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Remi Abgrall, Pietro Marco Congedo, Gianluca Geraci, Gianluca Iaccarino

**RESEARCH  
REPORT**

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Project-Team Bacchus





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**Abstract:** In this study, some preliminary results about the possibility to extend the classical polynomial Chaos (PC) theory to stochastic problems with non-classical probability distributions of the variables, *i.e.* outside the framework of the classical Wiener-Askey scheme [1], are presented. The proposed strategy allows to obtain an analytical representation of the solution in order to build a metamodel or to compute conditional statistics. Various numerical results obtained on some analytical problems are then provided to demonstrate the correctness of the presented approach.

**Key-words:** Polynomial Chaos, Collocation, Uncertainty Quantification, ANOVA, Conditional statistics

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# Développement non-polynomial pour des problèmes stochastiques avec des pdf non-classiques

**Résumé :** Dans cette étude, on présente des résultats préliminaires sur la possibilité d'utiliser la théorie classique du Chaos Polynomial pour des problèmes stochastiques avec des fonctions densité de probabilité non-classiques. La stratégie proposée permet de calculer une représentation analytique de la solution pour construire un metamodelle ou calculer les statistiques. Plusieurs résultats numériques sont présentés pour illustrer la validité de l'approche proposée.

**Mots-clés :** Chaos Polynomial, Collocation, Quantification des incertitudes, ANOVA

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## 1 Introduction

In recent years the growing interest in Uncertainty Quantification (UQ) in the numerical field has led to many different numerical methods or strategies to quantify the statistics in presence of stochastic inputs. One of the most popular method is the Polynomial Chaos (PC) both in its version intrusive or non-intrusive [2]. This class of methods has been shown to be very efficient, compared to Monte Carlo or collocation strategies, if the model to represent is smooth enough. More recently with the aim to extend the classical PC theory to real application cases the so called multi-element PC (me-PC) has been introduced by Karniadakis et al. (see for instance [3]) allowing the representation of probability distributions that fall outside the so-called Wiener-Askey scheme. This opens the way to the representation of inputs characterized by probability distributions that can be extracted from experiments. However the implementation of a me-PC code could be not so straightforward even if a PC code is already at disposal and, until this moment, the effectiveness of this approach to obtain statistical moments higher than the variance has not been done yet. In particular a simple extension of the simple link between the ANOVA representation and the PC expansion (see for instance [4]) is still missing. In the present work we would like to reinterpret the problem to extend the PC to non classical pdf in a more direct way recovering all the common features of the classical PC, as for instance the link between the expansion and the ANOVA decomposition to compute conditional statistics. We propose a strategy based on a mapping of the original problem on an equivalent uniform stochastic space on which applying the PC analysis. This strategy leads to a non orthogonal and non polynomial (in the general case) representation that reflects in a loss of efficiency if compared to the PC in the case of classical pdfs. However as will be clear later the loss of orthogonality does not affect the computation of the coefficient of the representation but only the statistical moments computation. We expect anyway to improve these preliminary results with some simple further steps, as a coupling with a Sparse Grid algorithm and a parallel implementation, in a short term. The remaining part of the work is organized as follows. In the section §2 the mathematical setting is presented and the higher statistical moments are defined. An analytical definition of the ANOVA expansion and how it reflects in the computation of conditional statistics is also provided. An introduction on the classical PC is furnished with the aim to make the work as possible self-contained in section §3. The heart of the work is the section §4 in which our strategy (nPC) is proposed. Some results on the link between the PC and nPC are then presented and the link between the nPC expansion and the ANOVA decomposition is described for the first order terms of the conditional variances. Finally some numerical results are presented for analytical problems in dimension up to three for different kind of custom defined pdfs in section §5. Concluding remarks and future perspective works are reported as closure in §6.

## 2 Mathematical and problem setting

Consider the following problem for an output of interest  $u(\mathbf{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega}))$ :

$$\mathcal{L}(\mathbf{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega}); u(\mathbf{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega}))) = \mathcal{S}(\mathbf{x}, t, \boldsymbol{\xi}(\boldsymbol{\omega})), \quad (1)$$



where the operator  $\mathcal{L}$  can be either an algebraic or a differential operator (in this case we need appropriate initial and boundary conditions). The operator  $\mathcal{L}$  and the source term  $\mathcal{S}$  are defined on the domain  $D \times T \times \Xi$ , where  $\mathbf{x} \in D \subset \mathbb{R}^{n_d}$ , with  $n_d \in \{1, 2, 3\}$ , and  $t \in T$  are the spatial and temporal dimensions. Randomness is introduced in (1) and its initial and boundary conditions in term of  $d$  second order random parameters  $\boldsymbol{\xi}(\boldsymbol{\omega}) = \{\xi_1(\omega_1), \dots, \xi_d(\omega_d)\} \in \Xi$  with parameter space  $\Xi \subset \mathbb{R}^d$ . The symbol  $\boldsymbol{\omega} = \{\omega_1, \dots, \omega_d\} \in \Omega \subset \mathbb{R}^d$  denotes realizations in a complete probability space  $(\Omega, \mathcal{F}, P)$ . Here  $\Omega$  is the set of outcomes,  $\mathcal{F} \subset 2^\Omega$  is the  $\sigma$ -algebra of events and  $P : \mathcal{F} \rightarrow [0, 1]$  is a probability measure. Random parameters  $\boldsymbol{\xi}(\boldsymbol{\omega})$  can have any arbitrary probability density function  $p(\boldsymbol{\xi}(\boldsymbol{\omega}))$ , in this way  $p(\boldsymbol{\xi}(\boldsymbol{\omega})) > 0$  for all  $\boldsymbol{\xi}(\boldsymbol{\omega}) \in \Xi$  and  $p(\boldsymbol{\xi}(\boldsymbol{\omega})) = 0$  for all  $\boldsymbol{\xi}(\boldsymbol{\omega}) \notin \Xi$ ; we can now drop the argument  $\boldsymbol{\omega}$  for brevity. The probability density function  $p(\boldsymbol{\xi})$  is defined as a joint probability density function from the independent probability function of each variable:  $p(\boldsymbol{\xi}) = \prod_{i=1}^d p_i(\xi_i)$ . This assumption allows to an independent polynomial representation for every direction in the probabilistic space with the possibility to recover the multidimensional representation by tensorization. In the present work the test cases are algebraic, steady equations with no physical space dependence (we can drop the spatial argument  $\mathbf{x}$ ), so we can write

$$\mathcal{L}(\boldsymbol{\xi}; f(\boldsymbol{\xi})) = 0 \quad (2)$$

then the aim is to find the statistical moments of the solution  $f(\boldsymbol{\xi})$ .

The (centered) statistical moments of degree  $n$ th are defined as

$$\mu^n(f) = \int_{\Xi} (f(\boldsymbol{\xi}) - E(f))^n p(\boldsymbol{\xi}) d\boldsymbol{\xi}, \quad (3)$$

where  $E(f)$  represents the expected value of the solution  $f(\boldsymbol{\xi})$

$$E(f) = \int_{\Xi} f(\boldsymbol{\xi}) p(\boldsymbol{\xi}) d\boldsymbol{\xi}. \quad (4)$$

In this work moments up to the degree four are considered and in the following we refer to the variance  $\text{Var}$ , skewness  $s$  and kurtosis  $k$  to indicate, respectively, the second, third and fourth order statistical moments.

