



**HAL**  
open science

## Recent advances in the control of PGD-based approximations

Ludovic Chamoin, Pierre Ladevèze, Florent Pled

► **To cite this version:**

Ludovic Chamoin, Pierre Ladevèze, Florent Pled. Recent advances in the control of PGD-based approximations. 6th International Conference on Adaptive Modeling and Simulation (ADMOS 2013), Jun 2013, Lisbon, Portugal. pp.170-181. hal-01057247

**HAL Id: hal-01057247**

**<https://hal.science/hal-01057247v1>**

Submitted on 21 Aug 2014

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# RECENT ADVANCES IN THE CONTROL OF PGD-BASED APPROXIMATIONS

LUDOVIC CHAMOIN\*, PIERRE LADEVEZE\*, AND FLORENT PLED\*

\*Laboratoire de Mécanique et Technologie (LMT-Cachan)  
Ecole Normale Supérieure de Cachan  
61 Avenue du Président Wilson, 94230 Cachan, France  
e-mail: {chamoin,ladeveze,pled}@lmt.ens-cachan.fr, www.lmt.ens-cachan.fr

**Key words:** Model reduction, Verification, Proper Generalized Decomposition, Constitutive relation error, Adjoint problem, Handbook techniques

**Abstract.** In this work, we define a verification procedure that enables to build guaranteed PGD-reduced models for linear elliptic or parabolic problems depending on many parameters. It is based on the general concept of constitutive relation error and provides for strict bounds on both global error and error on outputs of interest. Furthermore, it helps driving adaptive strategies by assessing contributions of various error sources. Consequently, virtual charts that may be constructed from the PGD approximate solution can be certified. Technicalities and performances of the control approach, in particular when dealing with a large set of model parameters, are detailed on a transient thermal problem.

## 1 INTRODUCTION

Due to the continuous advances in both modeling and computing resources, numerical simulation has become a common tool in science and engineering activities. Nowadays, it is numerically possible to deal with very complex models that aim at giving an accurate representation of the real world. However, due to an overwhelming computational effort, this practice remains difficult and often impossible when considering mathematical models with various fluctuating parameters. This case is for instance encountered when tackling stochastic or optimization problems in which a large amount of scenarios need to be considered. For such multi-parameter models, numerical simulation faces the so-called *curse of dimensionality* that leads to a huge number of degrees of freedom when using classical brute force (i.e. grid-based) approximation methods. Therefore, alternative computing approaches are necessary in this context.

During the last decade, model reduction techniques have been the object of a growing interest both in research and industry. They 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. Model reduction techniques, that distinguish themselves by the way of defining and constructing the reduced basis, are thus an appropriate computing tool for addressing multi-parameter models. In particular, an appealing model reduction technique called Proper Generalized Decomposition (PGD) has recently emerged and is currently the topic of various research works [1]. It is based on separation of variables within a spectral resolution approach, and contrary to the well-known POD, no partial knowledge on the solution is required which is a major asset. PGD basis functions (or modes) are computed on the fly, once for all and in an offline process, by solving a series of manageable mono-parameter problems. The obtained PGD approximation, that explicitly depends on all model parameters, can then be used in an online optimization process.

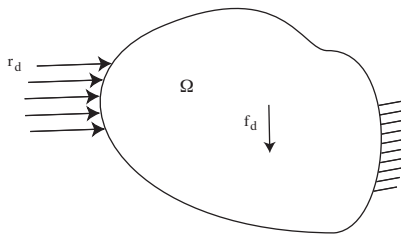
Performances of PGD have been shown in many applications for which variations in loading, boundary or initial conditions, material behavior, geometry,...were taken into account as additional model coordinates [2, 3, 4, 5]. However, a major difficulty for its transfer and intensive use in industry is the control of the PGD-reduced model. Indeed, certifying the accuracy of the PGD solution is a fundamental issue in order to perform robust and reliable design. This control requires mastering the number of PGD modes which are computed, but also the numerical methods which are employed in these computations.

There are actually very few works which have addressed the control of PGD-based approximations until now. Basic results on a priori error estimation for representations with separation of variables are given in [6], whereas a pioneering work mostly devoted to adaptivity can be found in [7]. A first robust approach for PGD verification, using the concept of Constitutive Relation Error (CRE) [8, 9], was proposed recently [10]. It applies to linear elliptic or parabolic problems depending on parameters, and provides for guaranteed PGD-reduced models for both global error and error on specific outputs of interest [11, 12]. Furthermore, the approach enables to assess contributions of various error sources (space and time discretizations, truncation of the PGD decomposition, etc.), which can help driving adaptive strategies.

