} \int_0^T \lambda_{m_0} \mu_{m_0} \dot{\lambda}_k \mu_k \, dt \, d\theta \right] \psi_k \psi^* \, d\Omega \quad \forall \psi^* \in \mathcal{V}_h \end{aligned} \quad (23)$$

It follows that for $m_0 \in [1, m]$, term:

$$\mathbf{Q}_{m_0} \equiv \int_{\Theta} \int_0^T \lambda_{m_0} \mu_{m_0} (\mathbf{q}_d - k \nabla u_{m_0}) \, dt \, d\theta \quad (24)$$

equilibrates $\sum_{k=1}^{m_0} \left[\int_{\Theta} \int_0^T \lambda_{m_0} \mu_{m_0} \dot{\lambda}_k \mu_k \, dt \, d\theta \right] \psi_k$ in a FE sense. By a simple inversion of the system, one obtains that a term of the form $\sum_{j=1}^m R_{ij} \mathbf{Q}_j$ equilibrates ψ_i in the FE sense ($i = 1, \dots, m$). Consequently,

$$\mathbf{q}_m = \mathbf{q}_d - \sum_{i=1}^m \sum_{j=1}^m \dot{\lambda}_i \mu_i R_{ij} \mathbf{Q}_j \quad (25)$$

satisfies the FE equilibration (18) (or (21)). Moreover, it admits a PGD description:

$$\mathbf{q}_m = \mathbf{q}_d + \sum_{i=1}^q \mathbf{q}_i(\mathbf{x}) z_i(t) s_i(\boldsymbol{\theta}) \quad (26)$$

Then, usual techniques to build an equilibrated flux $\hat{\mathbf{q}}$ (verifying (2)) from \mathbf{q}_m can be used. Full details on these techniques can be found in [17–20]; here, we specifically use the new technique introduced in [19, 20] which defines local problems on patches of elements, and represents a nice compromise between robustness, computational cost, and implementation facilities. We also refer to [21] for other approaches enabling to construct a statically admissible field. In the non material parameter case, the used technique is completely detailed in [14].

4.3 Specific error indicators

To control the computation process, specific error indicators are suitable. The indicator on the PGD error (i.e. the error due to truncation of the sum in the PGD representation (10)) is derived from the Constitutive Relation Error method considering as the reference problem the discretized (in space and time) one. This idea, not restricted to the PGD framework, has been applied in other works (see [17] for instance). The reference problem is then here of the form:

$$\mathbf{U}_h^1 = \mathbf{0} \quad ; \quad \mathbb{M} \frac{\mathbf{U}_h^{p+1} - \mathbf{U}_h^p}{\Delta t} + \mathbb{K} \mathbf{U}_h^p = \mathbf{F}_h^p \quad \forall p \in [1, P - 1] \quad (27)$$

where P is the number of time steps. A pair which is admissible for this problem is (u_m, \mathbf{q}_m) and the corresponding constitutive relation error reads:

$$E_{PGD}^2 = \frac{1}{2} \| \mathbf{q}_m - k \nabla u_m \|_q^2 \quad (28)$$

One then defines the error indicator on time and space discretizations by:

$$E_h^2 \equiv E_{CRE}^2 - E_{PGD}^2 \quad (29)$$

4.4 Illustration

We consider the 2D structure of Figure 2 which presents two rectangular holes in which a fluid circulates. Using symmetries, we keep a quarter of the 2D domain (upper right quarter) that we denote Ω . It is subjected to a given flux $r_d(t) = -1$ on the hole boundary, a zero flux on symmetry planes, and a given temperature $u_d = 0$ on other boundaries. A source term of the form $f_d(x, y) = 200xy$ is also applied in Ω .