Higher order statistics (from order two) can be computed knowing only expectancies of the model function  $f$  and its values raised to the desired order

$$\begin{aligned} \text{Var} &= E(f^2) - E(f)^2 \\ s &= E(f^3) - 3E(f)\text{Var} - E(f)^3 \\ k &= E(f^4) - 4E(f^3)E(f) + 6E(f^2)E(f)^2 - 3E(f)^4. \end{aligned} \quad (5)$$

This representation of the higher moments will be employed to compare the strategy with a collocation approach. The key idea, leading to this last approach, is to compute the expectancy for the functions  $f$ ,  $f^2$ ,  $f^3$  and  $f^4$ , obtained directly from the values of the model  $f$  and then combine these expectancy to obtain high order statistics. A direct, brutal-force, collocation approach could be to compute directly all the integrals contained in the equations (5) evaluating each term by the precedent statistical moment. The problem reduce to compute only four integral. This can be done efficiently if the number of quadrature points is high enough. Anyway this approach cannot provide a metamodel of

the function and an expansion of the solution on which conditional statistics can be computed (see for instance [5]). The theoretical framework on which the conditional statistics can be obtained based on an ANOVA representation is the subject of the following section.

## 2.1 ANOVA decomposition and sensitivity indexes

Let us consider to have a given equation, or a systems of equations, to solve and to have an output of interest  $f = f(\boldsymbol{\xi})$ . The output of the system is dependent by  $d$  uncertainties parameters  $\xi_i$  assumed so that  $\boldsymbol{\xi} = \{\xi_1, \dots, \xi_d\} \in \Xi \subset \mathbb{R}^d$ . In this work we assume independent distributed random variables  $\xi_i \in \Xi_i$  and, consequently, the space  $\Xi$  can be obtained by tensorization of their monodimensional spaces, i.e.  $\Xi_i \subset \mathbb{R}$ ,  $\Xi = \Xi_1 \times \dots \times \Xi_d$ .

From the independence of the random variables follows directly  $p(\boldsymbol{\xi}) = \prod_i p(\xi_i)$ . Assuming  $f(\boldsymbol{\xi}) \in L^2(\boldsymbol{\xi}, p(\boldsymbol{\xi}))$  then a Sobol unique functional decomposition exists:

$$f(\boldsymbol{\xi}) = \sum_{\mathbf{u} \subseteq \{1, \dots, d\}} f_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) \quad (6)$$

where  $\mathbf{u}$  is a set of integers with cardinality  $v = |\mathbf{u}|$  and  $\boldsymbol{\xi}_{\mathbf{u}} = \{\xi_{u_1}, \dots, \xi_{u_v}\}$ . Each function  $f_{\mathbf{u}}$  is computed by the relation [4]:

$$f_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) = \int_{\Xi_{\bar{\mathbf{u}}}} f(\boldsymbol{\xi}) p(\boldsymbol{\xi}_{\bar{\mathbf{u}}}) d\boldsymbol{\xi}_{\bar{\mathbf{u}}} - \sum_{\mathbf{w} \subset \mathbf{u}} f_{\mathbf{w}}(\boldsymbol{\xi}_{\mathbf{w}}) \quad (7)$$

where  $\Xi_{\bar{\mathbf{u}}}$  is the space  $\Xi$  without the dimensions contained in  $\mathbf{u}$  and  $\boldsymbol{\xi}_{\bar{\mathbf{u}}}$  is the vector  $\boldsymbol{\xi}$  without the variables in  $\mathbf{u}$ .

By definition

$$f_0 = \int_{\Xi} f(\boldsymbol{\xi}) p(\boldsymbol{\xi}) d\boldsymbol{\xi} \quad (8)$$

is the mean of the function  $f(\boldsymbol{\xi})$ . This functional decomposition is called ANOVA if each of the  $2^d$  elements of the decomposition, except  $f_0$ , verifies for every  $\xi_i$ :

$$\int_{\Xi_i} f_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) p(\xi_i) d\xi_i = 0, \quad \forall i \in \mathbf{u} \quad (9)$$

Directly from eq. 9 follows the orthogonality:

$$\int_{\Xi} f_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) f_{\mathbf{w}}(\boldsymbol{\xi}_{\mathbf{w}}) p(\boldsymbol{\xi}) d\boldsymbol{\xi} = 0, \quad \mathbf{u} \neq \mathbf{w} \quad (10)$$

### 2.1.1 Sobol sensitivity indices

Employing the ANOVA decomposition it is possible to decompose the variance of  $f = f(\boldsymbol{\xi})$ :

$$\text{Var}(f) = \sum_{\substack{\mathbf{u} \subseteq \{1, \dots, d\} \\ \mathbf{u} \neq \emptyset}} D_{\mathbf{u}}(f_{\mathbf{u}}) \quad (11)$$

where

$$D_{\mathbf{u}}(f_{\mathbf{u}}) = \int_{\Xi_{\mathbf{u}}} f_{\mathbf{u}}^2(\boldsymbol{\xi}_{\mathbf{u}}) p(\boldsymbol{\xi}_{\mathbf{u}}) d\boldsymbol{\xi}_{\mathbf{u}} \quad (12)$$

and  $\Xi_{\mathbf{u}} = \Xi_{u_1} \times \cdots \times \Xi_{u_v}$ .

The Sobol sensitivity indices (SI), are defined as:

$$S_{\mathbf{u}} = \frac{D_{\mathbf{u}}}{\text{Var}} \quad (13)$$

measuring the sensitivity of the variance due to the  $v$ -order ( $v = |\mathbf{u}|$ ) interaction between the variables in  $\xi_{\mathbf{u}}$ . It is evident that the summation of the  $2^d - 1$  Sobol indices is equal to one.

### 3 Classical Polynomial Chaos approach

In this section we refer briefly to the main results relative to the high order statics computation by the classical PC approach with further extensions for higher statistical moments provided by the same authors; for exhaustive details refer to [5].

The solution is expanded as

$$f(\xi) = \sum_{k=0}^P \beta_k \Psi_k(\xi), \quad (14)$$

where  $\Psi_k$  is the polynomial basis orthogonal to the probability density distribution  $p(\xi)$ .

Each of the  $P + 1 = (n_0 + d)/(n_0!d!)$  coefficients of the expansion (of total degree  $n_0$ ) can be computed as projection of the model function  $f(\xi)$  with the polynomial basis exploiting the orthogonality conditions, i.e. the polynomial basis is chosen in accord to the Wiener-Askey scheme to be orthogonal to the probability distribution  $p(\xi)$

$$\beta_k = \frac{\int_{\Xi} f(\xi) \Psi_k(\xi) p(\xi) d\xi}{\int_{\Xi} \Psi_k(\xi) \Psi_k(\xi) p(\xi) d\xi}. \quad (15)$$

The problem is to compute the integral at numerator while for the denominator the value could be known analytically.