In previous works [10, 11, 12], performances were shown with only few parameters. Here, we present new advances which have been performed in this PGD-verification method. We particularly focus on cases with numerous model parameters. We also use a non-intrusive procedure for the solution of the adjoint problem, in order to limit implementation issues. Therefore, virtual charts associated with quantities of interest and computed from PGD models can now fully benefit from the verification method to satisfy a prescribed accuracy. Numerical experiments on a transient thermal model with fluctuating material parameters are conducted to 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  $\Omega \subset R^d$  ( $d = 1, 2, 3$ ), 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  $\overline{\partial_u\Omega \cup \partial_q\Omega} = \partial\Omega$ ; (ii) a source term  $f_d(\mathbf{x}, t)$  in  $\Omega$ .



**Figure 1:** Representation of the reference problem.

For the sake of simplicity, we consider that initial conditions are set to zero. The material that composes  $\Omega$  is assumed to be isotropic but heterogeneous and partially unknown. Therefore, diffusion coefficient  $k$  and thermal capacity  $c$  depend on space variable  $\mathbf{x}$  but also on a set of  $N$  parameters  $\mathbf{p} = [p_1, p_2, \dots, p_N]$  belonging to a given bounded domain  $\Theta = \Theta_1 \times \Theta_2 \times \dots \times \Theta_N$ .

The associated mathematical problem consists of finding the temperature-flux pair  $(u(\mathbf{x}, t, \mathbf{p}), \boldsymbol{\varphi}(\mathbf{x}, t, \mathbf{p}))$ , with  $(\mathbf{x}, t, \mathbf{p}) \in \Omega \times \mathcal{I} \times \Theta$ , that verifies :

- the thermal constraints :

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

- the equilibrium equations :

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

- the constitutive relation :

$$\boldsymbol{\varphi} = -k \nabla u \quad \forall (\mathbf{x}, t, \mathbf{p}) \in \Omega \times \mathcal{I} \times \Theta \quad (3)$$

- the initial conditions :

$$u|_{t=0+} = 0 \quad \forall (\mathbf{x}, \mathbf{p}) \in \Omega \times \Theta \quad (4)$$

$\mathbf{n}$  denotes the outgoing normal to  $\Omega$ . 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  $\boldsymbol{\varphi} \rightarrow -\boldsymbol{\varphi}$  which leads, in particular, to the new constitutive relation

$$\boldsymbol{\varphi} = k \nabla u.$$

Defining  $\mathcal{V} = H_0^1(\Omega) = \{v \in H^1(\Omega), v|_{\partial_u \Omega} = 0\}$ , the weak formulation in space of the previous problem reads for all  $(t, \mathbf{p}) \in \mathcal{I} \times \Theta$  :

$$\text{Find } u(\mathbf{x}, t, \mathbf{p}) \in \mathcal{V} \text{ such that } b(u, v) = l(v) \quad \forall v \in \mathcal{V} \quad (5)$$

with  $u|_{t=0^+} = 0$ . Bilinear form  $b(\bullet, \bullet)$  and linear form  $l(\bullet)$  are defined as :

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

As regards the full weak formulation, we introduce the functional spaces  $\mathcal{T} = L^2(\mathcal{I})$ ,  $\mathcal{P}_i = L^2(\Theta_i)$ , and  $L^2(\mathcal{I}, \Theta; \mathcal{V}) = \mathcal{V} \otimes \mathcal{T} \otimes_{n=1}^N \mathcal{P}_n$ . We therefore search solution  $u \in L^2(\mathcal{I}, \Theta; \mathcal{V})$ , with  $\frac{\partial u}{\partial t} \in L^2(\mathcal{I}, \Theta; L^2(\Omega))$ , such that :

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

with

$$\begin{aligned} B(u, v) &= \int_{\Theta} \left[ \int_{\mathcal{I}} b(u, v) dt + \int_{\Omega} cu(\mathbf{x}, 0^+)v(\mathbf{x}, 0^+)d\Omega \right] d\mathbf{p} \\ L(v) &= \int_{\Theta} \int_{\mathcal{I}} l(v) dt d\mathbf{p} \end{aligned} \quad (8)$$

The exact solution of (7), which is usually out of reach, is denoted  $u_{ex}$  (and  $\boldsymbol{\varphi}_{ex} = k \nabla u_{ex}$ ). It is classically approximated using the FEM in space associated with a time integration scheme and a given grid in the parameter space  $\Theta$ .

