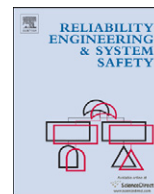




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Short communication

On convergence of moments in uncertainty quantification based on direct quadrature

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ABSTRACT

Theoretical results for the convergence of statistical moments in numerical quadrature based polynomial chaos computational uncertainty quantification are presented in this work. This is accomplished by considering the computation of the moments through a direct numerical quadrature method, which is shown to be equivalent to stochastic collocation. For problems which involve output variables which have a polynomial dependence on the random input variables, lower bound expressions are derived for the number of quadrature points required for convergence of arbitrary order moments. In addition, an error expression is derived for when this lower bound is used for problems which have a higher degree of continuity than what was assumed when the bounds are computed. The theoretical results are demonstrated through a simple random algebraic problem and a nonlinear plate problem. The results presented in this work provide further insight into the widely used polynomial chaos expansion method of uncertainty quantification along with presenting simple expressions which can be used for uncertainty quantification code verification.

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1. Introduction

The process of uncertainty quantification (UQ) results in a measure of the effect of uncertainty in a system input on the system response quantities of interest. In the design of engineering systems, the information produced from uncertainty quantification can be used as a tool for enabling quantitative risk analysis [1]. When the so-called system involves a computational model, this is accomplished through the propagation of model input uncertainty through the computational model to determine the statistics of the model outputs. These statistics can then be used to determine the probability of undesirable events (outputs) which in turn can be used to give a measure of the risk involved in a given “activity”. Several examples of the application of uncertainty quantification for problems (activities) of interest to the engineering community are discussed in Refs. [2–4].

When discussing types of model input uncertainty, the classification provided in Ref. [5] is often used. In this classification three types of uncertainty are recognized: aleatory or irreducible uncertainty; epistemic uncertainty; and uncertainty due to human error. When considering computational uncertainty the first two are relevant [6,7] and relate to a lack of knowledge in the true physics of the problem (epistemic) and randomness in a

system (model) parameters (aleatory). Aleatory uncertainty can normally be put in the framework of a probabilistic description while epistemic uncertainty is often difficult to quantify. In this paper we will deal only with aleatory uncertainty.

Computational uncertainty quantification methods can be intrusive or non-intrusive. Most intrusive methods can be thought of as weighted-residual methods whereby the (random) response variables in a differential equation are expanded in a finite series of basis functions (functions of the random input variables) and then the error in the approximation is forced to be orthogonal to a “test” functional space (from considerations of error minimization). This results in a set of deterministic (differential) equations for the coefficients in the expansion. On the other hand in non-intrusive methods, deterministic simulation tools can be treated as “black boxes” and hence simulation code modification is not required. A typical non-intrusive uncertainty quantification scheme consists of, similar to intrusive methods, expanding the random response variable in a finite series of basis functions whose coefficients are then computed by sampling the black box simulation and then using spectral projection or linear regression [8]. For either method, intrusive or non-intrusive, once the coefficients in the expansion are found they can be used to reconstruct the response which then can be used to determine statistical quantities of interest.

The most common functional spaces used in the expansions correspond to what is called generalized polynomial chaos [9–14] and can be generated using the Wiener–Askey scheme. The first

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instance of this was introduced by Wiener [15] as the span of the Hermite polynomial functionals of a Gaussian random process and is often called Wiener's polynomial chaos or Homogeneous chaos. Depending on the type of continuous random variable, the Wiener–Askey scheme generates polynomials which are orthogonal to the measure of the random variable.

When using uncertainty quantification analysis for an engineering system, an important objective should be the determination of a set of design criteria which can be used in a probabilistic context so that a reliability analysis is permitted [16–18]. In this context, the statistical moments (including mean, variance, skewness, kurtosis) of the system response can provide bounds about its expected range along with giving meaningful information about the reliability of the system with random inputs. The moments can also be used together with some expansion, such as the Edgeworth expansion [19], to approximate the probability distribution function of the response process. In order for the uncertainty quantification analysis to provide useful information about system reliability, the moments of interest should be estimated accurately to within a user-defined tolerance. Some key questions which should then be asked are: (a) *what smart choices can the analyst make in an a priori sense to ensure that moments up to a desired order are estimated accurately?* and (b) *how many samples are necessary for accurate uncertainty quantification, including asymptotic convergence in (point estimates of) the probability density of the system output and convergence in moments up to an arbitrarily high order?* In other words (regarding question (a)), if something is known about the functional dependence of the random response on the random input, can the minimum number of samples in a non-intrusive uncertainty quantification analysis be chosen ahead of time such that all moments up to a given order are guaranteed to be converged? It appears that convergence in probability density functions of system outputs (regarding question (b)) is dependent on the type of reconstruction approach used (e.g. Edgeworth series, Maximum Entropy approach) to determine the probability density function based on the underlying moments (up to a known order).