Assuming to know the coefficients  $\beta_k$  of the expansion the four statistical

moments are [5]

$$\begin{aligned}
 E(f) &= \beta_0 \\
 \text{Var} &= \sum_{i=1}^P \beta_i^2 \langle \Psi_i^2(\boldsymbol{\xi}) \rangle \\
 s &= \sum_{k=1}^P \beta_k^3 \langle \Psi_k^3(\boldsymbol{\xi}) \rangle + 3 \sum_{i=1}^P \beta_i^2 \sum_{\substack{j=1 \\ j \neq i}}^P \beta_j \langle \Psi_i^2(\boldsymbol{\xi}), \Psi_j(\boldsymbol{\xi}) \rangle \\
 &+ 6 \sum_{i=1}^P \sum_{j=i+1}^P \sum_{k=j+1}^P \beta_i \beta_j \beta_k \langle \Psi_i(\boldsymbol{\xi}), \Psi_j(\boldsymbol{\xi}) \Psi_k(\boldsymbol{\xi}) \rangle \\
 k &= \sum_{i=1}^P \beta_i^4 \langle \Psi_i^4 \rangle + 4 \sum_{i=1}^P \beta_i^3 \sum_{\substack{j=1 \\ j \neq i}}^P \beta_j \langle \Psi_i^3, \Psi_j \rangle + 3 \sum_{i=1}^P \beta_i^2 \sum_{\substack{j=1 \\ j \neq i}}^P \beta_j^2 \langle \Psi_i^2, \Psi_j^2 \rangle \\
 &+ 12 \sum_{i=1}^P \beta_i^2 \sum_{\substack{j=1 \\ j \neq i}}^P \beta_j \sum_{\substack{k=j+1 \\ k \neq i}}^P \beta_k \langle \Psi_i^2, \Psi_j \Psi_k \rangle \\
 &+ 24 \sum_{i=1}^P \sum_{j=i+1}^P \sum_{k=j+1}^P \sum_{h=k+1}^P \beta_i \beta_j \beta_k \beta_h \langle \Psi_i \Psi_j, \Psi_k \Psi_h \rangle
 \end{aligned} \tag{16}$$

The expression reported in (16) are obtained thanks to the orthogonality of the polynomial basis, *i.e.*

$$\int_{\Xi} \Psi_i(\boldsymbol{\xi}) \Psi_j(\boldsymbol{\xi}) p(\boldsymbol{\xi}) d\boldsymbol{\xi} = \delta_{ij} \langle \Psi_i^2 \rangle. \tag{17}$$

### 3.1 Sensitivity computation from PC expansion

The computation of the Sobol indices is possible using every sample stochastic method (Monte Carlo, quasi-Monte Carlo) but can be done in a very efficient way when a polynomial expansion of the solution is adopted. The idea is to compute the expansion of the solution (truncated) and compute the Sobol indices from the expansion instead of computing them on the real function. Remember the polynomial expansion:

$$f(\boldsymbol{\xi}) = \tilde{f}(\boldsymbol{\xi}) + \mathcal{O}_T = \sum_{k=0}^P \beta_k \Psi_k(\boldsymbol{\xi}) + \mathcal{O}_T, \tag{18}$$

with a number of terms related to the maximum degree of the polynomial reconstruction  $n_o$  and the dimension of the system  $d$ :  $P+1 = \frac{(n_o+d)!}{n_o!d!}$ . Each element  $f_{\mathbf{u}}$  of the functional decomposition of  $f(\boldsymbol{\xi})$  is approximated by the relative term  $\tilde{f}_{\mathbf{u}}$ :

$$f_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) \approx \tilde{f}_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) = \sum_{k \in K_{\mathbf{u}}} \beta_k \Psi_k(\boldsymbol{\xi}_{\mathbf{u}}), \tag{19}$$

where the set of indices  $K_{\mathbf{u}}$  is given by

$$K_{\mathbf{u}} = \left\{ k \in \{1, \dots, P\} \mid \Psi_k(\boldsymbol{\xi}_{\mathbf{u}}) = \prod_{i=1}^{|\mathbf{u}|} \phi_{\alpha_i^k}(\xi_{u_i}), \alpha_i^k > 0 \right\} \tag{20}$$

and  $\phi_{\alpha_i^k}(\xi_{u_i})$  are the monodimensional polynomials for every direction  $\xi_i$  of degree  $k$  chosen with respect to the so-called Wiener-Askey scheme [1].

Thanks to the orthogonality it is possible to obtain directly the variance  $\tilde{\text{Var}}(f) = \text{Var}(\tilde{f}) \approx \text{Var}(f)$  and the conditional variance  $\tilde{D}_{\mathbf{u}}(f_{\mathbf{u}}) = D_{\mathbf{u}}(\tilde{f}_{\mathbf{u}}) \approx D_{\mathbf{u}}(f_{\mathbf{u}})$  from the following relations:

$$\begin{aligned}\tilde{\text{Var}}(f) &= \sum_{k=1}^P \beta_k^2 \langle \Psi_k, \Psi_k \rangle \\ \tilde{D}_{\mathbf{u}}(f_{\mathbf{u}}) &= \sum_{k \in K_{\mathbf{u}}} \beta_k^2 \langle \Psi_k, \Psi_k \rangle.\end{aligned}\quad (21)$$

Sobol sensitivity indices follows directly from eq. 21:

$$S_{\mathbf{u}} \approx \tilde{S}_{\mathbf{u}} = \frac{\tilde{D}_{\mathbf{u}}(f_{\mathbf{u}})}{\tilde{\text{Var}}(f)} = \frac{\sum_{k \in K_{\mathbf{u}}} \beta_k^2 \langle \Psi_k, \Psi_k \rangle}{\sum_{k=1}^P \beta_k^2 \langle \Psi_k, \Psi_k \rangle}.\quad (22)$$

If custom defined probability distribution function are employed the orthogonality properties of the basis cannot be exploited anymore to compute the coefficients of the polynomial expansion. In the following section we describe a strategy to recover a solution expansion with respect a non polynomial basis, in the general case, in which the orthogonality of a support basis is employed to compute the coefficients of the expansion.

## 4 Handling whatever form of pdf for the computation of higher order statistics

The state-of-the-art to compute statistics moments for non classical pdf is the so-called multi-element method me-PC [3]. This family of techniques allows to efficiently compute, thanks to a partition of the stochastic space, the (piecewise) polynomial approximations of the model function  $f(\boldsymbol{\xi})$ . Despite to the possibility to compute expectancy and variance efficiently to compute high order statistics this method encounter the same problems of the classical PC approach: high number of integrals to compute as in the direct approach (see equations (16)) or sampling convergence issues as a metamodel approach. At the same time a very strong computational effort must be devoted to adapt an existing PC code to a multi-element capable one. Anyway the effective possibility to link the me-PC method to the ANOVA decomposition has not been yet provided to compute conditional statistics.

To tackle this problem we proposed a *mapping* procedure that allows to obtain a polynomial representation of a function depending on a custom defined distributed random vector. This procedure allows a straightforward implementation starting from an existing PC code.

The procedure is the same of the classical PC approach, i.e. a polynomial approximation of the model is computed and then all the statistical moments are computed directly from this polynomial expansion. Obviously conditional statistics can be computed too.