*Remark* : in the steady-state case, we merely consider :

$$b(u, v) = \int_{\Omega} k \nabla u \cdot \nabla v d\Omega \quad ; \quad B(u, v) = \int_{\Theta} b(u, v) d\mathbf{p} \quad ; \quad L(v) = \int_{\Theta} l(v) d\mathbf{p} \quad (9)$$

### 3 CONSTRUCTION OF THE PGD APPROXIMATION

We now introduce the recently called *Proper Generalized Decomposition* (PGD) technique [1] which constitutes an *a priori* construction of a separated variables representation of the solution of (7). The approximate PGD solution is searched under the form :

$$u(\mathbf{x}, t, \mathbf{p}) \approx u_m(\mathbf{x}, t, \mathbf{p}) \equiv \sum_{i=1}^m \psi_i(\mathbf{x}) \lambda_i(t) \Gamma_i(\mathbf{p}) \quad \text{with } \Gamma_i(\mathbf{p}) = \prod_{n=1}^N \gamma_{i,n}(p_n) \quad (10)$$

$m$  is the order (i.e. number of modes) of the representation, whereas space functions  $\psi_i(\mathbf{x})$ , time functions  $\lambda_i(t)$ , and parameter functions  $\gamma_{i,n}(p_n)$  respectively belong to  $\mathcal{V}$ ,  $\mathcal{T}$ , and

$\mathcal{P}_n$ . An attractive feature of the PGD technique is that the construction of modes does not require any knowledge on  $u$ . Neither  $\psi_i(\mathbf{x})$  nor  $\lambda_i(t)$  nor  $\gamma_{i,n}(p_n)$  are initially given; these are computed on the fly. In the following, we give a classical version of the PGD technique, called *progressive Galerkin-based PGD* and inspired from classical fixed-point algorithms used to solve eigenvalue problems.

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

$$u_m(\mathbf{x}, t, \mathbf{p}) = u_{m-1}(\mathbf{x}, t, \mathbf{p}) + \psi(\mathbf{x})\lambda(t)\Gamma(\mathbf{p}) \quad \text{with } \Gamma(\mathbf{p}) = \prod_{n=1}^N \gamma_n(p_n) \quad (11)$$

$\psi$ ,  $\lambda$ , and  $\gamma_n$  ( $n = 1, \dots, N$ ) are a priori unknown functions belonging respectively to discretized subsets  $\mathcal{V}_h$ ,  $\mathcal{T}_h$ , and  $\mathcal{P}_{nh}$ ; we assume  $\mathcal{V}_h$  and  $\mathcal{T}_h$  respect kinematic constraints and initial conditions, respectively. Starting from an initialization  $\psi^{(0)}(\mathbf{x})\lambda^{(0)}(t)\Gamma^{(0)}(\mathbf{p})$ , one builds a new mode representation  $\psi^{(1)}(\mathbf{x})\lambda^{(1)}(t)\Gamma^{(1)}(\mathbf{p})$  thanks to the following sub-iteration :

- determine  $\lambda^{(1)} \in \mathcal{T}_h$  such that :

$$B(u_{m-1} + \psi^{(0)}\lambda^{(1)}\Gamma^{(0)}, \psi^{(0)}\lambda^*\Gamma^{(0)}) = L(\psi^{(0)}\lambda^*\Gamma^{(0)}) \quad \forall \lambda^* \in \mathcal{T}_h \quad (12)$$

- for  $n_0 = 1, \dots, N$ , determine  $\gamma_{n_0}^{(1)} \in \mathcal{P}_{n_0h}$  such that :

$$B(u_{m-1} + \psi^{(0)}\lambda^{(1)}\gamma_{n_0}^{(1)}\Gamma_{/n_0}^{(1,0)}, \psi^{(0)}\lambda^{(1)}\gamma^*\Gamma_{/n_0}^{(1,0)}) = L(\psi^{(0)}\lambda^{(1)}\gamma^*\Gamma_{/n_0}^{(1,0)}) \quad \forall \gamma^* \in \mathcal{P}_{n_0h} \quad (13)$$

$$\text{with } \Gamma_{/n_0}^{(1,0)} = \prod_{n=1}^{n_0-1} \gamma_n^{(1)} \times \prod_{n=n_0+1}^N \gamma_n^{(0)};$$

- determine  $\psi^{(1)} \in \mathcal{V}_h$  such that :

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

Few sub-iterations are performed in practice; in the following numerical results, the process has been stopped after 4 sub-iterations. Furthermore, time function  $\lambda^{(j)}(t)$  and parameter functions  $\gamma_n^{(j)}(p_n)$  are normalized at each sub-iteration  $j$ .

