Computational aspects for constructing realizations of polynomial chaos in high dimension

Christian Soize, Christophe Desceliers

COMPUTATIONAL ASPECTS FOR CONSTRUCTING REALIZATIONS OF POLYNOMIAL CHAOS IN HIGH DIMENSION

C. SOIZE* AND C. DESCELIERS†

Abstract. This paper deals with computational aspects related to the construction of realizations of polynomial chaos expansion in high dimension. The method proposed consists (1) in constructing the realizations of the multivariate monomials using a generator of independent realizations of the germs whose probability distribution is the given arbitrary measure and (2) in performing an orthogonalization of the realizations of the multivariate monomials with an algorithm different from the Gram-Schmidt orthogonalization algorithm which is not stable in high dimension. A brief review of polynomial chaos expansion with arbitrary measure is given. The statistically independent realizations of multivariate monomials are introduced. The centered statistically independent realizations of orthonormal multivariate polynomials are developed. Finally, a quantification of the errors induced by the usual methods is given.

Key words. Polynomial chaos expansion, high dimension, computation.

AMS subject classifications. 60H35, 60H15, 60H25, 60H40, 65C50

1. Introduction. The Polynomial Chaos Expansion (PCE), firstly introduced by Wiener [52] for stochastic processes, is a powerful tool for constructing a stochastic representation of a random vector, of a random matrix or a random tensor, of a stochastic process or a random field. A general methodology has been introduced in [17, 18] for the PCE construction of a stochastic process or a random field (for such a construction of a polynomial chaos expansion with respect to an arbitrary measure, see for instance [46]).

In the last decade, the polynomial chaos expansions of stochastic processes and random fields have been used in many works to study stochastic boundary value problems (see for instance, [1] to [16], [19] to [44], [47, 50, 51, 53, 54]). An excellent and exhaustive synthesis of all the works on spectral methods for uncertainty quantification can be found in the recent book [24].

This paper is devoted to the computational aspects related to the numerical calculation of realizations $\boldsymbol{X}_N(\theta_\ell) = \sum_{j=1}^N \boldsymbol{x}_j \, \Psi_j(\boldsymbol{\Xi}(\theta_\ell))$ of a given polynomial chaos expansion $\boldsymbol{X}_N = \sum_{j=1}^N \boldsymbol{x}_j \, \Psi_j(\boldsymbol{\Xi})$ in high dimension and for an arbitrary measure. The "high dimension" terminology means that the family $\{\Psi_j(\boldsymbol{\Xi}), j = 1, \ldots, N\}$ of polynomials contains polynomials having a high degree N_d (for instance 20) with simultaneously a significant value of the germ dimension N_g (for instance 4), inducing a high value of the total dimension N. Such situation is encountered when a high value of N is required in order to achieve convergence of the PCE. The "arbitrary measure" terminology means that the germ $\boldsymbol{\Xi} = (\Xi_1, \ldots, \Xi_{N_g})$ is a vector-valued random variable whose probability distribution $P_{\boldsymbol{\Xi}}(d\boldsymbol{\xi})$ is arbitrary on $\mathbb{R}^{N_g}$.

The main objective of the paper is not directly related to the construction of a polynomial chaos expansion of stochastic processes or random fields in order to solve a stochastic equation by using the Galerkin method (spectral method) which requires, for instance, the use of collocation methods. The objective of the manuscript is to propose a new methodology to compute independent realizations (in preserving the orthogonality properties) of the polynomial chaos expansion of a stochastic process or of a random field when the convergence consideration implies a high dimension expansion and for an arbitrary probability measure

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of the germ. For instance, such a situation is met to identify (by solving stochastic inverse problems) the polynomial chaos representation of unknown stochastic processes and random fields. In such a case the coefficients are estimated using the maximum likelihood method for which the probability density functions are estimated by the Monte Carlo method requiring the calculation of independent realizations of the polynomial chaos expansion (see for instance [1, 4, 7, 45]).

In this paper, the method proposed is very useful for analyzing the two following cases. The first one corresponds to the case for which the system of orthogonal polynomials $\{\Psi_j(\boldsymbol{\xi}), j = 1, \ldots, N\}$ is explicitly known (for instance, for the Gaussian measure, the system is constituted of the Hermite polynomials). The second one corresponds to the case for which the system of orthogonal polynomials $\{\Psi_j(\boldsymbol{\xi}), j = 1, \ldots, N\}$ is not explicitly known because the measure $P_{\boldsymbol{\Xi}}(d\boldsymbol{\xi})$ does not correspond to a usual measure which is explicitly known.

Sometimes, for $\ell = 1, \ldots, \nu$, realizations $\boldsymbol{X}_N(\theta_\ell) = \sum_{j=1}^N \boldsymbol{x}_j \, \Psi_j(\boldsymbol{\Xi}(\theta_\ell))$ must be computed for high polynomial degrees in order to achieve convergence of the PCE. Such a situation can arise for the identification of the coefficients $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ of the PCE $\boldsymbol{X}_N = \sum_{j=1}^N \boldsymbol{x}_j \, \Psi_j(\boldsymbol{\Xi})$ corresponding to an unknown stochastic model for which N and coefficients $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ are unknown and must be identified using observed data. For instance, this is the case for a stochastic reduced-order model of a random field having a relatively short correlation length with respect to the domain size.