In this paper we will present analysis which addresses question (a). Specifically, we will provide theoretical results on the necessary conditions for the number of samples needed in a non-intrusive polynomial chaos expansion (PCE) to provide statistical moments of a response variable within a given error bound. For random response variables which are given in terms of polynomials of the random input variables, these conditions provide a lower bound on the number of samples needed for an exact evaluation of the statistical moments. In addition an expression is developed for the error incurred if this lower bound is used for a problem which has a higher degree of continuity than which was assumed when the bound was computed. In order to produce these results, we will develop the non-intrusive uncertainty quantification process directly in terms of numerical quadrature of the statistical moments [20], the result of which will be shown to be equivalent to stochastic collocation [8]. In addition to aiding in the development of the theoretical results, the authors feel that presenting the computation of statistical moments from a direct quadrature perspective presents a simple, straightforward way of introducing the topic. The theoretical results on the number of samples needed for statistical moment convergence will be demonstrated using a simple numerical example. It may be noted that in our analysis (regarding determination of minimum number of samples needed for convergence of moments up to a desired order), we assume that the exact functional dependence of the system response on the system input is known and can be represented via polynomials. Although this may not often be the case, the present analysis serves as an important tool for code verification and validation. As this work is particularly focused on

identifying the conditions for accurate estimation of moments (of arbitrary order) using quadrature, it could complement many methods in reliability analysis that involve moment dependent (e.g. variance based) or moment independent (e.g. entire output distribution) uncertainty measures [17,18,13,14].

2. Theory

In this section we will present the salient theoretical details which are needed to derive the theoretical results for the PCE method. Further details on the generalized PCE can be found, for example, in Refs [3,10].

2.1. A direct quadrature view of the computation of moments of random response

The n th moment of a random variable u which is a function of N independent random variables, denoted here as $\xi(\theta) = \{\xi_1(\theta), \xi_2(\theta), \dots, \xi_N(\theta)\}$, is given by the expression

$$\langle u^n(\xi) \rangle = \int_{\Omega} u(\xi(\theta))^n p(\xi(\theta)) d\xi(\theta), \quad (1)$$

where θ is a random event and Ω and $p(\xi(\theta))$ denote the support and probability density (respectively) corresponding to ξ .

The basis of the direct quadrature computation is to use numerical (Gauss) quadrature to compute the integral in Eq. (1). Using Gauss quadrature a one-dimensional integral of the form

$$\int_a^b f(x)w(x) dx \quad (2)$$

is approximated with the M -point quadrature formula given by

$$\int_a^b f(x)w(x) dx \approx \sum_{i=1}^M f(x_i)\tilde{w}_i. \quad (3)$$

The evaluation point x_i corresponds to the i th root of the orthogonal polynomials with the weighting function $w(x)$. Common weighting functions (with the corresponding support) include 1 (Gauss–Legendre), $1/(\sqrt{1-x^2})$ (Gauss–Chebyshev) and e^{-x^2} (Gauss–Hermite). Higher dimensional integrals can be computed using tensor products of one-dimensional formulas or, if the dimension is large, a sparse grid technique such as Smolyak quadrature [21]. If $f(x)$ is continuous on $[a, b]$, then it can be shown [22] that the approximations in Eq. (3) converge to the integral as $M \rightarrow \infty$.

For a function $f(x) \in C^{2M}[a, b]$ the error in Eq. (3) is given by

$$E = \frac{f^{2M}(\zeta)}{(2M)!} \langle \Phi_M, \Phi_M \rangle, \quad (4)$$

where $f^{2M}(\zeta)$ corresponds to the $2M$ th derivative of f and $a < \zeta < b$. Also $\langle \Phi_M, \Phi_M \rangle$ corresponds to the inner product of the M th-order polynomial which is orthogonal to the weighting function $w(x)$ in Eq. (3). From Eq. (4) it can be shown that M point Gauss quadrature is exact for a polynomial of degree at most $2M-1$.

For clarity of presentation we will now restrict ourselves to $N=1$, i.e. a one-dimensional space of a single random variable (ξ). Additional consideration of results for higher dimensions will be given where necessary. For one dimension, Eq. (1) can now be approximated using numerical quadrature as

$$\begin{aligned} \langle u^n(\xi) \rangle &= \int_a^b u(\xi(\theta))^n p(\xi(\theta)) d\xi(\theta) \\ &\approx \sum_{i=1}^M u(\xi_i)^n \tilde{w}_i, \end{aligned} \quad (5)$$

where the quadrature points ξ_i and weights \tilde{w}_i could correspond to quadrature rules which have $p(\xi)$ as the weighting function $w(x)$ in Eq. (3). For example if $p(\xi)$ is a Gaussian distribution or a uniform distribution, Gauss–Hermite and Gauss–Legendre quadrature would be used. Alternatively, if a quadrature rule does not exist for the given $p(\xi)$, Eq. (5) can be rewritten in such a way as to use a known quadrature rule e.g.

