Generalized spectral decomposition method for solving stochastic finite element equations: Invariant subspace problem and dedicated algorithms

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A B S T R A C T

Stochastic Galerkin methods have become a significant tool for the resolution of stochastic partial differential equations (SPDE). However, they suffer from prohibitive computational times and memory requirements when dealing with large scale applications and high stochastic dimensionality. Some alternative techniques, based on the construction of suitable reduced deterministic or stochastic bases, have been proposed in order to reduce these computational costs. Recently, a new approach, based on the concept of generalized spectral decomposition (GSD), has been introduced for the definition and the automatic construction of reduced bases. In this paper, the concept of GSD, initially introduced for a class of linear elliptic SPDE, is extended to a wider class of stochastic problems. The proposed definition of the GSD leads to the resolution of an invariant subspace problem, which is interpreted as an eigen-like problem. This interpretation allows the construction of efficient numerical algorithms for building optimal reduced bases, which are associated with dominant generalized eigenspaces. The proposed algorithms, by separating the resolution of reduced stochastic and deterministic problems, lead to drastic computational savings. Their efficiency is illustrated on several examples, where they are compared to classical resolution techniques.

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1. Introduction

Computer simulations have become an essential tool for the quantitative prediction of the response of physical models. The need to improve the reliability of numerical predictions often requires taking into account uncertainties inherent to these models.

Uncertainties, either epistemic or aleatory, are commonly modeled within a probabilistic framework. For many physical models, it leads to the resolution of a stochastic partial differential equation (SPDE) where the operator, the right-hand side, the boundary conditions or even the domain, depend on a set of random variables. Many numerical methods have been proposed for the approximation of such SPDEs. In particular, stochastic Galerkin methods [1–4] have received a growing interest in the last decade. They allow the obtention of a decomposition of the solution on a suitable approximation basis, the coefficients of the decomposition being obtained by solving a large system of equations. These methods, which lead to high quality predictions, rely on a strong mathematical basis. That allows deriving *a priori* error estimators [5–7] but also *a posteriori* error estimators [8,9] and therefore to develop adaptive approximation techniques. However, many complex applications require a fine discretization at both deterministic and stochastic levels. This dramatically increases the dimension of approximation spaces and therefore of the resulting system of equations. The use of classical solvers in a black box fashion generally leads to prohibitive computational times and memory requirements. The reduction of these computational costs has now become a key question for the development of stochastic Galerkin methods and their transfer towards large scale and industrial applications.

Some alternative resolution techniques have been investigated over the last years in order to drastically reduce computational costs induced by the use of Galerkin approximation schemes. Some of these works rely on the construction of reduced deterministic bases or stochastic bases (sets of random variables) in order to decrease the size of the problem [3,10,11]. These techniques usually start from the assertion that optimal deterministic and stochastic bases can be obtained by using a classical spectral decomposition of the solution (namely a Karhunen–Loève or Hilbert Karhunen–Loève expansion). The solution being not known *a priori*, the basic idea of these techniques is to compute an approximation of the "ideal" spectral decomposition by ad hoc numerical strategies. The obtained set of deterministic vectors (resp. random variables) is then considered as a good candidate for a reduced deterministic (resp. stochastic) basis on which the initial stochastic problem can be solved at a lower cost. Let us here mention that this kind of decomposition has already been introduced in various domains of application such as functional data analysis [12], image analysis [13], dynamical model reduction [14,15], etc. In other contexts, it is also known as Principal Component Analysis, Proper Orthogonal Decomposition or Singular Value Decomposition.

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In [16], a new approach has been proposed to define and compute suitable reduced bases, without *a priori* knowing the solution nor an approximation of it. This method, which is inspired by a technique for solving deterministic evolution equations [17–19], is based on the concept of generalized spectral decomposition (GSD). It consists in defining an optimality criterion of the decomposition based on the operator and right-hand side of the stochastic problem. In the case of a linear elliptic symmetric SPDE, the obtained decomposition can be interpreted as a generalized Karhunen–Loève expansion of the right-hand side in the metric induced by the operator. In [16], it has been shown that corresponding optimal reduced bases were solution of an optimization problem on a functional which can be interpreted as an extended Rayleigh quotient associated with an eigen-like problem. In order to solve this problem, a power-type algorithm has been proposed. This algorithm, by separating the resolution of reduced deterministic problems and reduced stochastic problems, has led to significant computational savings.

The aim of this paper is to extend the concept of generalized spectral decomposition to a wider class of stochastic problems and to provide ad hoc efficient numerical strategies for its construction. The proposed definition of the GSD leads to the resolution of an invariant subspace problem, which in fact can be interpreted as an eigen-like problem. This interpretation allows the development of suitable algorithms for the construction of the decomposition. Algorithms are inspired by resolution techniques for classical eigenproblems, such as subspace iterations or Arnoldi techniques [20]. Significant computational savings are obtained with these new algorithms, in comparison with classical resolution techniques but also with previous GSD algorithms proposed in [16].

The proposed method will be presented on a generic discretized linear problem, encountered in many physical situations, without taking care of the initial "continuous problem" and of the discretization techniques at the deterministic and stochastic levels. In this paper, we consider that the solution of the fully discretized problem is our reference solution. The proposed method then leads to an approximation of this reference approximate solution. The study of approximation error, i.e. the distance between the reference solution and the solution of the continuous problem, is beyond the scope of this paper. For details, the reader can refer to [4–9].