In this paper, the method proposed has been developed in the context of a research recently published [45] which was devoted to the identification of high dimensional polynomial chaos expansions with random coefficients for non-Gaussian tensor-valued random fields using partial and limited experimental data. In this work, the number N of coefficients to be identified were about seven millions corresponding to $N_g = 4$ and $N_d = 22$ and allowing the convergence of the polynomial expansion to be achieved. In [45], the computation of the realizations of the polynomial chaos for this high dimension case using either the computational recurrence formula or the algebraic explicit representation did not give good results. This is the reason why the new methodology presented below has been developed and has allowed the computation of the case in high dimension to be carried out. This new methodology is not presented in [45] but is developed and validated in the present paper.

It should be noted that such problems are not trivial at all. For instance, as it will be shown in the last section, the use of the explicit algebraic formula (for instance, constructed with a symbolic Toolbox) or the use of a recurrence relation with respect to the degree, to evaluate the realizations $\{\Psi_j(\boldsymbol{\Xi}(\theta_\ell))$ for $j = 1, \ldots, N$ and for $\ell = 1, \ldots, \nu\}$ with high polynomial degrees, induces important numerical noise and the orthogonality property defined by $E\{\Psi_j(\boldsymbol{\Xi}) \, \Psi_k(\boldsymbol{\Xi})\} \simeq \frac{1}{\nu} \sum_{\ell=1}^{\nu} \Psi_j(\boldsymbol{\Xi}(\theta_\ell)) \, \Psi_k(\boldsymbol{\Xi}(\theta_\ell)) = \delta_{jk}$ is lost.

The main idea of the proposed method is based (1) on the construction of the realizations $\mathcal{M}_j(\boldsymbol{\Xi}(\theta_\ell))$ of the monomials $\mathcal{M}_j(\boldsymbol{\Xi})$ using a generator of independent realizations $\boldsymbol{\Xi}(\theta_1), \ldots, \boldsymbol{\Xi}(\theta_\nu)$ of the germs whose probability distribution is the given arbitrary measure $P_{\boldsymbol{\Xi}}(d\boldsymbol{\xi})$ and (2) on the construction of a Gram-Schmidt orthogonalization of the family of vectors made up of the realizations of the monomials. Unfortunately, when N and $\nu > N$ are large (several ten thousands), the Gram-Schmidt algorithm is not stable. We then propose an alternative way to perform the orthogonalization of the monomials.

With the method proposed, independent realizations are constructed in preserving the orthogonality properties. It should be noted that, if an orthogonalization was performed on the realizations constructed with the usual methods (computational recurrence formula or algebraic explicit representation) in order to obtain the orthogonality properties, then the statistical independence would be lost. With the new method proposed in this paper, the realizations are statistically independent. Concerning the sources of the numerical noise, it

seems that the major contribution is not due to the evaluation of the monomials (products) but is due to the evaluation of the polynomials (summation of monomials of different degrees).

In a first section, a brief review on the polynomial chaos expansion with an arbitrary measure is given. Then, the statistically independent realizations of multivariate monomials are introduced. In the following section, the centered statistically independent realizations of the orthonormal multivariate polynomials are developed. The last section deals with a validation of the proposed method.

2. Brief review of the polynomial chaos expansion with respect to an arbitrary measure. Let $\mathbb{N} = \{0, 1, 2, \ldots\}$ be the set of all the null and positive integers. Let $\mathbb{R}^{N_g}$ be the Euclidean space for which the generic point is $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_{N_g})$. Let $d\boldsymbol{\xi} = d\xi_1 \ldots d\xi_{N_g}$ be the Lebesgue measure on $\mathbb{R}^{N_g}$. Let $\boldsymbol{\Xi} = (\Xi_1, \ldots, \Xi_{N_g})$ be a $\mathbb{R}^{N_g}$-valued random vector defined on a probability space $(\Theta, \mathcal{T}, \mathcal{P})$ with probability distribution $P_{\boldsymbol{\Xi}}(d\boldsymbol{\xi})$ on $\mathbb{R}^{N_g}$. Let

$$\{\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})\,,\, \boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_{N_g}) \in \mathbb{N}^{N_g}\,,\, |\boldsymbol{\alpha}| = \alpha_1 + \ldots + \alpha_{N_g} \in \mathbb{N}\} \quad , \tag{2.1}$$

be a family of multivariate orthonormal real polynomials $\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \Psi_{\alpha_1}(\xi_1) \times \ldots \times \Psi_{\alpha_{N_g}}(\xi_{N_g})$ with respect to the arbitrary probability measure $P_{\boldsymbol{\Xi}}(d\boldsymbol{\xi})$ on $\mathbb{R}^{N_g}$ such that for all $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ in $\mathbb{N}^{N_g}$,

$$\int_{\mathbb{R}^{N_g}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})\, \Psi_{\boldsymbol{\beta}}(\boldsymbol{\xi})\, P_{\boldsymbol{\Xi}}(d\boldsymbol{\xi}) = E\{\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\Xi})\, \Psi_{\boldsymbol{\beta}}(\boldsymbol{\Xi})\} = \delta_{\boldsymbol{\alpha}\boldsymbol{\beta}} \quad . \tag{2.2}$$

In Eq. (2.2), E is the mathematical expectation and $\delta_{\boldsymbol{\alpha}\boldsymbol{\beta}} = 0$ if $\boldsymbol{\alpha} \neq \boldsymbol{\beta}$ and $= 1$ if $\boldsymbol{\alpha} \neq \boldsymbol{\beta}$. For $\boldsymbol{\alpha} = \mathbf{0}$, $\Psi_{\mathbf{0}}(\boldsymbol{\xi}) = 1$ is the constant normalized polynomial.