First of all the  $P + 1$  coefficients must be computed. If the probability distribution fall outside the so-called Wiener-Askey scheme a proper orthogonal basis cannot be employed as in the generalized-PC method.

Let us assume to recast the probability density function  $p(\boldsymbol{\xi})$  as

$$p(\boldsymbol{\xi}) = \frac{p(\boldsymbol{\xi})\bar{p}}{\bar{p}}, \quad (23)$$

where  $\bar{p}$  is an equivalent uniform distribution on the space  $\Xi$

$$\bar{p} = \frac{1}{\int_{\Xi} d\boldsymbol{\xi}}. \quad (24)$$

All the integral of the kind  $\int f(\boldsymbol{\xi})p(\boldsymbol{\xi})d\boldsymbol{\xi}$  can be re-interpreted as statistics of a function  $\bar{f}(\boldsymbol{\xi})$  defined by

$$\bar{f}(\boldsymbol{\xi}) = \frac{f(\boldsymbol{\xi})p(\boldsymbol{\xi})}{\bar{p}}, \quad (25)$$

with an uniform distribution  $\bar{p}$  on  $\Xi$  of the parameter vector.

At this stage a polynomial representation of the function  $\bar{f}(\boldsymbol{\xi})$  can be obtained employing a Legendre basis orthogonal on a stochastic space embedded with an uniform distribution.

The  $P + 1$  coefficients of the series can be computed as

$$\beta_k = \frac{\int_{\Xi} \bar{f}(\boldsymbol{\xi})\Psi_k(\boldsymbol{\xi})\bar{p}d\boldsymbol{\xi}}{\int_{\Xi} \Psi_k(\boldsymbol{\xi})\Psi(\boldsymbol{\xi})\bar{p}d\boldsymbol{\xi}}, \quad (26)$$

where the orthogonality of the polynomial basis allows to avoid to compute the mixed terms, i.e. terms of the kind  $\int_{\Xi} \Psi_i\Psi_j\bar{p}d\boldsymbol{\xi}$ .

The  $P + 1$  terms of the polynomial approximation of the function  $\bar{f}(\boldsymbol{\xi})$ , obtained on the Legendre basis, could be employed easily to obtain a polynomial expansion of  $f(\boldsymbol{\xi})$  on a set of  $P+1$  (non orthogonal) term on the stochastic space with distribution  $p$ . The procedure is the following

$$\bar{f}(\boldsymbol{\xi}) = f(\boldsymbol{\xi})\frac{p(\boldsymbol{\xi})}{\bar{p}} = \sum_{i=0}^P \beta_k \Psi_k(\boldsymbol{\xi}) \quad \rightarrow \quad f(\boldsymbol{\xi}) = \sum_{i=0}^P \beta_k \Psi_k \frac{\bar{p}}{p(\boldsymbol{\xi})} = \sum_{i=0}^P \beta_k \bar{\Psi}_k, \quad (27)$$

this is made possible if, as is the case, no holes in the domain are present,  $p(\boldsymbol{\xi}) > 0$ . We remark that the basis  $\{\bar{\Psi}_i\}_{i=0}^P$  is not polynomial if the probability distribution  $p(\boldsymbol{\xi})$  is not polynomial and, in the general case  $\int_{\Xi} \bar{\Psi}_i\bar{\Psi}_j p(\boldsymbol{\xi})d\boldsymbol{\xi} \neq \delta_{ij} \int_{\Xi} \bar{\Psi}_i^2 p(\boldsymbol{\xi})d\boldsymbol{\xi}$ .

However this expansion allows to compute statistics (eventually conditional) and also the metamodel for the function  $f(\boldsymbol{\xi})$ . Even in the case of time dependent pdf the points on which evaluate the model are always the zeros of the Legendre polynomial associated to the space. Despite to the possibility to compute the expansion even for a known distribution as for instance a Beta distribution, this technique is expected to perform worst in this case in which a proper optimal basis, in term of convergence, can be chosen. A discussion on the relation of the classical gPC method with this non polynomial chaos expansion is reported in the next section.

#### 4.1 On the relation between polynomial and non polynomial chaos approach

In the previous section a novel technique has been presented to compute the expansion of the solution for a whatever form of pdf.

Let assume to have a polynomial function  $f(\boldsymbol{\xi}) \in \mathbb{P}^r$  with a distribution of the vector parameter  $\boldsymbol{\xi} \sim \text{Beta}(\alpha, \beta)$ . We recall here that a  $\text{Beta}(\alpha, \beta)$  distribution is described as

$$p(\xi) = \frac{(\xi + 1)^{\alpha-1}(1 - \xi)^{\beta-1}}{B(\alpha, \beta)2^{\alpha+\beta-1}}, \quad (28)$$

where the function  $B(\alpha, \beta)$  is

$$B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha + \beta)} \quad (29)$$

and the gamma function is  $\Gamma(n) = (n - 1)!$

In the generalized-PC case the Jacobi base can be employed and the number of points  $n$  needed to compute the integral of order  $2r$  (product of the function and the Jacobi polynomial of degree  $r$ th) is  $2r = 2n - 1$ , then  $n = r + 1$  (for each dimension). If the non polynomial chaos is employed the integrand should be of the order  $2r + \alpha + \beta$ . Of course the regularity of the integrand becomes the same of the PC case in case of uniform distribution ( $\alpha = \beta = 0$ ). In the general case an higher number of points is needed to solve correctly the integrals with respect the general case. However in a general case the model function is not polynomial and then the advantage of a Gaussian quadrature based on the polynomial orthogonal basis is less evident. Of course this techniques make sense in the case of non standard (eventually time dependent) pdfs in which case the PC techniques cannot be applied without a multi-element technique. We remark here that in the case of discontinuous pdf this procedure could still be applied even if the convergence could be slower or even prevented in the worst cases.

The other difference with respect a standard PC technique is in the computation of the statistical moments. The basis  $\{\bar{\Psi}_i\}_{i=0}^P$  is not orthogonal on the space  $\Xi$  with respect the distribution  $p(\boldsymbol{\xi})$  and then the mixed terms of the expansion must be considered. When the expansion for  $f(\boldsymbol{\xi})$  is obtained (see

equation (27)) the statistics can be computed as (see [5] for the orthogonal case)

