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Development of error criteria for adaptive multi-element polynomial chaos approaches

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ABSTRACT

This paper presents and compares different methodologies to create an adaptive stochastic space partitioning in polynomial chaos applications which use a multi-element approach. To implement adaptive partitioning, Wan and Karniadakis first developed a criterion based on the relative error in local variance. We propose here two different error criteria: one based on the residual error and the other on the local variance discontinuity created by partitioning. The methods are applied to classical differential equations with long-term integration difficulties, including the Kraichnan–Orszag three-mode problem, and to simple linear and nonlinear mechanical systems whose stochastic dynamic responses are investigated. The efficiency and robustness of the approaches are investigated by comparison with Monte-Carlo simulations. For the different examples considered, they show significantly better convergence characteristics than the original error criterion used.

1. Introduction

In various applications, engineers and researchers use complex modelling techniques and simulations to predict behaviour of structures and optimise their design process. However, in order to incorporate more realistic data into their models, it is necessary to take uncertainties into account within the design stage and to predict their influence. Different stochastic or probabilistic procedures are used for modelling these uncertainties. A review on the numerical methods for stochastic prediction can be found for instance in [1], or more recently in [2,3].

The most straightforward statistical method based on Monte Carlo (MC) simulation [4] is often used as reference. It relies on the calculation of the direct problem for a large sample. The main drawback is probably that its accuracy relies heavily on the sample size and it is therefore computationally expensive. To confront these difficulties and minimise the sampling size, dedicated methods have been developed such as Latin hypercube [5] or quasi-Monte Carlo SOBOL [6] sampling. On the other hand, non-statistical methods that are not based on very large sampling, have also been developed. For instance, the perturbation methods [7] are based on a Taylor series expansion of the random field around its mean value. However such methods cannot handle accurately uncertainty with high discrepancy because the theory is based on assumed small perturbations. Furthermore it implies that the function derivative around its mean is finite up to a given order, which may not be possible for not-smooth functions.

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The Homogeneous Chaos is another branch of non-statistical methods, initiated by Wiener [8] who used Hermite polynomials to model stochastic processes with Gaussian random variables. Ghanem and Spanos then introduced polynomial chaos with a finite element method to model uncertainty in solid mechanics [9]. They showed exponential convergence rate for Gaussian stochastic processes. The non-intrusive stochastic collocation approach [10] uses direct deterministic, but small, samplings at collocation points in the random space and recreates the stochastic response by constructing local polynomial interpolations. In order to deal with discontinuities in the probability or physical space, it was later extended to the multi-element stochastic reduced basis methods [11], the multi-element probabilistic collocation method (MEPCM) [12,13], an adaptive hierarchical sparse grid collocation method [14], or the simplex stochastic collocation [15]. The intrusive approach also makes use of polynomials to model uncertainties. The main idea of the method is to expand the random solution spectrally in the polynomial basis and subsequently use a Galerkin projection scheme to transform the original stochastic problem into a set of deterministic algebraic equations with more unknowns. Xiu and Karniadakis [16] introduced the concept of generalised polynomial chaos (gPC) using different polynomial bases defined with the correspondence between the probability density functions of random variables and the weight functions of the scalar product that orthogonalises the basis. It is a generalisation of the original Wiener's Hermite-chaos and can deal with non-Gaussian random inputs efficiently. Soize and Ghanem later proposed a proper mathematical frame to address the chaos representation of vector-valued random variables with arbitrary distributions [17]. More recently, Wan and Karniadakis [18] showed how to create orthogonal polynomials on the fly to extend the procedure to arbitrary random distributions.

Depending on the problem, one can be confronted with quantities whose variations with respect to the random parameters are not continuous. gPC has difficulties for converging for such discontinuous distributions in the stochastic space. Increasing the maximum degree of the chosen basis (p-refinement) may help but it cannot always overcome those convergence difficulties. It also enlarges the size of the system to solve and makes the solution of the stochastic problem more complex. It is known for instance that gPC fails to converge for long-term integration (see the Kraichnan–Orszag problem in [19]). The reason is that a certain shape of solution is assumed at the initial time, but this does not necessarily correspond to the real shape or distribution at later times. For long term integration, the method called time-dependent generalised polynomial chaos (TDgPC) [20] recalculates the polynomial basis after a certain time, which helps for convergence.

The regularity or irregularity of the solution with respect to the stochastic space affects the convergence rate of gPC expansion and is usually not known *a priori* in many cases. One of the strategies to tackle this problem is to divide the stochastic space (h-refinement) and use a relatively low degree of expansion on each element of the partition, which corresponds to a piecewise polynomial approximation fitting. This has motivated Wan and Karniadakis to propose the multi-element generalised polynomial chaos (MEgPC) method [19]. The space of random inputs is decomposed in small elements. In each element, a new random variable is created and the standard gPC method is applied. Their mesh adaptation scheme to decompose the space of random inputs is based on the relative error in the variance prediction. The partitioning process is performed by dividing each element which does not satisfy the criterion in two equal-size elements.

As far as the authors know, the error criterion proposed in [19] is the only one that was used in MEgPC problems. It was for instance re-used later by the same authors in [18] for solving differential equations, and more recently in the field of robotics by Kewlani and Iagnemma [21], or to predict limit-cycle oscillations of an elastically mounted airfoil [22]. However, as it will be discussed in further detail in this manuscript, this error criterion has some inherent drawbacks. Further developments in multi-element polynomial chaos partitioning methodology are therefore needed and these are the main objectives of the present manuscript. Two new error criteria are proposed here to enhance polynomial chaos capabilities for the solution of stochastic differential or algebraic equations.

The manuscript is organised as follows. The mathematical formulation of the generalised polynomial chaos (gPC) and its extension to multi-elements are briefly presented in Section 2. Then, the proposed error criteria are described in Sections 3. Numerical results and comparison with reference studies provided in [19] are discussed in detail in Section 4.

2. Polynomial chaos and its extension to multi-element approaches

This section briefly describes the principles of polynomial chaos expansion and its extension to a multi-element approach when considering the uncertainty propagation in a problem initially defined by a set of deterministic governing equations. It is assumed that uncertainty affects some parameters of these governing equations and that the stochastic model of these *input variables or parameters* is known. The polynomial chaos is then applied in order to obtain a stochastic description of some other quantities of interest which will be referred to as *output variables*.

In what follows, two types of governing equations are considered: sets of algebraic governing equations, denoted $H(u) = 0$ and ordinary differential equations (ODE) denoted $\dot{u} = f(u, t)$.

2.1. Probability space and notations

Let us define $(\Theta, \mathcal{A}, \mathbb{P})$ a probability space with Θ being the event space, $\mathcal{A}$ being the σ-algebra on Θ and $\mathbb{P}$ being a probability measure. The probability density function (pdf) associated to a random variable U is denoted p_U. U expected