Let $\boldsymbol{\xi} \mapsto \boldsymbol{f}(\boldsymbol{\xi}) = (f_1(\boldsymbol{\xi}), \ldots, f_n(\boldsymbol{\xi}))$ be a measurable mapping from $\mathbb{R}^{N_g}$ into $\mathbb{R}^n$ such that the $\mathbb{R}^n$-valued random variable $\boldsymbol{X} = (X_1, \ldots, X_n) = \boldsymbol{f}(\boldsymbol{\Xi})$ is a second-order random variable, that is to say, is such that

$$E\{\|\boldsymbol{X}\|^2\} = E\{\|\boldsymbol{f}(\boldsymbol{\Xi})\|^2\} = \int_{\mathbb{R}^{N_g}} \|\boldsymbol{f}(\boldsymbol{\xi})\|^2\, P_{\boldsymbol{\Xi}}(d\boldsymbol{\xi}) < +\infty \quad , \tag{2.3}$$

in which $\|\boldsymbol{X}\|^2 = \sum_{j=1}^{n} X_j^2$. Consequently, the random variable $\boldsymbol{X} = \boldsymbol{f}(\boldsymbol{\Xi})$ admits the following polynomial chaos expansion with respect to the probability measure $P_{\boldsymbol{\Xi}}(d\boldsymbol{\xi})$,

$$\boldsymbol{X} = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^{N_g}} \boldsymbol{x}_{\boldsymbol{\alpha}}\, \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\Xi}) \quad , \tag{2.4}$$

in which the family of vectors $\{\boldsymbol{x}_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha} \in \mathbb{N}^{N_g}}$ in $\mathbb{R}^n$ is such that

$$\boldsymbol{x}_{\boldsymbol{\alpha}} = E\{\boldsymbol{f}(\boldsymbol{\Xi})\, \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\Xi})\} \quad . \tag{2.5}$$

The right-hand side of Eq. (2.4) is mean-square convergent. In this paper, the summation over the multi-index $\boldsymbol{\alpha}$, in Eq. (2.4), is renumbered in using a mono-index such that $\boldsymbol{X} = \sum_{j=1}^{+\infty} \boldsymbol{x}_j\, \Psi_j(\boldsymbol{\Xi})$ and Eq. (2.5) is rewritten as $\boldsymbol{x}_j = E\{\boldsymbol{f}(\boldsymbol{\Xi})\, \Psi_j(\boldsymbol{\Xi})\}$.

3. Statistically independent realizations of multivariate monomials. Let $\boldsymbol{\Xi} = (\Xi_1, \ldots, \Xi_{N_g})$ be the $\mathbb{R}^{N_g}$-valued random vector of the independent centered random variables $\Xi_1, \ldots, \Xi_{N_g}$ for which the probability density functions (with respect to the Lebesgue measure $d\xi$ on the real line) are denoted by $p_{\Xi_1}(\xi), \ldots, p_{\Xi_{N_g}}(\xi)$. For all $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_{N_g})$ in $\mathbb{N}^{N_g}$ (including the null multi-index $(0, \ldots, 0)$) and for all $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_{N_g})$ belonging to $\mathbb{R}^{N_g}$, the multivariate monomial $\mathcal{M}_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$ is defined by

$$\mathcal{M}_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \xi_1^{\alpha_1} \times \ldots \times \xi_{N_g}^{\alpha_{N_g}} \quad . \tag{3.1}$$

Let us consider the set $\{\mathcal{M}_{\boldsymbol{\alpha}}(\boldsymbol{\xi})\,,\,\boldsymbol{\alpha}\,;\,|\boldsymbol{\alpha}|=0,\ldots,N_d\}$ which contains $N=(N_d+N_g)!/(N_d!\,N_g!)$ multivariate monomials. This set of multivariate monomials is renumbered as $\mathcal{M}_1(\boldsymbol{\xi}),\ldots,\mathcal{M}_N(\boldsymbol{\xi})$ such that the set $\{\mathcal{M}_{\boldsymbol{\alpha}}(\boldsymbol{\xi})\,,\,\boldsymbol{\alpha}\,;\,|\boldsymbol{\alpha}|=0,\ldots,N_d\}$ of length N is identified to the set $\{\mathcal{M}_1(\boldsymbol{\xi}),\ldots,\mathcal{M}_N(\boldsymbol{\xi})\}$. It is assumed that $\mathcal{M}_1(\boldsymbol{\xi})=1$ is the constant monomial. It should be noted that the random variables $\mathcal{M}_1(\boldsymbol{\Xi}),\ldots,\mathcal{M}_N(\boldsymbol{\Xi})$ are not normalized, centered or orthogonal. Let ν be an integer such that $\nu>N$. Let $\boldsymbol{\Xi}(\theta_1),\ldots,\boldsymbol{\Xi}(\theta_\nu)$ be ν independent realizations of random vector $\boldsymbol{\Xi}$. Then the ν independent realizations of the N random multivariate monomials $\mathcal{M}_1(\boldsymbol{\Xi}),\ldots,\mathcal{M}_N(\boldsymbol{\Xi})$ are represented by the $\nu\times N$ real numbers $\{\mathcal{M}_j(\boldsymbol{\Xi}(\theta_\ell))\}_{\ell j}$.