The outline of the paper is as follows. In Section 2, we briefly recall the principles of stochastic Galerkin methods leading to the definition of a fully discretized version of the stochastic problem. Section 3 introduces some possible strategies for building deterministic or stochastic reduced bases. In Section 4, the principles of the generalized spectral decomposition method (GSD) are introduced. In particular, some mathematical considerations allow us to exhibit the underlying eigen-like problem that defines the GSD. Section 5 is devoted to the presentation of different algorithms for building the GSD. In Sections 6 and 7, the method is applied to two model problems: the first one is a linear elasticity problem and the second one is based on transient heat equation. Those model problems illustrate the capabilities of the method respectively for elliptic and parabolic stochastic partial differential equations.

2. Stochastic Galerkin methods

2.1. Stochastic modeling and discretization

We adopt a probabilistic modeling of the uncertainties. We consider that the probabilistic content of the stochastic problem can be represented by a finite dimensional probability space $(\Theta, \mathscr{B}, P)$. $\Theta \subset \mathbb{R}^m$ is the space of elementary events, $\mathscr{B}$ an associated σ-algebra

and P the probability measure. We consider that a preliminary approximation step has been performed at the deterministic level and that the stochastic problem reduces to the resolution of the following system of stochastic equations: find a random vector $\mathbf{u} : \theta \in \Theta \mapsto \mathbf{u}(\theta) \in \mathbb{R}^n$ such that we have P-almost surely

$$\mathbf{A}(\theta)\mathbf{u}(\theta) = \mathbf{b}(\theta), \tag{1}$$

where $\mathbf{A} : \Theta \to \mathbb{R}^{n \times n}$ is a random matrix and $\mathbf{b} : \Theta \to \mathbb{R}^n$ is a random vector. For the sake of clarity and generality, we do not focus on the way to obtain this semi-discretized problem. In the following, we will admit that the continuous and discretized problems are well-posed, which means that the continuous problem and the approximation technique have "good mathematical properties". Sections 6 and 7 will illustrate two continuous model problems and associated approximation techniques that lead to a system of type (1) (by introducing usual spatial and temporal discretizations). Now, we introduce an ad-hoc real-valued random function space $\mathscr{S}$, classically the space of second order random variables $L^2(\Theta; dP)$, such that a weak formulation of the stochastic problem (1) can be introduced. This weak formulation, whose solution is not necessarily solution of (1), reads: find $\mathbf{u} \in \mathbb{R}^n \otimes \mathscr{S} \cong (\mathscr{S})^n$ such that

$$E(\mathbf{v}^T \mathbf{A} \mathbf{u}) = E(\mathbf{v}^T \mathbf{b}) \quad \forall \mathbf{v} \in \mathbb{R}^n \otimes \mathscr{S}. \tag{2}$$

Approximation technique at the stochastic level consists in introducing a suitable finite dimensional approximation space

$$\mathscr{S}_P = \left\{ v(\theta) = \sum_{\alpha \in \mathscr{I}_P} v_\alpha H_\alpha(\theta), v_\alpha \in \mathbb{R}, H_\alpha \in \mathscr{S} \right\}, \tag{3}$$

where $\{H_\alpha\}_{\alpha \in \mathscr{I}_P}$ is a basis of $\mathscr{S}_P$, and $\mathscr{I}_P = \{\alpha_i, i = 1, \ldots, P\}$ is a set of P indices. The approximate solution $\mathbf{u} \in \mathbb{R}^n \otimes \mathscr{S}_P$ then reads

$$\mathbf{u}(\theta) = \sum_{\alpha \in \mathscr{I}_P} \mathbf{u}_\alpha H_\alpha(\theta). \tag{4}$$

A classical way to define the approximation is to use a Galerkin orthogonality criterion reading

$$E(\mathbf{v}^T \mathbf{A} \mathbf{u}) = E(\mathbf{v}^T \mathbf{b}) \quad \forall \mathbf{v} \in \mathbb{R}^n \otimes \mathscr{S}_P, \tag{5}$$

where E denotes the mathematical expectation. System (5) is equivalent to the following system of $n \times P$ equations:

$$\sum_{\beta \in \mathscr{I}_P} E(\mathbf{A} H_\alpha H_\beta)\mathbf{u}_\beta = E(H_\alpha \mathbf{b}) \quad \forall \alpha \in \mathscr{I}_P. \tag{6}$$

Several choices have been proposed for the construction of a stochastic approximation basis in $L^2(\Theta; dP)$: polynomial chaos [1], generalized polynomial chaos [21,22], finite elements [6,4], or multi-wavelets [23,24]. Such a choice depends on the regularity of the solution at the stochastic level. Several techniques have been investigated for the adaptive choice of this basis, based on *a posteriori* error estimation with respect to the continuous model [25,7–9]. For well-posed approximate problems, the solution of (5) weakly converges with P (in a mean-square sense) towards the solution of problem (2). In this paper, we will consider that this approximation basis is given (fixed P). The approximate solution of the fully discretized problem (5) will then be considered as our reference solution. The study of the stochastic approximation error, i.e. the distance between solutions of Eqs. (5) and (2), is beyond the scope of this article.

2.2. Classical techniques to solve the discretized problem

System (6) can be written in the following block-matrix form:

$$\begin{pmatrix} E(\mathbf{A} H_{\alpha_1} H_{\alpha_1}) & \cdots & E(\mathbf{A} H_{\alpha_1} H_{\alpha_P}) \\ \vdots & \ddots & \vdots \\ E(\mathbf{A} H_{\alpha_P} H_{\alpha_1}) & \cdots & E(\mathbf{A} H_{\alpha_P} H_{\alpha_P}) \end{pmatrix} \begin{pmatrix} \mathbf{u}_{\alpha_1} \\ \vdots \\ \mathbf{u}_{\alpha_P} \end{pmatrix} = \begin{pmatrix} E(\mathbf{b} H_{\alpha_1}) \\ \vdots \\ E(\mathbf{b} H_{\alpha_P}) \end{pmatrix}. \tag{7}$$