## 4 GLOBAL ERROR ESTIMATION IN THE PGD FRAMEWORK

### 4.1 The Constitutive Relation Error method - Principle

The verification strategy we propose uses the concept of Constitutive Relation Error (CRE) (see [8] for full details). Let  $(\hat{u}, \hat{\varphi})$  be an admissible solution of the problem, i.e. verifying (1), (2), and (4). The CRE measure, that depends on  $\mathbf{p}$ , then reads :

$$E_{CRE}^2(\mathbf{p}) = \frac{1}{2} \int_{\mathcal{I}} \int_{\Omega} \frac{1}{k} [\hat{\varphi} - k \nabla \hat{u}] \cdot [\hat{\varphi} - k \nabla \hat{u}] d\Omega dt \equiv \frac{1}{2} \|\hat{\varphi} - k \nabla \hat{u}\|^2 \quad (15)$$

where  $||| \bullet |||$  is an energy norm in the space-time domain, and one has the extension of the Prager-Synge theorem :

$$|||\varphi_{ex} - \hat{\varphi}^*|||^2 + \frac{1}{2} \int_{\Omega} c(u_{ex} - \hat{u})|_T^2 d\Omega = \frac{1}{2} E_{CRE}^2 \quad (16)$$

with  $\hat{\varphi}^* = \frac{1}{2}[\hat{\varphi} + k\nabla\hat{u}]$ . The value of  $E_{CRE}$  can be used as an estimate of the global error between  $u_{ex}$  and  $u_m$ .

*Remark* : Again, in the steady-state case, we would consider :

$$E_{CRE}^2(\mathbf{p}) = \frac{1}{2} \int_{\Omega} \frac{1}{k} [\hat{\varphi} - k\nabla\hat{u}] \cdot [\hat{\varphi} - k\nabla\hat{u}] d\Omega \equiv \frac{1}{2} \|\hat{\varphi} - k\nabla\hat{u}\|^2 \quad (17)$$

$$\|\varphi_{ex} - \hat{\varphi}^*\|^2 = \frac{1}{2} E_{CRE}^2 \quad (18)$$

## 4.2 Construction of an admissible solution

We now explain how an admissible pair  $(\hat{u}_m, \hat{\varphi}_m)$  can be obtained as a post-processing of all information available from the computation of the PGD solution  $u_m$ . Constructing the kinematically admissible field  $\hat{u}_m(\mathbf{x}, t, \mathbf{p})$  is rather simple, and one usually takes  $\hat{u}_m = u_m$ . Getting  $\hat{\varphi}_m(\mathbf{x}, t, \mathbf{p})$  is more difficult and technical. In order to use classical tools that enable to compute equilibrated fluxes (in particular the prolongation condition, see [8, 13]), one should first construct a field  $\varphi_m(\mathbf{x}, t, \mathbf{p})$  which satisfies the following FE equilibrium for all  $(t, \mathbf{p}) \in \mathcal{I} \times \Theta$  :

$$\int_{\Omega} \varphi_m \cdot \nabla u^* d\Omega = \int_{\Omega} (f_d - c \frac{\partial \hat{u}_m}{\partial t}) u^* d\Omega - \int_{\partial_q \Omega} r_d u^* dS \quad \forall u^* \in \mathcal{V}_h \quad (19)$$

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

$$(f_d(\mathbf{x}, t), r_d(\mathbf{x}, t)) = \sum_{j=1}^J \alpha_j(t) (f_d^j(\mathbf{x}), r_d^j(\mathbf{x})) \quad (20)$$

We thus compute, for each couple  $(f_d^j, r_d^j)$ , a field  $\varphi_d^j(\mathbf{x})$  verifying the FE equilibrium :

$$\int_{\Omega} \varphi_d^j \cdot \nabla u^* d\Omega = \int_{\Omega} f_d^j u^* d\Omega - \int_{\partial_q \Omega} r_d^j u^* dS \quad \forall u^* \in \mathcal{V}_h \quad (21)$$

It is in practice obtained using the finite element method in displacement, i.e. by searching  $v^j \in \mathcal{V}_h$  with  $\varphi_d^j = \nabla v^j$ . It follows that  $\varphi_d = \sum_{j=1}^J \alpha_j(t) \varphi_d^j(\mathbf{x})$  can be introduced in the calculation of  $\varphi_m$ , which should then verify for all  $(t, \mathbf{p}) \in \mathcal{I} \times \Theta$  :

$$\int_{\Omega} (\varphi_m - \varphi_d) \cdot \nabla u^* d\Omega = - \int_{\Omega} c \frac{\partial \hat{u}_m}{\partial t} u^* d\Omega = - \sum_{i=1}^m c \lambda_i \Gamma_i \int_{\Omega} \psi_i u^* d\Omega \quad \forall u^* \in \mathcal{V}_h \quad (22)$$