4. Centered statistically independent realizations of orthonormal multivariate polynomials. We introduce the estimation $\{\underline{\mathcal{M}}_j, j=1,\ldots,N\}$ of the mean values of the realizations $\{\mathcal{M}_j(\boldsymbol{\Xi}(\theta_\ell)), j=1,\ldots,N\}$ such that $\underline{\mathcal{M}}_1=0$ and such that, for all j in $\{2,\ldots,N\}$, $\underline{\mathcal{M}}_j=\nu^{-1}\sum_{\ell=1}^{\nu}\mathcal{M}_j(\boldsymbol{\Xi}(\theta_\ell))$. We then introduce the $(\nu\times N)$ real matrix $[\mathcal{M}]$ of the centered realizations such that

$$[\mathcal{M}]_{\ell j}=\mathcal{M}_j(\boldsymbol{\Xi}(\theta_\ell))-\underline{\mathcal{M}}_j \quad . \tag{4.1}$$

The main idea is to construct a $(N\times N)$ real matrix $[A\,]$ such that the independent realizations $[\Psi]_{\ell j}=\Psi_j(\boldsymbol{\Xi}(\theta_\ell))$ of the polynomial chaos $\Psi_j(\boldsymbol{\Xi})$ can be written as

$$[\Psi]=[\mathcal{M}]\,[A\,] \quad . \tag{4.2}$$

With such a construction, the realizations $\{\Psi_j(\boldsymbol{\Xi}(\theta_\ell)),\ell=1,\ldots,\nu\}$ are independent, because $[\Psi]_{\ell j}=\sum_{k=1}^{N}[\mathcal{M}]_{\ell k}\,[A\,]_{kj}$ shows that the rows stay independent. In addition, due to Eq. (4.1), the estimation of the mean value of each polynomial chaos is zero except the constant polynomial chaos. It should be noted that $\{[\Psi]^T\,[\Psi]\}_{jk}/\nu$ is the estimation of $E\{\Psi_j(\boldsymbol{\Xi})\,\Psi_k(\boldsymbol{\Xi})\}$ which has to be equal to the Kronecker symbol δ_{jk}. Consequently, the orthogonality of the polynomial chaos will be preserved if $[\Psi]^T\,[\Psi]/\nu=[I_N]$ in which $[I_N]$ is the identity matrix. Substituting Eq. (4.2) into $[\Psi]^T\,[\Psi]/\nu=[I_N]$ yields

$$[A\,]^T\,[\mathcal{M}]^T\,[\mathcal{M}]\,[A\,]=\nu\,[I_N] \quad . \tag{4.3}$$

which shows that the matrix $[A\,]$ is related to the singular value decomposition of matrix $[\mathcal{M}]$. Below, we detail the algorithm for the direct construction of matrix $[\Psi]$ without explicitly constructing matrix $[A\,]$ and then, without performing the product $[\mathcal{M}]\,[A\,]$.

Let $[\mathcal{M}]=[\mathbb{U}]\,[\mathcal{S}]\,[V]^T$ be the singular value decomposition of matrix $[\mathcal{M}]$ in which $[\mathbb{U}]$ is a $(\nu\times\nu)$ real unitary matrix, where $[\mathcal{S}]$ is a $(\nu\times N)$ real matrix whose diagonal elements are nonnegative and are ordered in decreasing values, and where $[V]$ is a $(N\times N)$ real unitary matrix. Since $\nu>N$, there are $\nu-N$ zero singular values that we remove hereinafter. Therefore, let $[U]$ be the $(\nu\times N)$ real matrix whose N columns are made up of the N first columns of matrix $[\mathbb{U}]$. We then have

$$[U]^T\,[U]=[I_N] \quad . \tag{4.4}$$

Let $[S]$ be the diagonal $(N\times N)$ real matrix made up of the block of the non zero singular values of matrix $[\mathcal{S}]$. We can then write

$$[\mathcal{M}]=[U]\,[S]\,[V]^T \quad . \tag{4.5}$$

Multiplying Eq. (4.5) by the invertible matrix $([S]\,[V]^T)^{-1}$ which is $[V]\,[S]^{-1}$ yields $[\mathcal{M}]\,[V]\,[S]^{-1}=[U]$. Substituting $[U]=[\mathcal{M}]\,[V]\;[S]^{-1}$ into Eq. (4.4) and multiplying the result by