$$\begin{aligned} \langle u^n(\xi) \rangle &= \int_a^b u(\xi(\theta))^n p(\xi(\theta)) d\xi(\theta) \\ &= \int_c^d u(\xi(\theta))^n \frac{p(\xi(\theta))}{f(\xi(\theta))} f(\xi(\theta)) d\xi(\theta) \\ &\approx \sum_{i=1}^M \frac{u(\xi_i)^n}{f(\xi_i)} p(\xi_i) \tilde{w}_i, \end{aligned} \tag{6}$$

where the limits of integration c and d along with the weights \tilde{w}_i and quadrature points ξ_i correspond to the distribution (weighting) function $f(\xi(\theta))$ for which a quadrature rule exists.

2.2. Equivalence of the direct quadrature view with stochastic collocation

In the Stochastic Collocation (SC) method the response variable $u(\xi)$ is expanded in terms of a set of Lagrange polynomials with unknown coefficients. If we once again restrict ourselves to $N=1$, this can be written as

$$u(\xi) = \sum_{i=1}^M u_i L_i(\xi) = \sum_{i=1}^M u_i \prod_{j=1, j \neq i}^M \frac{\xi(\theta) - \xi_j}{\xi_i - \xi_j}, \tag{7}$$

where $L_i = \prod_{j=1, j \neq i}^M ((\xi - \xi_j)/(\xi_i - \xi_j))$ is the i th Lagrange polynomial. The expression for the n th moment of $u(\xi)$ is given by

$$\langle u(\xi)^n \rangle = \int_a^b \left(\sum_{i=1}^M u_i \prod_{j=1, j \neq i}^M \frac{\xi(\theta) - \xi_j}{\xi_i - \xi_j} \right)^n p(\xi(\theta)) d\xi(\theta), \tag{8}$$

which can be approximated using a M point numerical quadrature of the type given in Eq. (3)

$$\langle u(\xi)^n \rangle \approx \sum_{k=1}^M \left(\sum_{i=1}^M u_i \prod_{j=1, j \neq i}^M \frac{\xi_k - \xi_j}{\xi_i - \xi_j} \right)^n \tilde{w}_k. \tag{9}$$

If the stochastic collocation points in Eq. (9), ξ_j , correspond to the abscissa values for a quadrature rule which is appropriate for $p(\xi(\theta))$ the following is true:

$$\sum_{i=1}^M u_i \prod_{j=1, j \neq i}^M \frac{\xi_k - \xi_j}{\xi_i - \xi_j} = \begin{cases} u_k & i = k \\ 0 & i \neq k \end{cases}. \tag{10}$$

With this result Eq. (9) becomes

$$\langle u(\xi)^n \rangle \approx \sum_{k=1}^M \left(\sum_{i=1}^M u_i \prod_{j=1, j \neq i}^M \frac{\xi_k - \xi_j}{\xi_i - \xi_j} \right)^n \tilde{w}_k = \sum_{k=1}^M u_k^n \tilde{w}_k, \tag{11}$$

which is equivalent to Eq. (5).

2.3. Generalized polynomial chaos for computation of moments of random response

In generalized polynomial chaos, the random response variable is written as a truncated generalized Fourier series:

$$u(\xi(\theta)) \approx \sum_{j=0}^P u_j \Psi_j(\xi(\theta)), \tag{12}$$

where the basis functions Ψ_j are orthogonal polynomials which would correspond to the measure of the random input variable, for example Hermite polynomials for a Gaussian random variable.

These polynomials can be generated using the Askey-scheme [10] if standard distributions are used or numerically if correlation exists or the distribution is nonstandard. The coefficients u_j in Eq. (12) are computed by projecting the response against each basis function and using the orthogonal properties of Ψ_j

$$u_j = \frac{\langle u(\xi(\theta)), \Psi_j(\xi(\theta)) \rangle}{\langle \Psi_j(\xi(\theta)), \Psi_j(\xi(\theta)) \rangle}, \tag{13}$$

where the inner product for the measure of choice is defined as

$$\langle u(\xi(\theta)), v(\xi(\theta)) \rangle = \int_{\Omega} u(\xi(\theta)) v(\xi(\theta)) p(\xi(\theta)) d\xi(\theta). \tag{14}$$

As stated, Eq. (12) is a generalized Fourier series and hence if u is a L2 random variable, i.e. has finite variance, the series shows mean-square convergence [23]. It should be noted, however, that while convergence of the order 1 and 2 moments is guaranteed, Field and Grigoriu [24] showed that depending on how the function u depends on ξ , moments higher than 2 may or may not converge as the number of terms in Eq. (12) is increased.