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

$$B(u_{m_0}, \psi^* \lambda_{m_0} \Gamma_{m_0}) = L(\psi^* \lambda_{m_0} \Gamma_{m_0}) \quad \forall \psi^* \in \mathcal{V}_h \quad (23)$$

We thus get :

$$\begin{aligned} & \int_{\Omega} \left[ \int_{\Theta} \int_{\mathcal{I}} \lambda_{m_0} \Gamma_{m_0} (k \nabla u_{m_0} - \varphi_d) dt d\mathbf{p} \right] \nabla \psi^* d\Omega \\ &= - \int_{\Omega} \left[ \int_{\Theta} \int_{\mathcal{I}} c \lambda_{m_0} \Gamma_{m_0} \frac{\partial u_{m_0}}{\partial t} dt d\mathbf{p} \right] \psi^* d\Omega \quad \forall \psi^* \in \mathcal{V}_h \\ &= - \int_{\Omega} \sum_{i=1}^{m_0} \left[ \int_{\Theta} \int_{\mathcal{I}} c \lambda_{m_0} \Gamma_{m_0} \dot{\lambda}_i \Gamma_i dt d\mathbf{p} \right] \psi_i \psi^* d\Omega \quad \forall \psi^* \in \mathcal{V}_h \end{aligned} \quad (24)$$

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

$$\mathbf{Q}_{m_0} \equiv \int_{\Theta} \int_{\mathcal{I}} \lambda_{m_0} \Gamma_{m_0} (\varphi_d - k \nabla u_{m_0}) dt d\mathbf{p} \quad (25)$$

equilibrates  $\sum_{i=1}^{m_0} \left[ \int_{\Theta} \int_{\mathcal{I}} c \lambda_{m_0} \Gamma_{m_0} \dot{\lambda}_i \Gamma_i dt d\mathbf{p} \right] \psi_i$  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  $\psi_i$  in the FE sense ( $i = 1, \dots, m$ ). Consequently,

$$\varphi_m = \varphi_d - \sum_{i=1}^m \sum_{j=1}^m c \dot{\lambda}_i \Gamma_i R_{ij} \mathbf{Q}_j \quad (26)$$

satisfies FE equilibration (19) (or (22)).

Then, usual techniques [8, 13] can be used to build, from  $\varphi_m$ , a flux  $\hat{\varphi}_m$  that verifies the full equilibrium :

$$\int_{\Omega} \hat{\varphi}_m \cdot \nabla u^* d\Omega = \int_{\Omega} (f_d - c \frac{\partial \hat{u}_m}{\partial t}) u^* d\Omega - \int_{\partial_q \Omega} r_d u^* dS \quad \forall u^* \in \mathcal{V} \quad (27)$$

This flux reads  $\hat{\varphi}_m = \hat{\varphi}_d - \sum_{i=1}^m \sum_{j=1}^m c \dot{\lambda}_i \Gamma_i R_{ij} \hat{\mathbf{Q}}_j$  where  $\hat{\varphi}_d$  and  $\hat{\mathbf{Q}}_j$  are computed solving local problems on each element or patch of elements.



*Remark* : for the steady-state case, (23) reads :

$$B(u_{m_0}, \psi^* \Gamma_{m_0}) = L(\psi^* \Gamma_{m_0}) \quad \forall \psi^* \in \mathcal{V}_h \quad (28)$$

and we get :

$$\int_{\Omega} \left[ \int_{\Theta} \Gamma_{m_0} (k \nabla u_{m_0} - \varphi_d) d\mathbf{p} \right] \nabla \psi^* d\Omega = 0 \quad \forall \psi^* \in \mathcal{V}_h \quad (29)$$

Therefore,  $\mathbf{Q}_{m_0} \equiv \int_{\Theta} \Gamma_{m_0} (\varphi_d - k \nabla u_{m_0}) d\mathbf{p}$  is auto-equilibrated (in a FE sense), and  $\varphi_m$  and  $\hat{\varphi}_m$  can be defined as :

$$\varphi_m(\mathbf{x}, \mathbf{p}) = \varphi_d(\mathbf{x}) + \sum_{m_0=1}^m \beta_{m_0}(\mathbf{p}) \mathbf{Q}_{m_0}(\mathbf{x}) \quad ; \quad \hat{\varphi}_m(\mathbf{x}, \mathbf{p}) = \hat{\varphi}_d(\mathbf{x}) + \sum_{m_0=1}^m \beta_{m_0}(\mathbf{p}) \hat{\mathbf{Q}}_{m_0}(\mathbf{x}) \quad (30)$$

where  $\beta_{m_0}$  are coefficients, depending on  $\mathbf{p}$ , which are explicitly obtained by minimizing  $\int_{\Theta} E_{CRE}^2(\mathbf{p}) d\mathbf{p}$ .