ν yield

$$(\nu^{1/2}\,[V]\,[S]^{-1})^T\,[\mathcal{M}]^T\,[\mathcal{M}]\,(\nu^{1/2}\,[V]\,[S]^{-1}) = \nu\,[I_N] \quad . \tag{4.6}$$

Comparing with Eq. (4.3) with Eq. (4.6) yields a solution for $[A\,]$ which can be written as

$$[A\,] = \nu^{1/2}\,[V]\,[S]^{-1} \quad . \tag{4.7}$$

Substituting Eq. (4.7) into Eq. (4.2) yields $[\Psi] = \nu^{1/2}\,[\mathcal{M}]\,[V]\,[S]^{-1}$. Finally, substituting Eq. (4.5) into the last equation yields

$$[\Psi] = \sqrt{\nu}\,[U] \quad . \tag{4.8}$$

It should be noted that, in Eq. (4.8), matrix $[U]$ is directly constructed through the SVD of matrix $[\mathcal{M}]$. Summarizing, we have the following statistical estimations. Let j_0 be the column index such that $|[\Psi]_{\ell j_0}| = 1$ for all $\ell = 1, \ldots, \nu$ and corresponding to the ν independent realizations of the constant chaos polynomial $\Psi_{j_0}(\Xi) = 1$. We then have

$$E\{\Psi_{j_0}(\Xi)\} \simeq \frac{1}{\nu}\sum_{\ell=1}^{\nu}[\Psi]_{\ell j_0} = 1 \quad . \tag{4.9}$$

For j in $\{1, \ldots, N\}$ but different from j_0, we have

$$E\{\Psi_j(\Xi)\} \simeq \frac{1}{\nu}\sum_{\ell=1}^{\nu}[\Psi]_{\ell j} = 0 \quad . \tag{4.10}$$

For j and k in $\{1, \ldots, N\}$, we also have

$$E\{\Psi_j(\Xi)\,\Psi_k(\Xi)\} \simeq \frac{1}{\nu}\sum_{\ell=1}^{\nu}[\Psi]_{\ell j}\,[\Psi]_{\ell k} = \delta_{jk} \quad . \tag{4.11}$$

5. Quantification of the errors induced by the usual methods. The objective of this section is to present a quantification of the errors induced by the usual methods concerning the orthogonality properties while the proposed new method does not produce errors. This proposed method is mathematically proven and a numerical application is not required. The method is not proposed as an alternative method with respect to the existing methods but is devoted to a field of applications for which no method is available today. This section demonstrates that the use of the usual methods (computational recurrence formula or algebraic explicit representation of the polynomial chaos) are not efficient in high dimension with respect to the orthogonality properties. The usual methods are sensitive to the numerical noise, while the proposed method allows the numerical noise to be overcome (see the explanations given in Section 1). In order to quantify the errors, two cases are considered. For these two cases the germ is Gaussian and then the polynomials are the normalized Hermite polynomials. The first one is the most simple case for which $N_g = 1$ and $N_d = 1, \ldots, 30$, therefore $N = 1, \ldots, 30$. The number of independent realizations is $\nu = 10^6$. The second one corresponds to $N_g = 5$ and $N_d = 1, \ldots, 10$, therefore $N = 6, \ldots, 3,003$. The number of independent realizations is $\nu = 10^5$.

For $\alpha_j = 0$, we introduce $\Psi_{\alpha_j}(\xi_j) = H_0(\xi_j) = 1$ and for $\alpha_j = 1, 2, \ldots$, we introduce $\Psi_{\alpha_j}(\xi_j) = H_{\alpha_j - 1}(\xi_j)/\sqrt{(\alpha_j - 1)!}$ in which the polynomials $H_{\alpha_j}(\xi_j)$ are the Hermite

polynomials which are not normalized. Let $\boldsymbol{\Xi}(\theta_1), \ldots, \boldsymbol{\Xi}(\theta_\nu)$ be ν independent realizations of the normalized Gaussian $\mathbb{R}^{N_g}$-valued random variable $\boldsymbol{\Xi}$ with $\nu > N$. Let $\Psi^{alg}_{\alpha_j}(\Xi_j)$ be the polynomial $\Psi_{\alpha_j}(\Xi_j)$ for which the realization $\Psi^{alg}_{\alpha_j}(\Xi_j(\theta_\ell))$ is computed using the usual explicit algebraic formula of the polynomial $\Psi_{\alpha_j}(\Xi_j)$ (constructed, for instance, with a symbolic toolbox). Let $\Psi^{recur}_{\alpha_j}(\Xi_j)$ be the polynomial $\Psi_{\alpha_j}(\Xi_j)$ for which the realization $\Psi^{recur}_{\alpha_j}(\Xi_j(\theta_\ell)) = H^{recur}_{\alpha_j-1}(\Xi_j(\theta_\ell))/\sqrt{(\alpha_j-1)!}$ is computed using the usual recurrence formula which is written as

$$H^{recur}_{\alpha_j+1}(\Xi_j(\theta_\ell)) = \Xi_j(\theta_\ell)\, H^{recur}_{\alpha_j}(\Xi_j(\theta_\ell)) - \alpha_j\, H^{recur}_{\alpha_j-1}(\Xi_j(\theta_\ell)) \quad . \tag{5.1}$$

with, for $\alpha_j = 0$, $H^{recur}_{\alpha_j}(\Xi_j(\theta_\ell)) = 1$ and for $\alpha_j = 1$, $H^{recur}_{\alpha_j}(\Xi_j(\theta_\ell)) = \Xi_j(\theta_\ell)$. Finally, let $\Psi^{comp}_{\alpha_j}(\Xi_j)$ be the polynomial $\Psi_{\alpha_j}(\Xi_j)$ for which the realization $\Psi^{comp}_{\alpha_j}(\Xi_j(\theta_\ell))$ is computed using the new method presented in Sections 3 and 4.