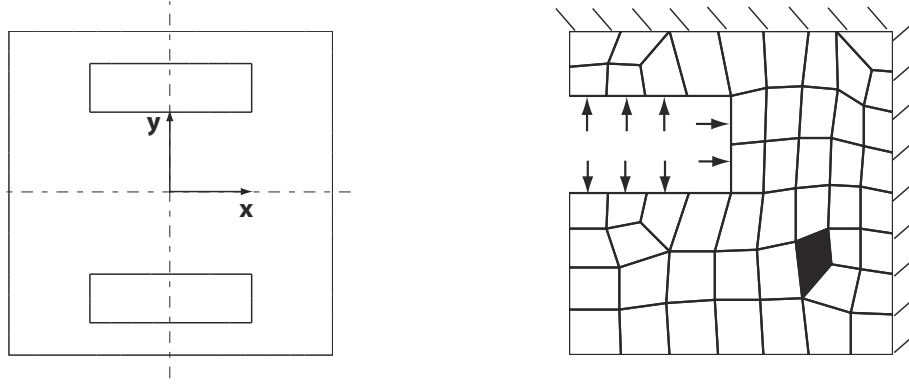


Figure 2. The 2D reference problem.

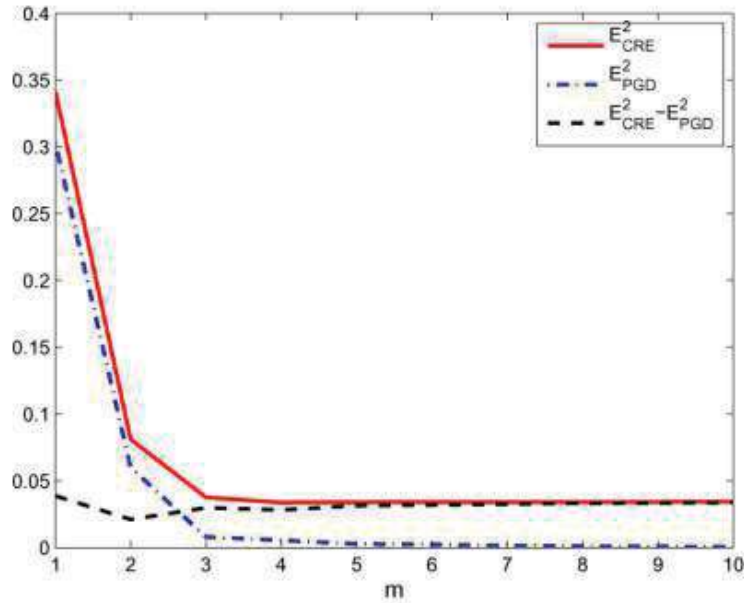


Figure 3. Error estimator and indicators with respect to the number m of PGD modes.

Figure 3 gives, for the case where $k = 1$ (no parameter θ), the constitutive relation error and specific error indicators with respect to the number of PGD modes taken in the approximation; we observe that after 3 modes, the only possibility to decrease the global error is to refine mesh and time discretizations.

5 UPPER ERROR BOUND ON AN OUTPUT OF INTEREST

Let I be an output of interest defined by extractor \mathbf{q}_Σ :

$$I(\theta) = \int_0^T \int_{\Omega} \mathbf{q}_\Sigma \cdot \nabla u(\mathbf{x}, t, \theta) d\Omega dt \quad (30)$$

$\mathbf{q}_\Sigma(\mathbf{x}, t)$ could be a Dirac distribution. Introducing the associated adjoint problem, the fundamental result for linear elliptic and parabolic problems is [22]:

$$|I_{ex} - I_h - I_{hh}| \leq E_{CRE} \tilde{E}_{CRE} \quad (31)$$

where I_{ex} (resp. I_h) is the exact (resp. approximated by PGD) value of the output of interest, I_{hh} is a correction term computed from approximate solutions of both reference and adjoint problems, and E_{CRE} (resp. \tilde{E}_{CRE}) is the constitutive relation error of the reference (resp. adjoint) problem. To solve the adjoint problem, one uses a PGD approximation following the progressive Galerkin technique used to solve the reference problem.

Two illustrations are given below, considering again the reference problem of Figure 2 and assuming now that k is probabilistic in $\omega \subset \Omega$ (black zone in Figure 2), i.e.:

$$k(\mathbf{x}, \theta) = 1 + 0.1 I_\omega(\mathbf{x}) \theta \quad (32)$$

where I_ω is the indicatrix function of ω , and $\theta \in [-2, 2]$ has a (truncated) normal distribution.