## 5 GOAL-ORIENTED ERROR ESTIMATION

### 5.1 Guaranteed bounding

Let  $I$  be an output of interest defined by the extraction pair  $(\varphi_{\Sigma}, \mathbf{f}_{\Sigma})$  :

$$I(\mathbf{p}) = \int_{\mathcal{I}} \int_{\Omega} \{ \varphi_{\Sigma} \cdot \nabla u + \mathbf{f}_{\Sigma} \cdot u \} d\Omega dt \quad (31)$$

$\varphi_{\Sigma}(\mathbf{x}, t)$  and  $\mathbf{f}_{\Sigma}(\mathbf{x}, t)$  can possibly be Dirac distributions. We therefore introduce the associated adjoint problem, and compute an approximate (resp. admissible) PGD solution  $(\tilde{u}_{\tilde{m}}, \tilde{\varphi}_{\tilde{m}})$  (resp.  $(\hat{u}_{\tilde{m}}, \hat{\varphi}_{\tilde{m}})$ ) for this problem. In practice, the PGD solution of the adjoint problem is performed using an order  $\tilde{m}$  possibly different from  $m$ , as well as introducing local enrichment functions in the vicinity of the space-time region where  $I$  is defined [14]. The fundamental result for linear elliptic and parabolic problems then reads (see [9]) :

$$|I_{ex} - I_m - I_{corr}| \leq E_{CRE} \tilde{E}_{CRE} \quad (32)$$

where  $I_{ex}(\mathbf{p})$  (resp.  $I_m(\mathbf{p})$ ) is the exact (resp. approximated by PGD) value of the output of interest,  $I_{corr}(\mathbf{p})$  is a correction term computed from approximate solutions of both reference and adjoint problems, and  $E_{CRE}(\mathbf{p})$  (resp.  $\tilde{E}_{CRE}(\mathbf{p})$ ) is the constitutive relation error of the reference (resp. adjoint) problem. Let us note that this bounding result does not use any Galerkin orthogonality property, but only properties of admissible solutions.

Consequently, strict bounds on the local error  $I_{ex} - I_m$  (or directly on  $I_{ex}$ ) can be obtained for any value  $\mathbf{p}$  of material parameters.

## 5.2 Specific indicators on error sources

In the problem we consider, the error  $I_{ex} - I_m$  comes from two main sources : (i) the truncation of the sum in the PGD representation (10) at a given order  $m$ ; (ii) discretizations used to compute modes. Indeed, the error reads :

$$I_{ex} - I_m = (I_{ex} - I_{dis}) + (I_{dis} - I_m) = \mathcal{E}_{dis} + \mathcal{E}_{PGD} \quad (33)$$

where  $I_{dis}$  is the value of the output of interest obtained after discretization of the reference problem inside all parameter domains, and  $\mathcal{E}_{dis}$  (resp.  $\mathcal{E}_{PGD}$ ) is part of the error due to discretization (resp. to truncation of the PGD representation). Furthermore, error due to discretization can also be split between contributions coming from the discretization of each parameter domain (space, time, ...).

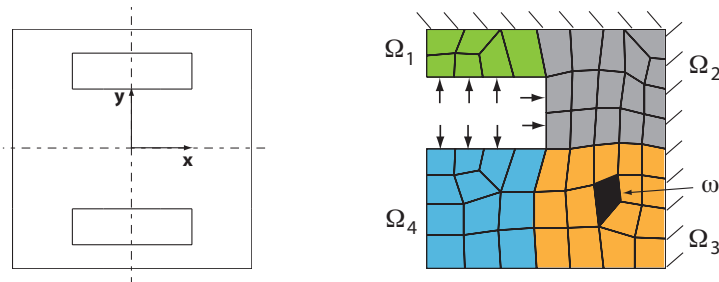
In order to control the computation process and lead adaptive strategies, we thus introduce an indicator for each error source. This is performed using verification tools presented previously, but considering additional (intermediate) reference problems obtained from a partial numerical method applied to the initial reference problem. For instance, assessing part  $\mathcal{E}_{PGD}$  of the error only due to truncation in the PGD representation can be done considering the discretized problem (i.e. the one providing for  $I_{dis}$ ) as the reference problem. It is of the form :

$$\mathbf{U}_h^1 = \mathbf{0} \quad ; \quad \mathbb{M} \frac{\mathbf{U}_h^{p+1} - \mathbf{U}_h^p}{\Delta t} + \mathbb{K} \mathbf{U}_h^p = \mathbf{F}_h^p \quad \forall p \in [1, P - 1] \quad (34)$$

where  $\Delta t$  is the time step size,  $P$  is the number of time steps, whereas  $\mathbb{M}$  and  $\mathbb{K}$  are classical matrices deriving from the FEM. Admissible pairs are then defined with respect to the new reference problems, and are in practice computed as a direct post-processing of available information.