Below, the multivariate polynomials are obtained by performing the tensorial product and, as explained at the end of Section 2, the multivariate polynomials are renumbered in using a mono-index j which belongs to $\{1, \ldots, N\}$.

Let $[Cor^{alg}(N)]$, $[Cor^{recur}(N)]$ and $[Cor^{comp}(N)]$ be the $(N \times N)$ matrices measuring the orthonormality of the polynomial chaos $\Psi^{alg}_j(\boldsymbol{\Xi})$, $\Psi^{recur}_j(\boldsymbol{\Xi})$ and $\Psi^{comp}_j(\boldsymbol{\Xi})$ defined and estimated by

$$[Cor^{alg}(N)]_{jk} = E\{\Psi^{alg}_j(\boldsymbol{\Xi})\, \Psi^{alg}_k(\boldsymbol{\Xi})\} \simeq \frac{1}{\nu} \sum_{\ell=1}^{\nu} \Psi^{alg}_j(\boldsymbol{\Xi}(\theta_\ell))\, \Psi^{alg}_k(\boldsymbol{\Xi}(\theta_\ell)) \quad , \tag{5.2}$$

$$[Cor^{recur}(N)]_{jk} = E\{\Psi^{recur}_j(\boldsymbol{\Xi})\, \Psi^{recur}_k(\boldsymbol{\Xi})\} \simeq \frac{1}{\nu} \sum_{\ell=1}^{\nu} \Psi^{recur}_j(\boldsymbol{\Xi}(\theta_\ell))\, \Psi^{recur}_k(\boldsymbol{\Xi}(\theta_\ell)) \quad . \tag{5.3}$$

$$[Cor^{comp}(N)]_{jk} = E\{\Psi^{comp}_j(\boldsymbol{\Xi})\, \Psi^{comp}_k(\boldsymbol{\Xi})\} \simeq \frac{1}{\nu} \sum_{\ell=1}^{\nu} [\Psi]_{\ell j}\, [\Psi]_{\ell k} \quad , \tag{5.4}$$

for which Eq. (4.11) has been used. By construction of the proposed new method, for any $\nu > N$, we have $[Cor^{comp}(N)]_{jk} = \delta_{jk}$ which corresponds to the orthonormality property. For ν sufficiently large, one could expect that $[Cor^{alg}(N)]_{jk} \simeq [Cor^{recur}(N)]_{jk} \simeq \delta_{jk}$. In fact, it is not the case. The orthonormality property is lost and we propose below to quantify the errors.

Let $\|.\|_F$ be the Frobenius norm of matrices. Let

$$N \mapsto \text{err}^{alg}(N) = \|[I_N] - [Cor^{alg}(N)]\|_F / \|[I_N]\|_F \quad , \tag{5.5}$$

$$N \mapsto \text{err}^{recur}(N) = \|[I_N] - [Cor^{recur}(N)]\|_F / \|[I_N]\|_F \quad , \tag{5.6}$$

$$N \mapsto \text{err}^{comp}(N) = \|[I_N] - [Cor^{comp}(N)]\|_F / \|[I_N]\|_F \quad , \tag{5.7}$$

be the error functions which measure the loss of the orthonormality property of the two usual methods (algebraic explicit representation and computational recurrence formula) and of the

proposed new method referenced as "comp". It should be noted that the error $\text{err}^{comp}(N)$ must be 0 for all N due to the orthonormality property which is preserved.

For the first case ($N_g = 1$ and $N_d = 30$), the estimations of quantities $[Cor^{alg}(N)]$, $[Cor^{recur}(N)]$ and $[Cor^{comp}(N)]$ presented in the figures are converged with respect to ν. Fig. 1 displays the graphs of the functions $N \mapsto \text{err}^{alg}(N)$, $N \mapsto \text{err}^{recur}(N)$, $N \mapsto \text{err}^{comp}(N)$ and $N \mapsto \text{err}^{theory}(N) = 0$ corresponding to the theoretical values. It can be seen that the level of the errors is the same for the two usual methods represented by the thin lines with circles. For $N = 5$, $N = 20$ and $N = 30$, the errors are about 7%, 72% and 80%. Consequently, for $N = N_d \geq 5$, the loss of the orthonormality property is very important for the usual methods (thin line with circles) while there is no error with the proposed new method (thick line) for which the computed error is 2.9×10^{-14} for $N = N_d = 30$. The new method coincides with the theoretical value which is zero (thick line). In order to