Once again we now will use $N=1$ in our derivations in order to simplify the presentation. Placing Eq. (12) into Eq. (1) results in the following expression for the approximation to the n th moment of a random response using generalized polynomial chaos:

$$\langle u(\xi(\theta))^n \rangle \approx \int_a^b \left[\sum_{j=1}^P u_j \Psi_j(\xi(\theta)) \right]^n p(\xi(\theta)) d\xi(\theta). \tag{15}$$

Replacing the coefficients u_j in Eq. (15) with the expressions in Eqs. (13) and (14) results in the following generalized polynomial chaos approximation for the n th moment of $u(\xi(\theta))$:

$$\begin{aligned} \langle u(\xi(\theta))^n \rangle \approx \int_a^b \left[\sum_{j=1}^P \left(\frac{\int_a^b u(\xi(\theta)) \Psi_j(\xi(\theta)) p(\xi(\theta)) d\xi(\theta)}{\int_a^b \Psi_j^2(\xi(\theta)) p(\xi(\theta)) d\xi(\theta)} \right) \Psi_j(\xi(\theta)) \right]^n \\ p(\xi(\theta)) d\xi(\theta). \end{aligned} \tag{16}$$

In Eq. (16) the variance of the orthogonal polynomials, i.e. the integral $\int_a^b \Psi_j^2(\xi(\theta)) p(\xi(\theta)) d\xi(\theta)$, can most often be computed analytically. The remaining integrals can be approximated using, for example, a numerical quadrature which has a weighting function corresponding to the measure of the random input variable. The resulting expression can be written as

$$\langle u(\xi(\theta))^n \rangle \approx \sum_{l=1}^M \left[\sum_{j=1}^P \left(\frac{\sum_{i=1}^M u(\xi_i(\theta)) \Psi_j(\xi_i(\theta)) \tilde{w}_i}{\langle \Psi_j, \Psi_j \rangle} \right) \Psi_j(\xi_i(\theta)) \right]^n \tilde{w}_l. \tag{17}$$

3. Theoretical results

Comparing PCE and the direct quadrature (SC) methods for computation of statistical moments, one can develop expressions for the commonly used PCE approach regarding the number of samples needed for an exact computation of arbitrary order moments for a known polynomial functional relationship between the output and input variables. These will now be developed.

Proposition 3.1. Given a random response variable $u(\xi(\theta)) \in \Pi_q$, where Π_q is the space of polynomials of degree at most q , which is a function of a single random variable $\xi(\theta)$ the n th moment of $u(\xi(\theta))$ for a P th order polynomial chaos approximation to $u(\xi(\theta))$ can be computed exactly using a numerical quadrature with at least M

samples where M is given by

$$M = \max\left(\frac{q+P+1}{2}, \frac{nq+1}{2}\right).$$

Mathematical reasoning for Proposition 3.1:

- (1) From Eq. (13) in order to evaluate the $P+1$ th coefficient u_{P+1} , an integrand of order $q+P$ must numerically be integrated. If this integration is to be exact then we must have $P+q+1 \leq 2M$ or $M \geq (P+q+1)/2$. If M satisfies this criteria then all other coefficients u_j will also be evaluated correctly.
- (2) By Eq. (4) in order to exactly compute the n th moment of $u(\xi(\theta))$ using the direct quadrature given in Eq. (5) the following relation must hold true between the number quadrature points (samples) M , n and q :

$$nq \leq 2M - 1 \tag{18}$$
- (3) If Eq. (17) is to be exact then Eq. (12) must be an equality and therefore Eqs. (17) and (5) are equivalent, i.e. the direct quadrature and generalized polynomial chaos expressions for the n th order moment are equivalent.
- (4) From steps 1, 2 and 3 (above) we arrive at the stated proposition.

It should be noted that Proposition 3.1 provides a lower bound but not necessarily an optimal value for M . In some circumstances, the value of M can be less than that given in the proposition. This can occur when, for example, odd functions in Eq. (5) integrate to zero negating an inexact evaluation of the u_j in Eq. (12).

A corollary resulting from Proposition 3.1 is the following.

Corollary 3.1. Given a random response variable $u(\xi(\theta))$ which is a function of N random variables with continuity in the i th random variable given by Π_{q_i} and which is expanded in a P_i th order polynomial chaos expansion for the i th random dimension, a lower bound on the number of samples needed to exactly represent the n th moment of $u(\xi(\theta))$ is given by

$$M = \max\left(\prod_{i=1}^N \left(\frac{q_i+P_i+1}{2}\right), \prod_{i=1}^N \left(\frac{nq_i+1}{2}\right)\right).$$

This corollary results from using (1) and (2) from the mathematical reasoning for Proposition 3.1 and the idea of anisotropic tensor product quadrature in multiple dimensions.