## 6 NUMERICAL RESULTS

As a simple example, we consider the 2D structure of Figure 2 which is a section presenting two rectangular holes in which a fluid circulates. It is subjected to a given source term  $f_d(x, y) = 200xy$ , a given flux  $r_d(t) = -1$  on the holes boundaries, and a zero temperature is imposed on other boundaries. Using symmetries, we only keep the upper right quarter of the structure that we denote  $\Omega$ .



**Figure 2:** The 2D reference problem.

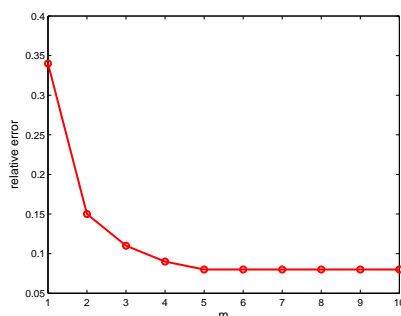
We consider that the diffusion coefficient  $k$  is fluctuating but remains piecewise homogeneous, i.e. it is homogeneous in each of the four non-overlapping subdomains  $\Omega_i$  ( $i = 1, 2, 3, 4$ ) defined in Figure 2 and such that  $\overline{\Omega_1 \cup \Omega_2 \cup \Omega_3 \cup \Omega_4} = \Omega$ . Furthermore, the thermal capacity  $c$  is supposed homogeneous in the whole domain  $\Omega$ . In the following, the two material coefficients are defined as :

$$k(\mathbf{x}, \theta_i) = 1 + \sum_{i=1}^4 g_i I_{\Omega_i}(\mathbf{x}) \theta_i \quad c(\mathbf{x}, \theta_5) = 1 + 0.2 \theta_5 \quad (35)$$

with  $[g_1, g_2, g_3, g_4] = [0.1, 0.1, 0.2, 0.05]$ ,  $\theta_i \in [-2, 2]$ , and  $I_{\Omega_i}(\mathbf{x})$  denoting the indicatrix function of subdomain  $\Omega_i$ .

The resulting solution  $u(\mathbf{x}, t, \theta_1, \theta_2, \theta_3, \theta_4, \theta_5)$  is searched using the PGD technique, with four-nodes quadrangular elements in space and a forward Euler time scheme.

Figure 3 gives the evolution of the constitutive relation error (seen as a global error estimate) with respect to the number  $m$  of PGD modes taken in the approximation ; this estimate is computed for  $\theta_i = 0$  ( $i = 1, \dots, 5$ ). We observe that after 5 modes, the error reaches an asymptotic value that corresponds to the discretization error.



**Figure 3:** Relative error estimate with respect to the number  $m$  of PGD modes.

Assuming that  $\theta_i$  are (truncated) centered reduced normal variables, and considering a given zone  $\omega \subset \Omega$  (see Figure 2), we study two quantities of interest :

- the mathematical expectation (in the probabilistic sense) of the mean value of  $u$  inside  $\omega$  at final time  $T$  :

$$I_1 = \mathbb{E} \left[ \frac{1}{|\omega|} \int_{\omega} u|_T d\Omega \right] \quad (36)$$

- the maximal value of the mean value of  $u$  inside  $\omega$  at final time  $T$  :

$$I_2 = \sup_{\theta_i} \frac{1}{|\omega|} \int_{\omega} u|_T d\Omega \quad (37)$$

We choose an order  $m = 3$  for the approximate PGD solution of the reference problem. For both  $I_1$  and  $I_2$ , obtained normalized upper bounds on  $I_{ex} - I_m - I_{corr}$  as well as specific error indicators are given in Figure 4 with respect to the number  $\tilde{m}$  of computed PGD modes for the adjoint solution.