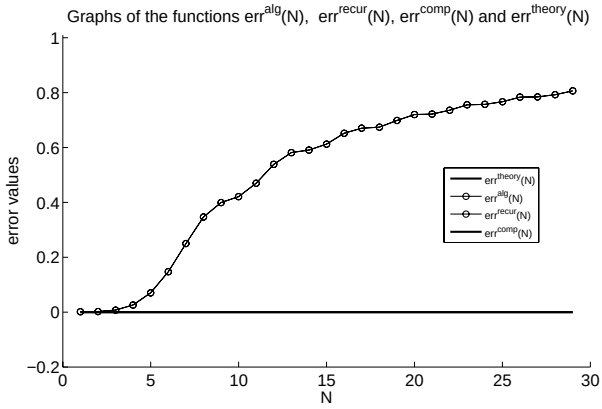

FIG. 5.1. *Graph of the error functions $N \mapsto err^{alg}(N)$ (thin line with circles), $N \mapsto err^{recur}(N)$ (thin line with circles), $N \mapsto err^{comp}(N)$ (thick line) and $N \mapsto err^{theory}(N)$ (thick line) for $N_g = 1$ and for $N_d = 1$ to 30 with $N = (N_d + N_g)!/\,(N_d!\,N_g!)$*

quantify more precisely the loss of the orthonormality property, we introduce the eigenvalue problems $[Cor^{name}(N)]\,\boldsymbol{x}^j = \lambda_j^{name}\boldsymbol{x}^j$ for $name = \{alg, recur, comp, theory\}$ and for $N = N_d = 30$. Fig. 2 displays the graphs of the functions $j \mapsto \lambda_j^{alg}$, $j \mapsto \lambda_j^{recur}$, $j \mapsto \lambda_j^{comp}$ and $j \mapsto \lambda_j^{theory} = 1$ corresponding to the theoretical values. It can be seen that the level of the errors is the same for the two usual methods(thin lines with circles). For these two usual methods, this figure shows that 6 eigenvalues have a value less that 10^{-6} instead of 1. For the second case ($N_g = 5$ and $N_d = 10$), the computation has been carried out with $\nu = 10^5$ independent realizations. We also have verified that, for $N = (N_d + N_g)!/\,(N_d!\,N_g!) = 3,003$, the estimations of quantities $[Cor^{alg}(N)]$, $[Cor^{recur}(N)]$ and $[Cor^{comp}(N)]$ shown in the figures are converged with respect to ν. Fig. 3 displays the graphs of the functions $N \mapsto \text{err}^{alg}(N)$, $N \mapsto \text{err}^{recur}(N)$, $N \mapsto \text{err}^{comp}(N)$ and $N \mapsto \text{err}^{theory}(N) = 0$ corresponding to the theoretical values. It can be seen that the level of the errors is not any more the same for the two usual methods represented by the thin lines with circles and squares. For $N = 56$ ($N_g = 5, N_d = 3$), $N = 792$ ($N_g = 5, N_d = 7$) and $N = 3,003$ ($N_g = 5, N_d = 10$), the errors are about 365%, 299% and 351% for the computational recurrence formula, and the errors are about 5.32%, 156% and 669% for the algebraic explicit representation. Consequently, the loss of the orthonormality property is very important for the usual methods (thin line with circles and squares) while there is no error

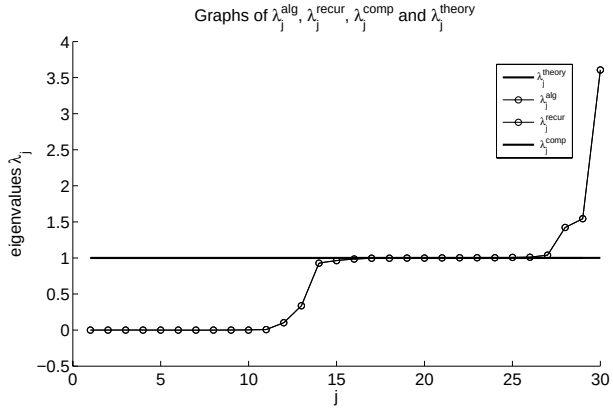

FIG. 5.2. *Graphs of $j \mapsto \lambda_j^{alg}$ (thin line with circles), $j \mapsto \lambda_j^{recur}$ (thin line with circles), $j \mapsto \lambda_j^{comp}$ (thick line) and $j \mapsto \lambda_j^{theory} = 1$ (thick line) corresponding to the theoretical values (for $N_g = 1$ and for $N_d = 30$)*

with the proposed new method (thick line) for which the computed error is 1.2×10^{-14} for $N = 3,003$ ($N_g = 5, N_d = 10$). The new method coincides with the theoretical value which is zero (thick line). Similarly to the first case, in order to quantify more precisely the loss