As it was shown that the direct quadrature view for statistical moments is equivalent to the result for these same quantities computed using stochastic collocation (SC), another way of viewing Proposition 3.1 (and Corollary 3.1) is that they represent the number of sample points which are needed for SC and PCE to be equivalent.

If instead the response variable $u(\xi(\theta))$ has a higher degree of continuity then C^q and can be expanded in a Taylor series, the following proposition can be stated.

Proposition 3.2. Given a random response variable $u(\xi(\theta)) \in C^q$ and if the $q+1$ th derivative $u^{(q+1)}$ exists on (a,b) then the choice for M stated in Proposition 3.1 results in an error which to leading order is given by

$$E_q = \int_a^b \left[\int_0^{\xi(\theta)} \frac{u^{(q+1)}}{t!} (\xi(\theta)-t)^q dt \right] p(\xi(\theta)) d\xi(\theta).$$

Mathematical reasoning for Proposition 3.2: If one expands the random variable $u(\xi(\theta))$ in a Taylor series about the point $\xi(\theta) = 0$, i.e.

$$u(\xi(\theta)) = \sum_{k=0}^q \frac{1}{k!} u^{(k)}(0) \xi^k(\theta) + E_q(\xi(\theta)), \tag{19}$$

$$E_q(\xi(\theta)) = \int_0^{\xi(\theta)} \frac{u^{(q+1)}}{t!} (\xi(\theta)-t)^q dt, \tag{20}$$

the n th moment given in Eq. (1) (for $N=1$) can be written as

$$\langle u^n(\xi(\theta)) \rangle = \int_a^b \left[\left[\sum_{k=0}^q \frac{1}{k!} u^{(k)}(0) \xi^k(\theta) \right] + \int_0^{\xi(\theta)} \frac{u^{(q+1)}}{t!} (\xi(\theta)-t)^q dt \right]^n p(\xi(\theta)) d\xi(\theta). \tag{21}$$

Expanding the expression in integrand and then writing the integral as the sum of two integrals results in the following expression for the $\langle u^n(\xi(\theta)) \rangle$:

$$\begin{aligned} \langle u^n(\xi(\theta)) \rangle &= \int_a^b \left(\left[\sum_{k=0}^q \frac{1}{k!} u^{(k)}(0) \xi^k(\theta) \right] \right)^n p(\xi(\theta)) d\xi(\theta) \\ &+ \int_a^b \left(\frac{1}{0!} u^{(0)}(0) \xi^0(\theta) \left[\int_0^{\xi(\theta)} \frac{u^{(q+1)}}{t!} (\xi(\theta)-t)^q dt \right] \right. \\ &+ \left. \frac{1}{1!} u^{(1)}(0) \xi^1(\theta) \left[\int_0^{\xi(\theta)} \frac{u^{(q+1)}}{t!} (\xi(\theta)-t)^q dt \right] + \dots \right) p(\xi(\theta)) d\xi(\theta). \end{aligned} \tag{22}$$

If higher order terms (in $\xi(\theta)$) are ignored in the second integral in Eq. (22) the mathematical reasoning needed for Proposition 3.2 is now complete as the first integral is exactly represented if the number of samples is chosen as stated in Proposition 3.1 and the first term in the second integral is exactly the error term given in Proposition 3.2. A similar result in multiple dimensions can be derived using a multidimensional Taylor series expansion.

The values of q_i and P_i in Corollary 3.1 are linked. This connection leads to the following idea. From a practical standpoint, if a PCE result is desired, the direct quadrature method of computation of moments can be used (along with Proposition 3.1 or Corollary 3.1) to determine the order of PCE and the number of sample points needed for an accurate computation of the n th moment of a response variable when q_i is unknown (as is usually the case for “real” problems). This is accomplished by varying the number of quadrature points in the i th random dimension while keeping fixed the number of quadrature points in the other dimensions. A converged value (to within some ϵ) of the mean for M_i quadrature points in the i th random dimension can then be used to determine a good approximation to q_i (and therefore P_i), i.e. $q_i = 2M_i - 1$. The error incurred by choosing a certain value of ϵ is related to Eq. (4). The samples used in the direct quadrature simulations could then be used directly to determine the coefficients in the PCE expansion if the number of samples used satisfies the result from Proposition 3.1/ Corollary 3.1. This idea could have potential limitations when the model response is non-differentiable and/or if the assumptions of Proposition 3.1 break down.

4. Numerical results

In order to demonstrate numerically the results from Proposition 3.1, a simple random algebraic problem (which has moments which can be computed analytically) is solved in one random dimension ($N=1$). The simulation involves the random algebraic equation given by $u(\xi(\theta)) = \xi(\theta)^q$ for q ranging from 1 to 8.