$$\begin{aligned}
 E(f) &= \beta_0 \\
 \text{Var} &= \beta_0^2 \langle (\bar{\Psi}_0^2 - 1) \rangle + \sum_{k=1}^P \beta_k^2 \langle \bar{\Psi}_k^2 \rangle + 2 \sum_{i=0}^P \sum_{j=i+1}^P \beta_i \beta_j \langle \bar{\Psi}_i, \bar{\Psi}_j \rangle \\
 s &= \sum_{k=0}^P \beta_k^3 \langle \bar{\Psi}_k^3(\boldsymbol{\xi}) \rangle + 3 \sum_{i=0}^P \beta_i^2 \sum_{\substack{j=0 \\ j \neq i}}^P \beta_j \langle \bar{\Psi}_i^2(\boldsymbol{\xi}), \bar{\Psi}_j(\boldsymbol{\xi}) \rangle \\
 &\quad + 6 \sum_{i=0}^P \sum_{j=i+1}^P \sum_{k=j+1}^P \beta_i \beta_j \beta_k \langle \bar{\Psi}_i(\boldsymbol{\xi}), \bar{\Psi}_j(\boldsymbol{\xi}) \bar{\Psi}_k(\boldsymbol{\xi}) \rangle \\
 k &= \sum_{k=0}^P \beta_k^4 \langle \bar{\Psi}_k^4(\boldsymbol{\xi}) \rangle + 4 \sum_{i=0}^P \beta_i^3 \sum_{\substack{j=0 \\ j \neq i}}^P \beta_j \langle \bar{\Psi}_i^3, \bar{\Psi}_j \rangle + 3 \sum_{i=0}^P \beta_i^2 \sum_{\substack{j=0 \\ j \neq i}}^P \beta_j^2 \langle \bar{\Psi}_i^2, \bar{\Psi}_j^2 \rangle \\
 &\quad + 12 \sum_{i=0}^P \sum_{\substack{j=0 \\ j \neq i}}^P \sum_{\substack{k=j+1 \\ k \neq i}}^P \beta_i^2 \beta_j \beta_k \langle \bar{\Psi}_i(\boldsymbol{\xi})^2, \bar{\Psi}_j(\boldsymbol{\xi}) \bar{\Psi}_k(\boldsymbol{\xi}) \rangle \\
 &\quad + 24 \sum_{i=0}^P \sum_{j=i+1}^P \sum_{k=j+1}^P \sum_{h=k+1}^P \beta_i \beta_j \beta_k \beta_h \langle \bar{\Psi}_i(\boldsymbol{\xi}), \bar{\Psi}_j(\boldsymbol{\xi}) \bar{\Psi}_k(\boldsymbol{\xi}) \bar{\Psi}_h(\boldsymbol{\xi}) \rangle.
 \end{aligned} \tag{30}$$

Obviously the number of integral to compute depends directly from the number of coefficients that is directly related to the dimension  $d$  of the problem and the total degree of approximation  $n_0$ . The number of terms for the non polynomial approach can be evaluated as

$$\begin{aligned}
 \bar{T}_{\text{Var}} &= P + 1 + \binom{P}{2} \\
 \bar{T}_s &= P + 1 + P(P + 1) + \binom{P + 1}{3} \\
 \bar{T}_k &= P + 1 + P(P + 1) + P(P + 1) + (P + 1) \binom{P}{2} + \binom{P + 1}{4},
 \end{aligned} \tag{31}$$

where the symbols  $\bar{T}_{\text{Var}}$ ,  $\bar{T}_s$  and  $\bar{T}_k$  indicate respectively the number of integral to compute for variance, skewness and kurtosis for the non polynomial approach.

The number of the mixed term to compute, which is equal to the difference between the number of integral to compute in the classical PC case (see equations (16)), can be shown to be equal to

$$\begin{aligned}
 \Delta_{\text{Var}} &= \binom{P}{2} + 1 \\
 \Delta_s &= 2P + 1 + \binom{P + 1}{3} - \binom{P}{3} \\
 \Delta_k &= P^2 + 3P + 1 + (P + 1) \binom{P}{2} + \binom{P + 1}{4} - \binom{P}{2} - P \binom{P - 1}{2} - \binom{P}{4},
 \end{aligned} \tag{32}$$



where  $P$  depends from both the stochastic dimension  $d$  and the total degree of the approximation (of the function  $\bar{f}(\boldsymbol{\xi})$ ).

The evolution of the number of the extra terms to compute is reported for the case with  $n_0 = 2$  and dimension between 2 and 10 in figure 1.

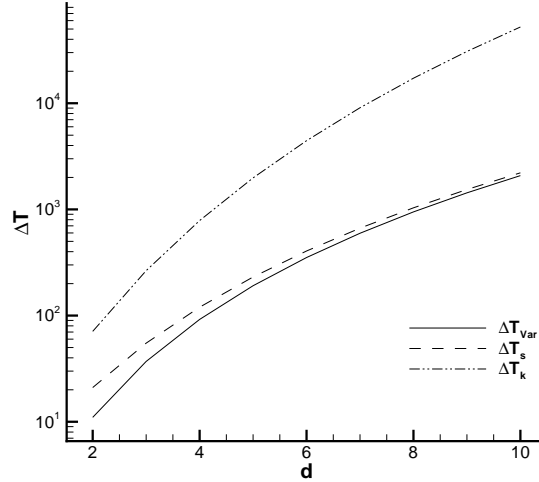


Figure 1: Evolution of the extra terms to compute in the non polynomial approach with respect the standard gPC method. The case reported is obtained with  $n_0 = 2$  and a dimension  $d$  between 2 and 10.

## 4.2 Computation of the conditional statistics by the nPC

The approach presented in this work allows to reproduce the structure of the solution  $f(\boldsymbol{\xi})$  in term of components even if these components are not orthogonal each other. For this reason the functional ANOVA decomposition cannot be derived in a straightforward way as showed in section §3.1 identifying directly the subset of indexes  $K_{\mathbf{u}}$  as showed in the equation (20). However the orthogonal basis of Legendre underlined above the series expansion of the solution allows to obtain in a relative simple way each first order term of the ANOVA expansion, *i.e.* terms associated to the subset  $\mathbf{u}$  with cardinality equal to one. Recalling the definition of these  $d$  terms of the ANOVA expansion, the equation (7) here reported only for convenience

$$f_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) = \int_{\Xi_{\bar{\mathbf{u}}}} f(\boldsymbol{\xi}) p(\boldsymbol{\xi}_{\bar{\mathbf{u}}}) d\boldsymbol{\xi}_{\bar{\mathbf{u}}} - \sum_{\mathbf{w} \subset \mathbf{u}} f_{\mathbf{w}}(\boldsymbol{\xi}_{\mathbf{w}}),$$

in the case of the first order terms, *i.e.* terms with  $\text{card}(\mathbf{u}) = 1$ , can be reduced in

$$f_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) = \int_{\Xi_{\bar{\mathbf{u}}}} f(\boldsymbol{\xi}) p(\boldsymbol{\xi}_{\bar{\mathbf{u}}}) d\boldsymbol{\xi}_{\bar{\mathbf{u}}} - f_0. \quad (33)$$

Inflating the expansion (27) into (33) one obtains

$$\begin{aligned} f_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) &= \sum_{k=0}^P \beta_k \int_{\Xi_{\bar{\mathbf{u}}}} \bar{\Psi}_k(\boldsymbol{\xi}) p(\boldsymbol{\xi}_{\bar{\mathbf{u}}}) d\boldsymbol{\xi}_{\bar{\mathbf{u}}} - f_0 \\ &= \sum_{k=0}^P \beta_k \int_{\Xi_{\bar{\mathbf{u}}}} \Psi_k(\boldsymbol{\xi}) \frac{p(\boldsymbol{\xi}_{\bar{\mathbf{u}}})}{p(\boldsymbol{\xi})} \bar{p} d\boldsymbol{\xi}_{\bar{\mathbf{u}}} - f_0. \end{aligned} \quad (34)$$

