NUMERICAL CHALLENGES IN THE USE OF POLYNOMIAL CHAOS REPRESENTATIONS FOR STOCHASTIC PROCESSES*

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Abstract. This paper gives an overview of the use of Polynomial Chaos expansions to represent stochastic processes in numerical simulations. Several methods are presented to perform arithmetic on, as well as to evaluate polynomial and non-polynomial functions of variables respresented with Polynomial Chaos expansions. These methods include TAYLOR series, a newly developed integration method as well as a sampling based spectral projection method for non-polynomial function evaluations. A detailed analysis of the accuracy of the Polynomial Chaos representations, and of the different methods for non-polynomial function evaluations is performed. It is found that the integration method offers a robust and accurate approach to evaluate non-polynomial functions, even when very high order information is present in the PC expansions.

Key words. Polynomial Chaos, Stochastic, Spectral Uncertainty Quantification

AMS subject classifications. 60G99, 65C20, 33C45, 37H10

1. Introduction. Stochastic processes and orthogonal polynomials are intimately related [24]. Early on, N. Wiener [26] discussed the role of HERMITE polynomials and homogeneous chaos in the integration theory with respect to Brownian motion. Recent developments in uncertainty quantification (UQ) have explored the use of Polynomial Chaos (PC), based on a suitable choice of orthogonal polynomial and its associated stochastic process, for stochastic representation of uncertainty. Polynomial chaos [5,26] is a member of the set of homogeneous chaos, first defined by Wiener [26]. It has since received increasing attention in a range of contexts [6, 7, 20, 21]. Ghanem and Spanos [16] implemented a PC expansion in terms of HERMITE polynomials of Gaussian random variables with a finite element method for UQ. This was applied in the modeling of transport in porous media [11], solid mechanics [12, 14] and structural [15] applications. The utility of the HERMITE-GAUSS PC for modeling non-Gaussian processes was also investigated in [13, 23]. Le Maître *et al.* [18, 19] extended the application of these techniques to thermo-fluid applications in the context of low Mach number flow. Xiu *et al.* [29] used generalized PC [28] for stochastic UQ in the modeling of flow-structure interactions, and for diffusion problems [27], where they examined various classes of orthogonal polynomials in the Askey scheme [3, 4, 24] and their associated stochastic processes. Debusschere *et al.* [8–10] used PC for UQ in the context of electrochemical flow in microfluidic systems. Reagan *et al.* [22] used PC for UQ in a Hydrogen-Oxygen reaction system. In these applications, stochastic

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dimensions are introduced to represent the variability in the model parameters due to, for example, experimental uncertainty or random variability in a material property.

In the specific case of *intrusive* spectral stochastic UQ methods, the PC expansions for model parameters and variables are substituted into the governing equations. Using a GALERKIN projection method, evolution equations are obtained for the spectral coefficients in the PC expansions. In this approach, all mathematical operations that are applied to the variables in the governing equations are now applied to the PC expansions that represent those variables. While elegant, the resulting "stochastic arithmetic" poses a number of challenges. These challenges include the accuracy of the (truncated) PC representations, truncation errors in the *pseudo–spectral* evaluation of polynomial functions and the evaluation of non-polynomial functions.

A first issue is the accuracy of the PC representations of random variables with probability density functions (PDFs) that deviate from the PDF of the random process that is associated with the chosen orthogonal polynomials insert ref. to Field and Grigoriu . For example representing strictly positive variables that have small mean values and large uncertainties can pose severe challenges for the accuracy and stability of the PC representation. Specifically, unless "sufficiently" high PC order is used, it is difficult to avoid non-zero probabilities of negative values of these variables under these conditions, which can destabilize the governing equations, *e.g.*, negative density or temperature. Under conditions with severe non-linearity, a sufficiently high PC order may be too computationally expensive to be practical.