The random variable is assumed to be Gaussian with zero mean and a standard deviation of 1 ($N(0,1)$).

It is important to note that Proposition 3.1 provides valuable information on the “minimum” number of sample points (M) needed for exact moment evaluation (for known functions) through the commonly used PCE approach for UQ. Shown in Table 1 are the comparisons of the value of M resulting from Proposition 3.1 and the corresponding value needed for an exact moment evaluation using PCE. Only nonzero moments are considered when evaluating Proposition 3.1. Various values of q, n and P are given in the table. For example the first row in Table 1 corresponds to the result (from Proposition 3.1 and the actual computation) for the number of sample points needed to compute the standard deviation of u (where $u = \xi(\theta)$) for a PCE of order 1. Similarly the third row corresponds to number of samples for the computation of the flatness value for an order 6 PCE solution. Only a small subset of all the results are shown in Table 1 (and Fig. 1). For all cases simulated, Proposition 3.1 always gives a result which either matches exactly with the numerically determined value or which is conservative (by no more than four sample points). Rows 3, 6, 8 and 14 in Table 1 are examples of when the proposition gives a conservative value for the number of samples. A verification of Proposition 3.1 is also illustrated in Fig. 1, which shows the convergence in kurtosis using both direct quadrature (DQ) and PCE approaches, for a random algebraic equation $u(\xi(\theta)) = \xi^5(\theta)$.

Table 1
PCE numerical simulation results for Proposition 3.1.

q	n	P	$\max\left(\frac{P+q+1}{2}, \frac{nq+1}{2}\right)$	Computational value of M
1	2	1	2	2
1	4	4	3	3
1	4	6	4	3
2	1	1	2	2
2	3	3	4	4
2	3	7	5	4
4	1	1	3	3
4	1	2	4	3
4	2	8	7	7
5	2	5	6	6
5	4	9	11	11
7	2	7	8	8
7	4	10	15	15
8	1	8	9	5
8	2	8	9	9

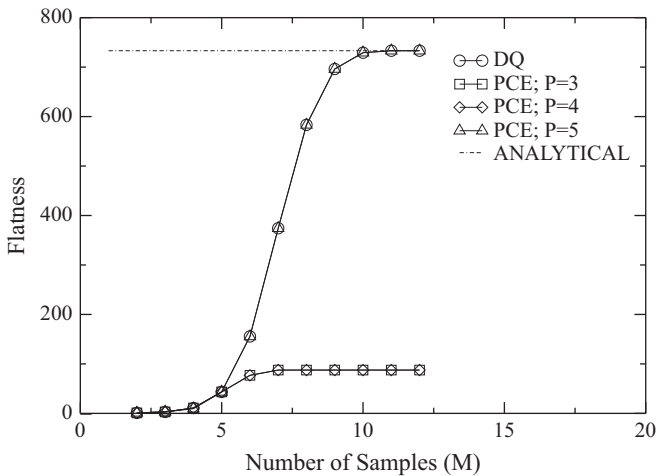


Fig. 1. Comparison of convergence in flatness factor for direct quadrature (DQ) and PCE approaches, using the random algebraic equation $u(\xi(\theta)) = \xi^5(\theta)$.

In order to demonstrate the application of DQ for higher dimensional (spatial and random) problems of relevance to engineering and risk analysis, an application in nonlinear mechanics is considered. A square plate (of length 1 m) constructed of aluminum material and which is clamped on all four sides (all degrees of freedom constrained) and subjected to a constant pressure load of 200 kPa. This example corresponds to the example problem given in Section 4.3 in Ref. [25]. The kinematic and strain formulations used here in the finite element spatial discretization of the problem correspond to the GL3 element from Ref. [25]. This formulation results in a problem where the strain depends on the displacement in a nonlinear manner. This element has been implemented into an in-house finite element solver which is used in conjunction with the software developed for the non-intrusive UQ analysis presented here. A coarse 4×4 mesh is used in the current work. The random input variables considered are the modulus of elasticity (ξ_1), thickness (ξ_2) and Poisson ratio (ξ_3) which have mean values of 72 GPa, 0.001 m and 0.30 respectively. The standard deviation for each random input variable is taken to be 10% of its mean. The exact functional dependence of the random output variable, which here was chosen to be the displacement at the center of the plate, on the random input variables is not known.