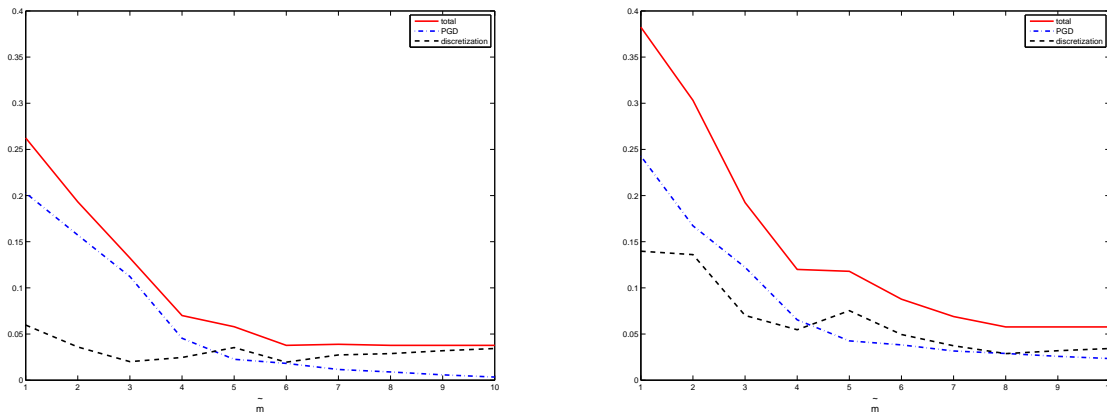


FIGURE 4: Normalized upper error bound and error indicators with respect to the number  $\tilde{m}$  of PGD modes used for the adjoint solution :  $I_1$  (left),  $I_2$  (right).

We observe that the correcting term  $I_{corr}$  enables to assess  $I_{ex}$  very effectively. The remaining asymptotic error could be decreased by improving discretizations used to compute PGD modes.

## 7 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. It can be applied in the case of numerous parameters (such as stochastic problems), even though optimizations when performing numerical integrations should be investigated in that case to decrease computational effort. It can also be directly extended to cases where the loading is defined with parameters.

**REFERENCES**

- [1] Chinesta, F., Ladevèze, P. and Cueto, E. A short review on model reduction based on Proper Generalized Decomposition. *Archives of Computational Methods in Engineering* (2011) **18**:395–404.
- [2] Nouy, A. A generalized spectral decomposition technique to solve a class of linear stochastic partial differential equations. *Computer Methods in Applied Mechanics and Engineering* (2007) **196**(45-48):4521–4537.
- [3] Nouy, A. A priori model reduction through Proper Generalized Decomposition for solving time-dependent partial differential equations. *Computer Methods in Applied Mechanics and Engineering* (2010) **199**(23-24):1603–1626.
- [4] Chinesta, F., Ammar, A. and Cueto, E. Recent advances and new challenges in the use of the Proper Generalized Decomposition for solving multidimensional models. *Archives of Computational Methods in Engineering* (2010) **17**(4):327–350.
- [5] Niroomandi, S., Alfaro, I. and Cueto, E. Accounting for large deformations in real-time simulations of soft tissues based on reduced-order models, *Computer Methods and Programs in Biomedicine* (2012) **105**(1):1–12.
- [6] Ladevèze, P. *Nonlinear Computational Structural Mechanics: New Approaches and Non-Incremental Methods of Calculation*. Springer (1998).
- [7] Ammar, A., Chinesta, F., Diez, P. and Huerta, A. An error estimator for separated representations of highly multidimensional models. *Computer Methods in Applied Mechanics and Engineering* (2010) **199**:1872–1880.
- [8] Ladevèze, P. and Pelle, J.P. *Mastering Calculations in Linear and Nonlinear Mechanics*. Springer NY (2004).
- [9] Ladevèze, P. Strict upper error bounds for calculated outputs of interest in computational structural mechanics. *Computational Mechanics* (2008) **42**(2):271–286.
- [10] Ladevèze, P. and Chamoin, L. On the verification of model reduction methods based on the Proper Generalized Decomposition. *Computer Methods in Applied Mechanics and Engineering* (2011) **200**:2032–2047.
- [11] Chamoin, L, Ladevèze, P. Robust control of PGD-based numerical simulations. *European Journal of Computational Mechanics* (2012) **21**(3-6):195–207.
- [12] Ladevèze, P. and Chamoin, L. *Toward guaranteed PGD-reduced models*. Bytes and Science, G. Zavarise & D.P. Boso (Eds.), CIMNE (2013).
- [13] Pled, F., Chamoin, L. and Ladevèze, P. On the techniques for constructing admissible stress fields in model verification: performances on engineering examples. *International Journal for Numerical Methods in Engineering* (2011) **88**(5):409–441.
- [14] Ladevèze, P. and Chamoin, L. Calculation of strict bounds for finite element approximations of non-linear pointwise quantities of interest. *International Journal for Numerical Methods in Engineering* (2010) **84**:1638–1664.