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A new non-intrusive polynomial chaos using higher order sensitivities

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Highlights

- New non-intrusive method for Polynomial Chaos Expansion called Polynomial Chaos Decomposition with Differentiation.
- Higher-order sensitivities.
- Higher order sensitivities calculation using sample responses in multi-dimensions.
- Sensitivities with varying order of truncation error.
- Number of samples equal to the polynomial chaos terms.

Abstract

This paper proposes a new non-intrusive method for uncertainty quantification called Polynomial Chaos Decomposition with Differentiation (PCDD) that uses higher-order sensitivities of the response. In PCDD, the polynomial chaos expansion (PCE) of the response is differentiated with respect to the basis random variables using multi-indices. This differentiation results in a system of linear equations which can then be solved to determine the expansion coefficients. Here, the higher accuracy, Modified Forward Finite Difference (ModFFD) that involves representation of the response using Taylor expansion of order equal to the chaos-order is used in combination with PCE. Therefore, the total number of samples required with this method is equal to the number of terms in the PCE. To verify the validity of this new technique, two analytical problems and two stochastic composite laminate problems were studied. The results of the analytical problems showed that the accuracy of PCDD using ModFFD is similar to that of PCDD using analytical sensitivities, which in addition is comparable to the exact results. For composite laminate problems, the PCDD displayed very high accuracy comparable to 50,000 Latin Hypercube Samples, which underlines the computational efficiency of this proposed method.

Keywords: Uncertainty quantification; Polynomial Chaos Expansion; Higher order sensitivities; Multi-indices; Finite-difference sensitivity

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1. Introduction

In Computational Mechanics, it is paramount to represent the physical problems with mathematical models, which are dependent on some input parameters. However, the mathematical models are not able to describe physical phenomenon precisely due to the factors like inherent randomness in the physical observation or input parameters (aleatoric uncertainties) and insufficient information due to the limited data and lack of full knowledge of the system (epistemic uncertainties) [1]. Therefore, it is judicious to take the uncertainties involved in the system into account and develop models in a probabilistic manner to obtain highly desirable designs. In fact, this has led to a considerable development of the techniques for Uncertainty Quantification (UQ) and Uncertainty propagation.

The Monte Carlo (MC) simulation used to be the preferred method for quantification of uncertainties [1,2]; however, the convergence rate for this approach is slow and requires an enormous number of simulations, which becomes infeasible for the expensive function evaluations. Therefore, efficient techniques such as Polynomial Chaos Expansion (PCE) have become more popular recently and are preferred over the MC approaches. Initially, the PC expansion or Wiener Chaos Expansion (WCE), which was first proposed by Wiener in his work 'The Homogeneous Chaos' [3] in 1938, used the Hermite polynomials in terms of Gaussian random variables as basis functions to expand the stochastic process in a random space. An L_2 convergence for a second order random process was proved by Cameron and Martin [4] for PCE. But as observed by Xiu and Karniadakis [5–7], the convergence rate using the Hermite polynomials for non-Gaussian processes is non-exponential. Hence, they proposed generalized Polynomial Chaos Expansion that uses orthogonal polynomials [8,9] associated with the distribution of random variables and can be chosen from the Askey-scheme.

The methods to obtain a stochastic response with PCE can be classified into two categories: intrusive and non-intrusive. The intrusive methods require modification of the governing equation that results in a system of coupled deterministic equations, which can be solved to obtain the expansion coefficients [10–15]. Hence, the non-intrusive methods that use deterministic codes as black boxes with a series of deterministic simulations for different realizations of uncertain parameters to obtain the PCE coefficients are preferred over the intrusive methods. The implementation of PCE using the intrusive approach in an engineering problem was initially carried out by Ghanem and Spanos [10,11] via finite element method and called it as Spectral Stochastic Finite Element Method (SSFEM). Ghanem also applied this method to the structural analysis using multiple non-Gaussian properties in [12], and later Sakamoto and Ghanem used it with non-Gaussian non-stationary processes [13]. In fluid dynamics, researchers have applied PCE for the study of uncertainties in flow simulations [5,14–18]. For composite structures, the PCE has been utilized to investigate the effect of uncertainties in the material and geometric properties as well as the boundary and loading conditions [19–21]. It has also been implemented in many other disciplines: stability and control [22], chemical reactions [23], and stochastic design optimization [24–26].

The non-intrusive method can be further classified into two types: Projection [16,27–31] and Collocation [16–18,32]. The Projection approach employs the orthogonality condition of multivariate polynomials whereas the Collocation approach uses regression to minimize the approximation error. The number of samples or function evaluations required to evaluate the integrals in the Projection approach increases exponentially with the increase of the dimensions, which is often referred to as the Curse of Dimensionality; however, Sparse Grids or Smolyak coarse tensorization [33–35] can be used to alleviate this problem. On the other hand, Latin Hypercube Sampling (LHS) and even roots of the orthogonal polynomials can be used for Collocation. It is mentioned in [17,18] that the minimum number of samples required to obtain accurate solutions is equal to twice the number of terms in PCE. Although this requires fewer samples than the Sparse Grids methods, the number of samples required becomes very large for large multidimensional problems. Therefore, the objective of this research is to propose a new non-intrusive method known as Polynomial Chaos Decomposition with Differentiation (PCDD) that requires a fewer number of samples but provides high accuracy.

The concept of Sensitivity Analysis (SA) tries to examine the importance of each input parameter or the combination of input parameters and can be classified as Local Sensitivity Analysis (LSA) and Global Sensitivity Analysis (GSA). The LSA focuses on the local impact of random input parameters on the model whereas GSA focuses on the impact of response uncertainty due to the uncertainties in random input parameters [36]. In PCDD, the higher-order sensitivities of the first type are required and depending on the nature of the function, different local sensitivity techniques can be used: analytical, automatic differentiation [37,38], complex-step [39–41], and finite-difference (FD) [42–44]. However, most of the commercial software available today cannot support automatic differentiation and complex-step sensitivity analysis. Hence, finite-difference (forward, central, and backward) or