Journal of Computational Physics 260 (2014) 54–84

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Grid and basis adaptive polynomial chaos techniques for sensitivity and uncertainty analysis

Zoltán Perkó *, Luca Gilli [1], Danny Lathouwers, Jan Leen Kloosterman

Delft University of Technology, Faculty of Applied Sciences, Department of Radiation Science and Technology, Section Nuclear Energy and Radiation Applications, Mekelweg 15, 2629 JB, Delft, The Netherlands

ARTICLE INFO

Article history:
Received 4 June 2013
Received in revised form 11 November 2013
Accepted 8 December 2013
Available online 18 December 2013

Keywords:
Polynomial chaos expansion
Generalized polynomial chaos
Adaptive sparse grids
Basis adaptivity
Uncertainty quantification
Sensitivity analysis

ABSTRACT

The demand for accurate and computationally affordable sensitivity and uncertainty techniques is constantly on the rise and has become especially pressing in the nuclear field with the shift to Best Estimate Plus Uncertainty methodologies in the licensing of nuclear installations. Besides traditional, already well developed methods – such as first order perturbation theory or Monte Carlo sampling – Polynomial Chaos Expansion (PCE) has been given a growing emphasis in recent years due to its simple application and good performance.

This paper presents new developments of the research done at TU Delft on such Polynomial Chaos (PC) techniques. Our work is focused on the Non-Intrusive Spectral Projection (NISP) approach and adaptive methods for building the PCE of responses of interest. Recent efforts resulted in a new adaptive sparse grid algorithm designed for estimating the PC coefficients. The algorithm is based on Gerstner's procedure for calculating multi-dimensional integrals but proves to be computationally significantly cheaper, while at the same it retains a similar accuracy as the original method.

More importantly the issue of basis adaptivity has been investigated and two techniques have been implemented for constructing the sparse PCE of quantities of interest. Not using the traditional full PC basis set leads to further reduction in computational time since the high order grids necessary for accurately estimating the near zero expansion coefficients of polynomial basis vectors not needed in the PCE can be excluded from the calculation. Moreover the sparse PC representation of the response is easier to handle when used for sensitivity analysis or uncertainty propagation due to the smaller number of basis vectors.

The developed grid and basis adaptive methods have been implemented in Matlab as the Fully Adaptive Non-Intrusive Spectral Projection (FANISP) algorithm and were tested on four analytical problems. These show consistent good performance both in terms of the accuracy of the resulting PC representation of quantities and the computational costs associated with constructing the sparse PCE. Basis adaptivity also seems to make the employment of PC techniques possible for problems with a higher number of input parameters (15–20), alleviating a well known limitation of the traditional approach. The prospect of larger scale applicability and the simplicity of implementation makes such adaptive PC algorithms particularly appealing for the sensitivity and uncertainty analysis of complex systems and legacy codes.

* Corresponding author. Tel.: +31 15 27 86618; fax: +31 15 27 86422.
E-mail addresses: Z.Perko@tudelft.nl (Z. Perkó), Gilli@nrg.eu (L. Gilli), D.Lathouwers@tudelft.nl (D. Lathouwers), J.L.Kloosterman@tudelft.nl (J.L. Kloosterman).
[1] Current address: Nuclear Research and consultancy Group, Utrechtseweg 310, 6800 ES Arnhem, The Netherlands.

0021-9991/$ – see front matter
http://dx.doi.org/10.1016/j.jcp.2013.12.025

1. Introduction

Present design and engineering processes heavily rely on numerical models in practically all branches of industry. This is especially true in the nuclear field, where experiments are particularly expensive and therefore computational tools are often favored. Such simulations are almost naturally augmented by extensive sensitivity and uncertainty (S&U) analysis. The former provides insight how the model input data affects the computed outputs, hence contributes to a deeper understanding of the investigated problem. The latter gives information about the uncertainty of the calculated responses arising from our incomplete knowledge of the input parameters, therefore is important and necessary to judge the reliability of the results.

As both the numerical models themselves and the associated S&U analysis techniques are computationally expensive there is an ever growing demand for the development of more accurate and faster methods. In the nuclear community this interest only intensified since the licensing of nuclear installations started to shift from conservatism to Best Estimate Plus Uncertainty methodologies [44]. A number of well-established approaches are already available for performing S&U analysis. Traditionally a distinction is made between deterministic methods – such as perturbation theory [42], generalized perturbation theory [14], forward and adjoint sensitivity analysis [20] – and statistical ones based on some form of Monte Carlo sampling [6]. All these techniques (and many more) are covered extensively in the literature, including quite a few books as well, just to give two excellent examples the interested reader is referred to the books of Saltelli et al. [37] and Cacuci et al. [5,7].