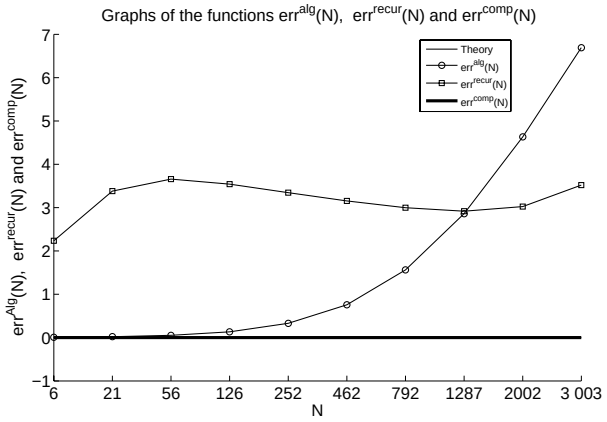

FIG. 5.3. *Graph of the error functions $N \mapsto err^{alg}(N)$ (thin line with circles), $N \mapsto err^{recur}(N)$ (thin line with circles), $N \mapsto err^{comp}(N)$ (thick line) and $N \mapsto err^{theory}(N)$ (thick line) for $N_g = 5$ and for $N_d = 1$ to 10 with $N = (N_d + N_g)!/\,(N_d!\,N_g!)$*

of the orthonormality property, we introduce the eigenvalue problems $[Cor^{\,name}(N)]\,\boldsymbol{x}^j = \lambda_j^{name}\boldsymbol{x}^j$ for $name = \{alg, recur, comp, theory\}$ and for $N = 3,003$ ($N_g = 5, N_d = 10$). Fig. 4 displays the graphs of the functions $j \mapsto \lambda_j^{alg}$, $j \mapsto \lambda_j^{recur}$, $j \mapsto \lambda_j^{comp}$ and $j \mapsto \lambda_j^{theory} = 1$ corresponding to the theoretical values. It can be seen that the level of the errors is not any more the same for the two usual methods(thin line and medium thick line). For these two usual methods, this figure shows that $2,251$ eigenvalues have a value less that 2×10^{-13} instead of 1 for the computational recurrence formula and $1,128$ eigenvalues have a value less that 10^{-1} instead of 1 for the algebraic explicit representation.

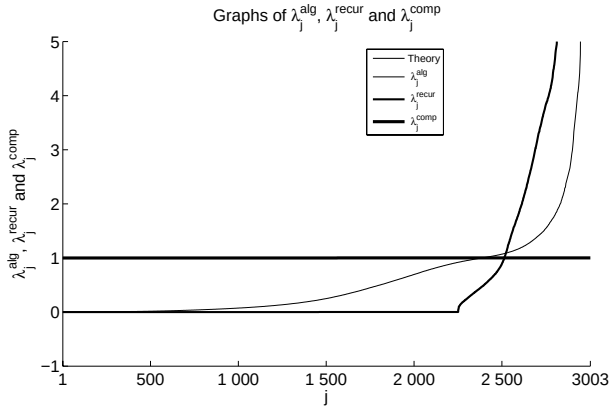

FIG. 5.4. *Graphs of $j \mapsto \lambda_j^{alg}$ (thin line with circles), $j \mapsto \lambda_j^{recur}$ (thin line with circles), $j \mapsto \lambda_j^{comp}$ (thick line) and $j \mapsto \lambda_j^{theory} = 1$ (thick line) corresponding to the theoretical values (for $N_g = 5$ and for $N_d = 10$)*

6. Additional comments about the proposed method. It should be noted that the proposed method allows the numerical calculation of realizations of a given polynomial chaos expansion in high dimension and for an arbitrary measure to be effectively performed. For such a case, the use of the algebraic explicit representation or the use of a recurrence relation to compute the realizations with high polynomial degrees, induces an important numerical noise and the orthogonality property is lost. For this case of the high dimension, there is in fact no alternative concerning the choice between the proposed method and the two usual methods. The proposed method has not been developed to replace the usual methods when there are available but proposes a new way to solve the cases for which the usual methods are not available. Consequently, the computational cost introduced by the proposed method with respect to the computational cost induced by the usual methods is not a criterium to evaluate the efficiency of the proposed method. Nevertheless, the computational cost induced by the proposed method is small enough with respect to the others computational costs induced by stochastic modeling in high dimension. For instance, for $N_g = 3$ and $N_d = 20$ yielding $N = 1,770$ and for $\nu = 2,000$, the total CPU time is 110 seconds using 1 processor; for $N_g = 4$ and $N_d = 20$ yielding $N = 10,626$ and for $\nu = 11,000$, the total CPU time is 4,800 seconds using 1 processor; finally, for $N_g = 5$ and $N_d = 20$ yielding $N = 53,130$ and for $\nu = 60,000$, the total CPU time is 6,600 minutes using 1 processor. It should be noted that the realizations can be computed as an initial step and can be used at any time of the computation.

7. Conclusion. This paper proposed a new methodology to compute a large number of independent realizations of a polynomial chaos expansion with respect to an arbitrary measure for the high dimension case and in preserving the orthogonality properties. Such a new tool is necessary to develop stochastic modeling in high dimension. For instance, the high dimension is required to construct the stochastic models of microstructures made up of complex materials and more generally, in order to construct stochastic multi-scale models of complex mechanical systems. Nowadays, this PCE range is perfectly attainable for many engineering applications. With the method proposed, the orthogonality properties are exactly satisfied for any value of the order of the polynomial chaos expansion. So, the convergence of polynomial chaos expansion can be analyzed. For the high dimension cases, it is proven that the computational recurrence formula and the algebraic explicit representation fail while

the new method proposed does not fail.

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