The ratio between the two probability density  $p(\boldsymbol{\xi}_{\bar{\mathbf{u}}})$  and  $p(\boldsymbol{\xi})$  can be computed as

$$\frac{p(\boldsymbol{\xi}_{\bar{\mathbf{u}}})}{p(\boldsymbol{\xi})} = \frac{p(\boldsymbol{\xi}_{\bar{\mathbf{u}}})}{p(\boldsymbol{\xi}_{\mathbf{u}})p(\boldsymbol{\xi}_{\bar{\mathbf{u}}})} = \frac{1}{p(\boldsymbol{\xi}_{\mathbf{u}})}, \quad (35)$$

where  $p(\boldsymbol{\xi}_{\mathbf{u}})$  is the probability density relative to the subset  $\mathbf{u}$ . The equivalent uniform distribution  $\bar{p}$ , in the same way, can be decomposed in the product between the equivalent uniform distribution relative to the set  $\mathbf{u}$  and the other variables as

$$\bar{p} = \bar{p}_{\mathbf{u}} \bar{p}_{\bar{\mathbf{u}}}. \quad (36)$$

These last two equation allow to recast the first order ANOVA term as

$$f_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) = \sum_{k=0}^P \beta_k \frac{\bar{p}_{\mathbf{u}}}{p(\boldsymbol{\xi}_{\bar{\mathbf{u}}})} \int_{\Xi_{\bar{\mathbf{u}}}} \Psi_k(\boldsymbol{\xi}) \bar{p}_{\bar{\mathbf{u}}} d\boldsymbol{\xi}_{\bar{\mathbf{u}}} - f_0. \quad (37)$$

The value of the integral in the last equation depends on the set associated to the index  $k$ . We can write

$$\int_{\Xi_{\bar{\mathbf{u}}}} \Psi_k(\boldsymbol{\xi}) \bar{p}_{\bar{\mathbf{u}}} d\boldsymbol{\xi}_{\bar{\mathbf{u}}} = \begin{cases} \Psi_k(\boldsymbol{\xi}) & \text{if } k \in K_{\mathbf{u}}^0 \\ 0 & \text{if } k \notin K_{\mathbf{u}}^0, \end{cases} \quad (38)$$

where the set  $K_{\mathbf{u}}^0$  is obtained as union of the set  $K_{\mathbf{u}}$  and the null multi-index element ( $k = 0$ ).

For the first order terms, *i.e.* if  $\text{card}(\mathbf{u}) = 1$ , we can write

$$f_{\mathbf{u}}(\boldsymbol{\xi}_{\mathbf{u}}) = \sum_{k \in K_{\mathbf{u}}^0} \beta_k \frac{\bar{p}_{\mathbf{u}}}{p(\boldsymbol{\xi}_{\bar{\mathbf{u}}})} \Psi_k(\boldsymbol{\xi}) - f_0, \quad (39)$$

obviously still holds  $f_0 = \beta_0$ .

To compute the conditional variance relative to each function  $f_{\mathbf{u}}$  the first step is to raise to the second power the equation (39) and then integrate over the space  $\Xi_{\mathbf{u}} \subset \Xi$  with the weight function  $p(\boldsymbol{\xi}_{\mathbf{u}})$ .

The equation (39) raised to the second power is

$$\begin{aligned} f_{\mathbf{u}}^2(\boldsymbol{\xi}_{\mathbf{u}}) &= \sum_{k \in K_{\mathbf{u}}^0} \beta_k^2 \frac{\bar{p}_{\mathbf{u}}^2}{p^2(\boldsymbol{\xi}_{\bar{\mathbf{u}}})} \Psi_k^2(\boldsymbol{\xi}) + 2 \sum_{i \in K_{\mathbf{u}}^0} \sum_{\substack{j \geq i+1 \\ j \in K_{\mathbf{u}}^0}} \beta_i \beta_j \frac{\bar{p}_{\mathbf{u}}^2}{p^2(\boldsymbol{\xi}_{\bar{\mathbf{u}}})} \Psi_i(\boldsymbol{\xi}) \Psi_j(\boldsymbol{\xi}) \\ &\quad - 2\beta_0 \sum_{k \in K_{\mathbf{u}}^0} \beta_k \frac{\bar{p}_{\mathbf{u}}}{p(\boldsymbol{\xi}_{\bar{\mathbf{u}}})} \Psi_k(\boldsymbol{\xi}) + \beta_0^2 \end{aligned} \quad (40)$$

The last equation need to be integrated and then, in the following, we analyze term by term the integration of the right hand side of the (40). The first term

of the right hand side integrated can be written as

$$\sum_{k \in K_u^0} \beta_k^2 \int_{\Xi_u} \frac{\bar{p}_u^2}{p^2(\xi_u)} \Psi_k^2(\xi) p(\xi_u) d\xi_u = \sum_{k \in K_u^0} \beta_k^2 \int_{\Xi_u} \frac{\bar{p}_u^2}{p(\xi_u)} \Psi_k^2(\xi) d\xi_u. \quad (41)$$

The second term can be treated in an analogue way

$$\begin{aligned} 2 \sum_{i \in K_u^0} \sum_{\substack{j \geq i+1 \\ j \in K_u^0}} \beta_i \beta_j \int_{\Xi_u} \frac{\bar{p}_u^2}{p^2(\xi_u)} \Psi_i(\xi) \Psi_j(\xi) p(\xi_u) d\xi_u = \\ 2 \sum_{i \in K_u^0} \sum_{\substack{j \geq i+1 \\ j \in K_u^0}} \beta_i \beta_j \int_{\Xi_u} \frac{\bar{p}_u^2}{p(\xi_u)} \Psi_i(\xi) \Psi_j(\xi) d\xi_u. \end{aligned} \quad (42)$$

The third term can be dramatically simplified as

$$\begin{aligned} 2\beta_0 \sum_{k \in K_u^0} \beta_k \int_{\Xi_u} \frac{\bar{p}_u}{p(\xi_u)} \Psi_k(\xi) p(\xi_u) d\xi_u = \\ 2\beta_0^2 \int_{\Xi_u} \frac{\bar{p}_u}{p(\xi_u)} p(\xi_u) d\xi_u + 2\beta_0 \sum_{k \in K_u} \beta_k \int_{\Xi_u} \frac{\bar{p}_u}{p(\xi_u)} \Psi_k(\xi) p(\xi_u) d\xi_u = 2\beta_0^2 \end{aligned} \quad (43)$$

The final form of the conditional variance, for the first order terms, is then obtained directly by summing up these simplified terms

$$\begin{aligned} D_u = \sum_{k \in K_u^0} \beta_k^2 \int_{\Xi_u} \frac{\bar{p}_u^2}{p(\xi_u)} \Psi_k^2(\xi) d\xi_u + \\ 2 \sum_{i \in K_u^0} \sum_{\substack{j \geq i+1 \\ j \in K_u}} \beta_i \beta_j \int_{\Xi_u} \frac{\bar{p}_u^2}{p(\xi_u)} \Psi_i(\xi) \Psi_j(\xi) d\xi_u - \beta_0^2. \end{aligned} \quad (44)$$

## 5 Numerical results

In this section some numerical results are reported for model problems with custom defined pdfs. All the results are provided with a comparison between the nPC and the collocation approach. We remark here that we expect a better behavior in term of convergence from the collocation approach, but the importance of the present nPC approach is to provide a metamodel of the solution and a framework to compute high order moments conditional statistics. Examples with dimensions up to three are here reported and the effectiveness of the strategy is verified with respect to the analytical solution.