In the pursuit for novel S&U analysis methods Polynomial Chaos (PC) techniques have received much attention lately. In the nuclear community this interest is relatively new [43,10,18,19], in contrast with several other disciplines – such as engineering mechanics [17] or fluid flow [22,25,46] – where research has been ongoing for a longer time. In simple terms the essence of PC schemes is nothing more than approximating a model output (i.e. a response of our interest) as a polynomial function of the model input parameters. Such a function, the Polynomial Chaos Expansion (PCE) of the response basically constitutes a metamodel of the original problem and can be used to describe the stochastic nature of the output in terms of its mean value, variance, covariance, distribution, etc. The idea was first introduced by Wiener to represent Gaussian processes by Hermite polynomials (see [41]), but later it was extended so that other types of stochastic processes could also be addressed using polynomials of the Askey family in the scope of generalized Polynomial Chaos (gPC) [45,11].

PC methods belong to a wider family of spectral techniques aimed at reconstructing the solution of a stochastic problem by a Fourier series like expansion [21]. Like any expansion such representation uses basis vectors and expansion coefficients. The basis vectors are predefined functionals of the random variables representing the stochastic input data, therefore they are random variables themselves. The expansion coefficients are deterministic and their efficient computation is the main issue. In traditional PC the basis vectors are multi-dimensional polynomials up to a certain order, hence the method inherently contains two limitations. On one hand, responses not smooth enough in the stochastic domain (i.e. being highly nonlinear in certain input variables) might require high polynomial orders to be properly reconstructed, moreover discontinuous responses are even impossible to represent with polynomials. On the other hand, even if the response is smooth with respect to all input variables, the PC metamodel is restricted by the predefined order of the expansion and it is difficult to judge what order is needed for an adequate representation.

The former difficulty can be overcome by employing local basis vectors instead of global polynomials. In multi-element gPC (ME-gPC) the stochastic space is decomposed into disjoint domains and on each of them polynomials with a local support are used as basis vectors [39,40]. The multi-element probabilistic collocation method (ME-PCM) is a variant of the same idea where a separate grid of points is used on each sub-domain of the stochastic space to interpolate the solution [13,12]. Employing wavelets is another promising method, the basic idea was demonstrated by Le Maître et al. in [23] using wavelets of the Haar family in the Wiener–Haar expansion, then was generalized in [24]. Ma and Zabaras introduced an adaptive collocation algorithm in [28] applying piecewise multi-linear hierarchical basis functions with which the response is interpolated on a locally refined mesh. All these techniques are mainly concerned with problems which experience sharp changes or discontinuities in the stochastic space. In many engineering problems however such rapid response variations are not encountered, hence the focus of this paper is on the other limitation associated with PC methods.

The predefined order of a traditional, full PCE confines the dependence of the response to a maximum mixed polynomial order (and therefore to a maximum order in any of the input variables) and to a maximum dimension, i.e. a maximum number of interacting parameters. Though the sparsity of effects principle (see [29]) suggests that responses are generally dominated by only a handful of inputs and low order interactions, usually it is not possible to know a priori what that polynomial order is and how many interacting parameters there are. Moreover with the increase of input parameters the full PC basis grows rapidly, hence typically only low order PC expansions of 2nd or 3rd order are used, obviously unable to catch higher order dependencies and interactions.

These problems can be alleviated by using an adaptively constructed polynomial basis instead of a predefined one. A brief discussion of such basis adaptivity was already presented by Li and Ghanem in [26], and later essentially the same idea was revived by Lucor and Karniadakis in [27], both papers dealing with a nonlinear oscillator subject to stochastic excitation. In these two articles the random variables used in the discretization of the excitation are separated at each time step based on their linear contribution to the solution (i.e. the norm of their linear component in the PCE) and only the most important ones are retained to produce the higher-order (nonlinear) terms. Another example of basis adaptivity can be found in the works of Todor and Schwab [38] and Bieri and Schwab [1], both papers considering elliptic stochastic partial differential