Figs. 2–5 show the absolute error, defined as the absolute value of the difference between a given result and what is taken as the exact value for this example ($e_{abs} = |\langle u^n \rangle_{DQ} - \langle u^n \rangle_{exact}|$),

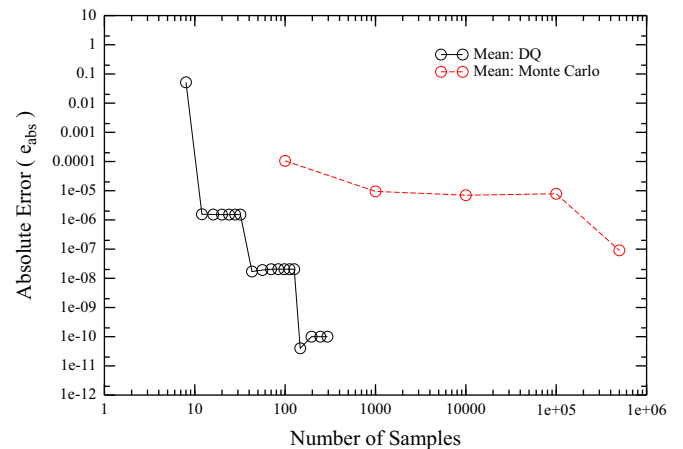


Fig. 2. Absolute error in mean versus number of samples for nonlinear plate problem.

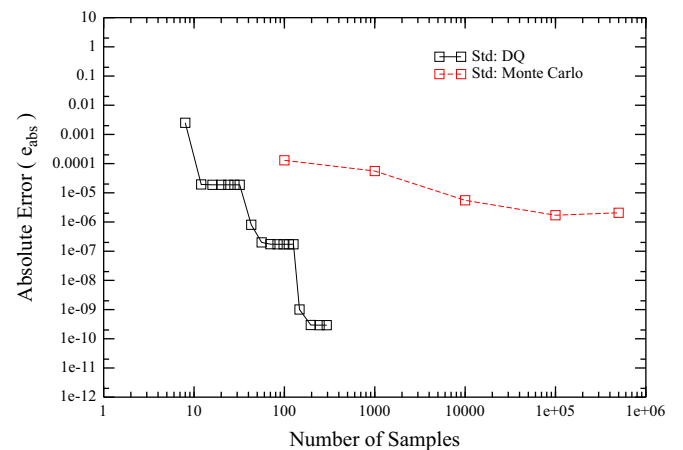


Fig. 3. Absolute error in standard deviation versus number of samples for nonlinear plate problem.

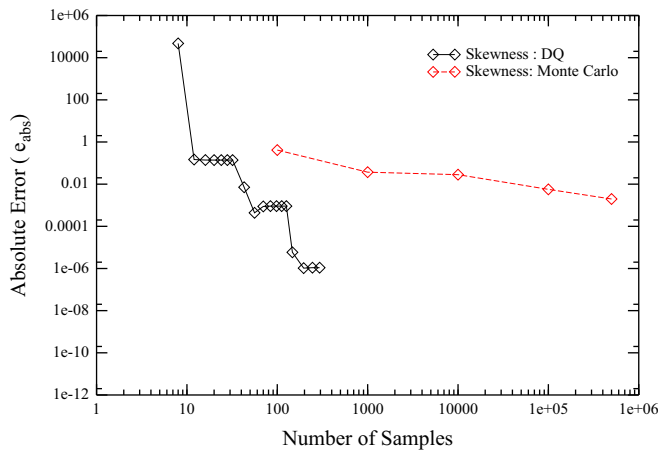


Fig. 4. Absolute error in skewness versus number of samples for nonlinear plate problem.

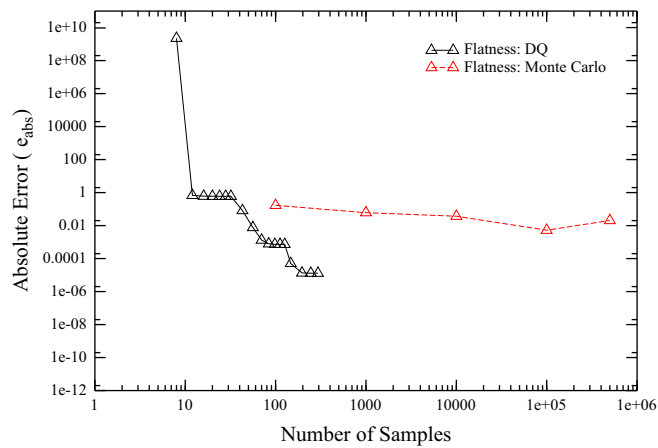


Fig. 5. Absolute error in flatness versus number of samples for nonlinear plate problem.

versus the number of samples for the mean, standard deviation, skewness and flatness respectively. The DQ and Monte Carlo results are shown in Figs. 2–5. The “exact” value for each of the standardized moments is taken to be the computed values from a DQ solution with 12 sample points in each of the three random variable dimensions. These values are 0.51707×10^{-1} , 0.25057×10^{-2} , 0.35912 and 0.32723×10^1 for the mean, standard deviation, skewness and flatness respectively. As expected, the convergence of the Monte Carlo results for higher order moments is very slow. The convergence of the Monte Carlo results also appears to be non-monotonic for the standard deviation and flatness. It should be noted that it may be possible to improve the estimation of moments using smoothing procedures (e.g see Ref. [26]).