Three different kind of custom pdfs are employed in this work (for a stochastic parameter defined in  $[-1, 1]$ ):

- a linear pdf  $p_1(\xi) = 1/2 + 1/3\xi$
- a quadratic pdf  $p_2(\xi) = \xi^2 + 1/2\xi + 1/6$
- a non polynomial pdf  $p_3(\xi) = 1/2 + 1/3 \sin(\pi\xi)$ .

In the case of multidimensional problems the pdf is obtained by tensorization of equal pdfs for each direction of the stochastic space.

The first model problem is a monodimensional function  $f(\xi) = \sin(\pi\xi) + e^{\xi^2}$  defined on  $\Xi = [-1, 1]$  with a probability distribution equal to  $p_1(\xi)$ .

The results obtained for the first model problem in term of percentage error with respect the analytical results are reported in figure 2. The collocation approach and the non polynomial approach show the same rate of convergence. As evident a lower error is reached by the collocation approach even if, in this case, a fully converged solution can be obtained for the problem in both cases.

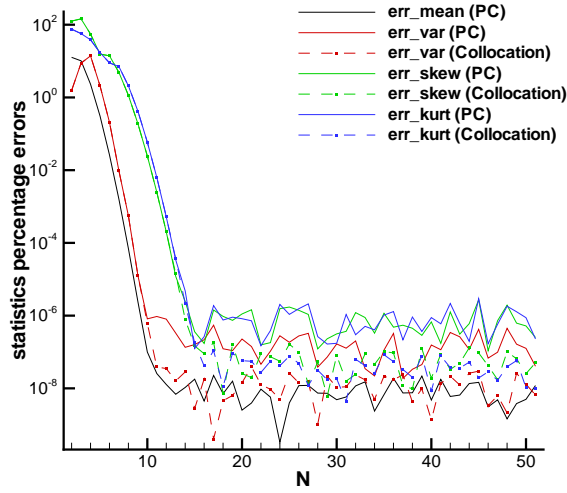


Figure 2: Comparison between the collocation approach and the non polynomial approach for the monodimensional problem.

In the following some multidimensional cases are reported with dimensions up to three. Two kind of function are employed

- a polynomial function  $f_{pol}(\boldsymbol{\xi}) = \prod_{i=1}^d (\xi_i/2 + 1)$
- a non polynomial function  $f_{np}(\boldsymbol{\xi}) = \prod_{i=1}^d \sin(\pi\xi_i)$ .

In particular the results for the polynomial function  $f_{pol}$  in dimension two with distributions (for each dimension)  $p_1(\boldsymbol{\xi})$ ,  $p_2(\boldsymbol{\xi})$  and  $p_3(\boldsymbol{\xi})$  are reported, respectively, in figures 3, 4 and 5.

The results for the polynomial function  $f_{pol}$  in dimension three with distributions (for each dimension)  $p_1(\boldsymbol{\xi})$  and  $p_2(\boldsymbol{\xi})$  are reported, respectively, in figures 6 and 7.

For the non polynomial function only the case with stochastic dimension equal to two is analyzed. In this case the three probability functions are employed and the percentage errors are reported respectively in the figures 8, 9 and 10.

The results obtained are in accord to our predictions: the solution converges slowly for higher moments with respect to the mean and variance and the con-

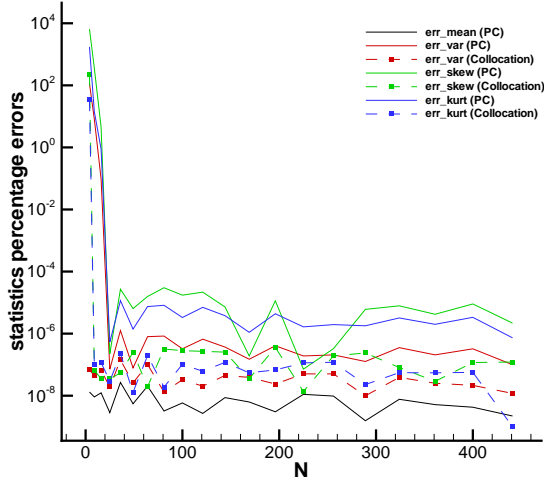


Figure 3: Comparison between the collocation approach and the non polynomial for the polynomial function  $f_{pol}$  with probability distribution  $p_1$  ( $d = 2$ ).

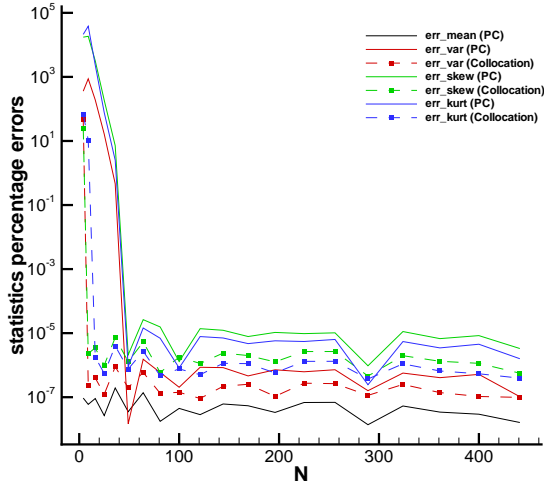


Figure 4: Comparison between the collocation approach and the non polynomial for the polynomial function  $f_{pol}$  with probability distribution  $p_2$  ( $d = 2$ ).

vergence is more stiff for problems with higher stochastic dimension and with non polynomial function or pdf.

Actually the home made code we employed is a sequential one and is very time demanding to obtain a fully converged solution for more stiff problems, but we aspect to improve the present results with a parallel implementation.

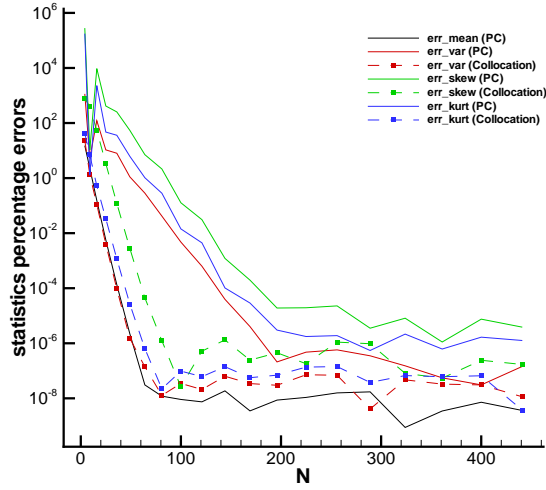


Figure 5: Comparison between the collocation approach and the non polynomial for the polynomial function  $f_{pol}$  with probability distribution  $p_3$  ( $d = 2$ ).