We first consider as an output of interest the mathematical expectation (in the probabilistic sense) of the mean value of u inside ω at time T :

$$I_1 = \mathbb{E} \left[\frac{1}{|\omega|} \int_\omega u|_T d\Omega \right] \quad (33)$$

where $E(\bullet) = \int_\Theta \bullet dP$, dP being the probability measure. The normalized upper bound $\int_\Theta E_{CRE} \tilde{E}_{CRE} dP / |I_{1h}|$ of the error, as well as specific error indicators, are given in Figure 4 (left) with respect to the number M of computed PGD modes for the adjoint solution.

We now consider as an output of interest the maximal value (over $\Theta = [-2, 2]$) of the mean value of u inside ω at time T :

$$I_2 = \sup_{\theta \in \Theta} \frac{1}{|\omega|} \int_\omega u|_T d\Omega \quad (34)$$

The normalized upper bound $\sup_{\theta \in \Theta} (E_{CRE} \tilde{E}_{CRE}) / |I_{2h}|$ of the error, as well as specific error indicators, are given in Figure 4 (right) with respect to the number M of computed PGD modes for the adjoint solution.

Let us finally notice that the proposed verification approach, when related to a quantity of interest I , yields for all $\theta \in \Theta$:

$$\epsilon(\theta) = |I_{ex} - I_h - I_{hh}| \leq E_{CRE} \tilde{E}_{CRE} \quad (35)$$

A convenient manner to control the error $\epsilon(\theta)$ is thus to control the error on the adjoint problem alone. This is easy to perform if the output of interest is local in space variable. However, a refined discretization should be used in the zone of interest, and that should be done in a black box manner.

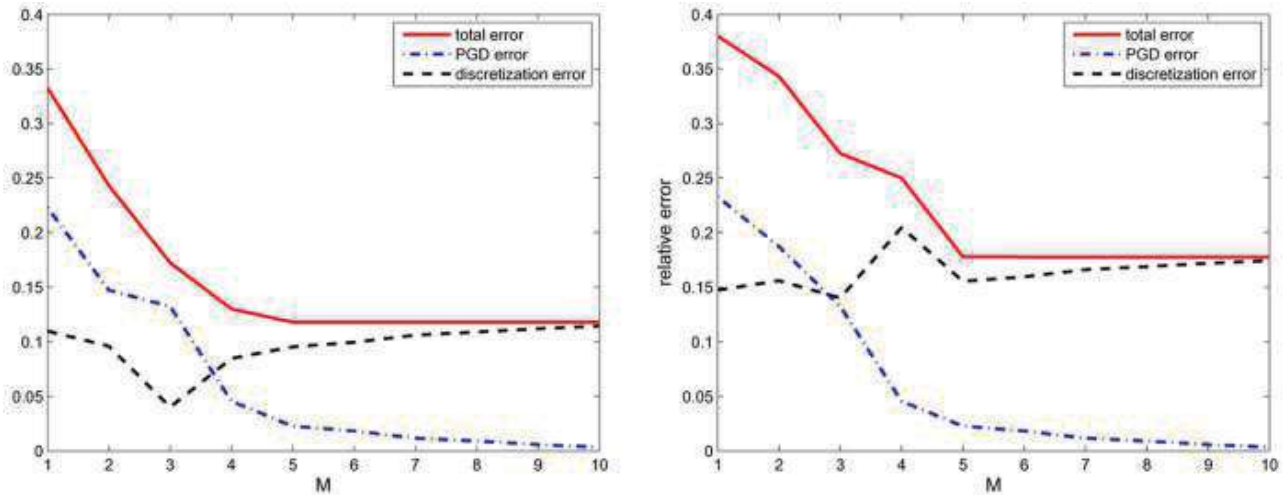


Figure 4. Normalized upper error bound and error indicators with respect to the number M of PGD modes used for the adjoint solution: I_1 (left), I_2 (right).

6 CONCLUSIONS

PGD-reduced models are a promising tool for solving complex engineering problems. However, a central and main question is to guarantee their accuracy. The verification method described here is a first attempt to address this challenge for elliptic and parabolic problems.

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