Table 2 gives values for the mean and standard deviation from a DQ solution for various number of quadrature points (M_1 , M_2 and M_3) in each of the random dimensions. The values are taken out to 10 places after the decimal point in order to correspond to the magnitude of the absolute error values reported in Figs. 2–5. The product of M_1 , M_2 and M_3 in Table 2 corresponds to the abscissa values in Figs. 2–5. Although arbitrary, as stated previously the first random dimension in the simulations corresponds to the modulus of the elasticity, the second the thickness and the third is the Poisson’s ratio. From Table 2 and Fig. 2 one can see that the mean is within 1.0×10^{-10} of the “exact” solution with seven quadrature points in the first and second random

Table 2
Mean and standard deviation for nonlinear plate problem for various number of quadrature points in each random dimension.

M_1	M_2	M_3	Mean $\times 10^1$	Standard deviation $\times 10^2$
3	2	2	0.5170515204	0.2486268980
4	2	2	0.5170518824	0.2486876808
5	2	2	0.5170518952	0.2486903195
6	2	2	0.5170518958	0.2486904634
7	2	2	0.5170518958	0.2486904726
8	2	2	0.5170518958	0.2486904735
7	3	2	0.5170669650	0.2504881992
7	4	2	0.5170673270	0.2505485432
7	5	2	0.5170673398	0.2505511627
7	6	2	0.5170673404	0.2505513056
7	7	2	0.5170673404	0.2505513147
7	8	2	0.5170673404	0.2505513156
7	7	3	0.5170671351	0.2505684581
7	7	4	0.5170671345	0.2505685293
7	7	5	0.5170671345	0.2505685297
12	12	12	0.5170671355	0.2505685590

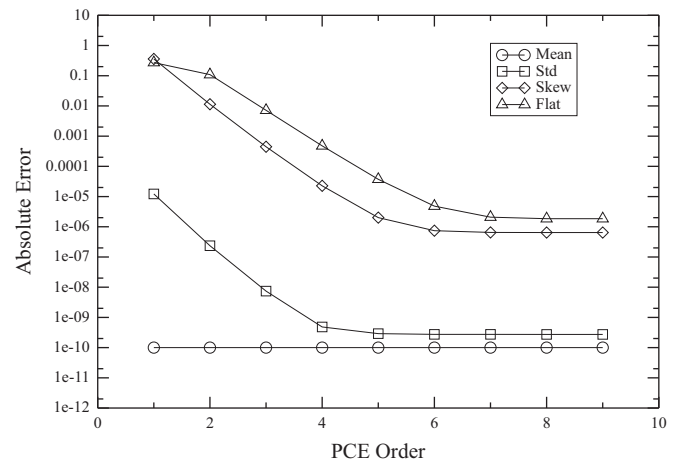


Fig. 6. Absolute error in first four standardized moments versus PCE order with nine quadrature points in each random dimension for nonlinear plate problem.

dimension and four quadrature points in the third dimension. From this one can infer that a polynomial chaos solution which uses an order four expansion in the first and second random dimensions and order three in the third dimension should be sufficient to capture the functional dependence of the output on the random inputs. Fig. 6 shows the absolute error in the PCE result versus PCE order (equal in each random dimension) for the first four standardized moments. The number of samples is based upon Proposition 3.1 with $q=4$ and $n=4$ hence the value of M in each dimension is taken to be 9. From Fig. 6 it appears that in order to accurately compute the mean only an order 1 PCE expansion is needed for this problem. However, the higher order moments require at least an order four expansion in order for the absolute error to be within 1.0×10^{-3} of the exact result.

5. Conclusions

Risk analysis often involves the use of computational modeling along with uncertainty analysis to determine the statistics of undesirable events which can give a quantitative measure for the risk involved with a certain activity. The results presented in this paper provide further insight into methods currently used in computational uncertainty quantification and therefore directly support reliability and risk analysis activities currently being

pursued in the engineering community. Theoretical results are given for the convergence of statistical moments computed using the quadrature-based non-intrusive polynomial chaos expansion method. These results are derived by considering directly, the numerical quadrature of the statistical moments, the result of which can be considered equivalent to the expression for the moments which would result from a stochastic collocation method. Expressions are presented for the lower bound on the number of samples needed to exactly compute, using a quadrature-based polynomial chaos expansion, a given order moment for a random output variable with a known polynomial dependence on the random inputs. Additionally a result is derived for the error incurred if this lower bound is used for a problem with a higher degree of continuity than what was assumed when the bound was computed. The theoretical results are demonstrated numerically using a simple random algebraic problem and a nonlinear plate problem.

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