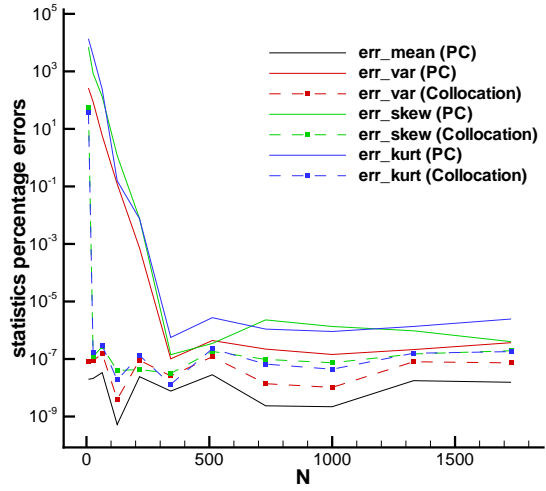


Figure 6: Comparison between the collocation approach and the non polynomial for the polynomial function  $f_{pol}$  with probability distribution  $p_1$  ( $d = 3$ ).

However as a general rule we can notify, that as we expected, a simple collocation is more efficient in term of simulations in practically all the cases. However the present approach retain its interest in the possibility to obtain a metamodel of the solution and an estimation of the conditional statistics.

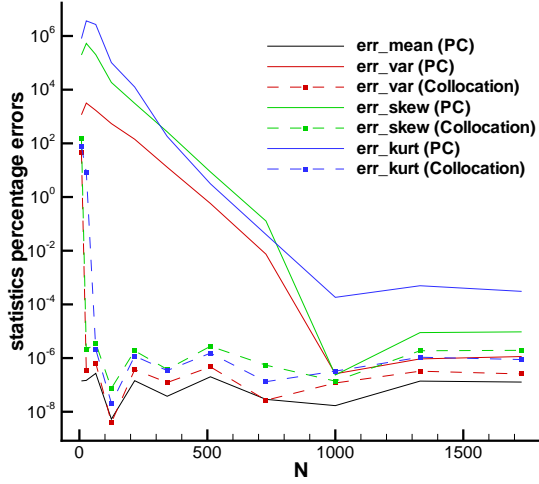


Figure 7: Comparison between the collocation approach and the non polynomial for the polynomial function  $f_{pol}$  with probability distribution  $p_2$  ( $d = 3$ ).

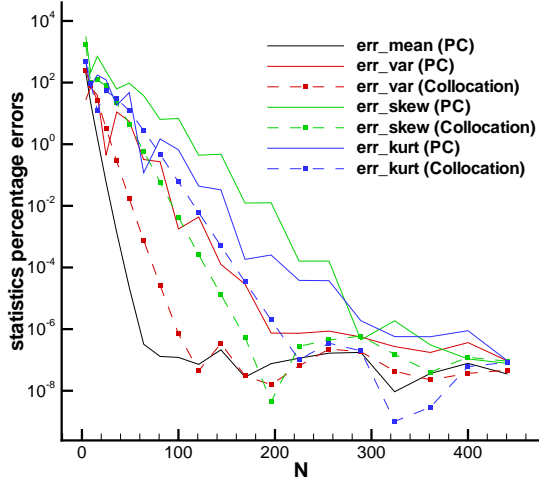


Figure 8: Comparison between the collocation approach and the non polynomial for the polynomial function  $f_{np}$  with probability distribution  $p_1$  ( $d = 2$ ).

## 6 Conclusions and perspective

In the present work a novel approach has been presented to extend the polynomial chaos expansion to the case of non classical defined pdfs, *i.e.* pdfs that fall outside the so-called Wiener-Askey scheme. The strategy is based on the clas-

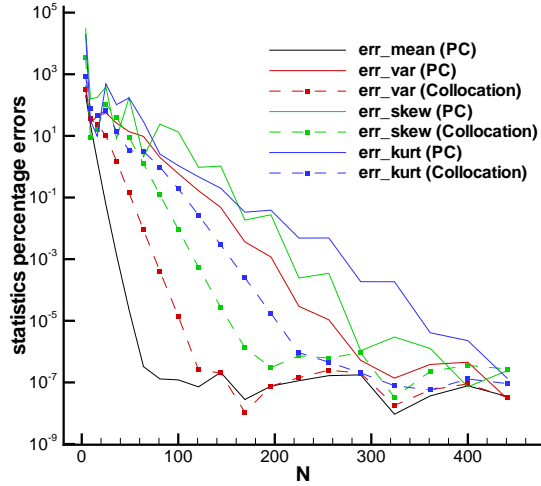


Figure 9: Comparison between the collocation approach and the non polynomial for the polynomial function  $f_{np}$  with probability distribution  $p_2$  ( $d = 2$ ).

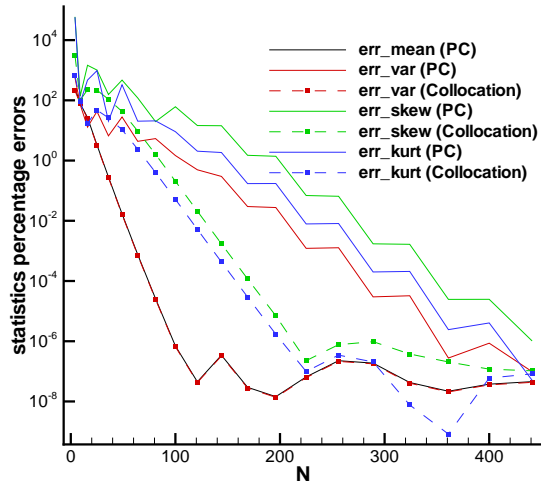


Figure 10: Comparison between the collocation approach and the non polynomial for the polynomial function  $f_{np}$  with probability distribution  $p_3$  ( $d = 2$ ).

sical PC approach but uniform equivalent distributions are employed to re-map the original problem in an uniform one irrespectively of the true probability distribution. This approach eventually degrades the convergence of the classical approach, in term of number of simulations required to estimate the statistics, if a classical pdf is employed. This is due to a quadrature rule optimal only in



the case of polynomial functions with uniform distribution. However this drawback is not much influent in real applications cases because the model function is, often, not polynomial. Another drawbacks could emerge if one compare the present strategy to a brutal force collocation strategy in which every statistical moments is decomposed in expectancies of the function and all the functions itself raised to a power equal to the degree of the maximum statistical moment required. This last approach allows to reduce dramatically the number of integrals to be computed. Anyway the present strategy is motivated because the advantage despite to the higher computational cost is to provide, at the same time, a complete metamodel of the model function and a known structure of the function on which is possible to compute conditional statistics. This possibly is not completely explored in this work and only the first order conditional variances are explicitly shown. At the present time only an home made sequential code is at our disposal and this limits the possibility to compute high order statistics for more complex problems in higher dimension than two. To allow more real application cases, in which the single cost of each computation can be much more expensive, we expect to really increase the efficiency coupling the present strategy with a Smolyak algorithm to compute the set of quadrature points on which the simulations must be performed. In the case of smooth model functions and probability distribution, for high dimension problems, the coupling between our novel nPC approach and the sparse grid is straightforward.

## 7 Acknowledgements

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