Closely related to this are truncation errors, which frequently surface in the evaluation of high-order powers of random variables. In order to perform polynomial function evaluations of random variables represented with PC expansions, high powers of those variables may be required. A pseudo–spectral approach is used in this work to calculate such high powers efficiently, as will be discussed below. However, this methodology can introduce non-negligible truncation errors if the order of the PC representation is not sufficiently high.

Non-polynomial function evaluations of PC variables present a challenge since the GALERKIN projection method cannot be applied directly to determine the PC coefficients of the function result. One approach to circumvent this is to use TAYLOR series approximations for the non-polynomial functions. While this approach is straightforward and generally cost-effective, it can become grossly inaccurate when high order PC expansions are required to represent the physical variability. For many functions, this approach is also limited by the theoretical range of convergence of the TAYLOR series. In this work, we discuss the shortcomings of this approach and we develop a more robust and accurate technique that evaluates non-polynomial functions by integrating their derivatives. This approach can be applied to all functions $u(x)$ where $\frac{\mathrm{d}u}{\mathrm{d}x}$ can be expressed as a rational function of x and/or $u(x)$. As a third option, sampling-based methods such as the non-intrusive spectral projection method [15,19,22] can be used to accurately evaluate functions of PC variables. However, those methods can be very computationally expensive and do not scale well with the number of stochastic dimensions in the problem. Therefore, this paper focuses mainly on the "intrusive" TAYLOR series and integration approaches, which operate directly on the PC coefficients, even though we will use sampling-based methods to evaluate the accuracy of those intrusive methods.

In the next section, we introduce the mathematical formulation for various elementary operations on PC expansions of random variables, as well as the TAYLOR series, integration, and sampling approaches for non-polynomial function evaluations.

We also highlight the main aspects of the implementation of these operations. Next, we discuss in detail issues regarding PC representation accuracy and truncation errors as well as a rigorous comparison between the various sampling, TAYLOR series, and integration approaches for non-polynomial function evaluations. The main conclusions are summarized at the end.

2. Formulation and Implementation.

2.1. Polynomial Chaos Expansions. Under specific conditions [24], a stochastic process can be expressed as a spectral expansion in terms of suitable orthogonal eigenfunctions with weights associated with a particular density. A well-studied example is the Wiener process (Brownian motion) which can be written as a spectral expansion in terms of HERMITE polynomials and the Normal distribution. Other examples include Charlier polynomials and the Poisson distribution, and the Laguerre polynomials and the Gamma distribution [24]. In the present context, we will generally refer to these spectral expansions as Polynomial Chaos (PC) expansions following Wiener [26], and we will exclusively focus on the HERMITE-GAUSS PC. Moreover, while these expansions are infinite series, we will consider only PC expansions truncated at some suitably high order.

Consider a real second-order random variable a, *i.e.*, a LEBESGUE-measurable mapping from a probability space (Ω, Θ, P) into $\mathbb{R}$, where Ω is the set of elementary events, Θ a σ-algebra on Ω and P a probability measure on (Ω, Θ) [16]. This random variable can be approximated by its truncated HERMITE-GAUSS PC expansion as follows [16, 26]:

$$\widehat{a} = \sum_{k=0}^{P} a_k H_k^N(\boldsymbol{\xi}). \tag{2.1}$$

In this expansion $N \in \mathbb{N}^*$ is the dimension of the stochastic space, $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_N)$ where the ξ_i are assumed to be uncorrelated random variables with a Gaussian distribution, the $H_k^N \in \mathbb{R}[X_1, X_2, \ldots, X_N]$ are N-dimensional HERMITE polynomials, and the coefficients a_k are the (deterministic) spectral coefficients, here called *PC coefficients*. For example, if only one stochastic dimension is considered, one-dimensional HERMITE polynomials, which belong to $\mathbb{R}[X]$, are used and the first of them are given in normalized form as:

$$H_0^1 = 1,\ H_1^1 = X,\ H_2^1 = X^2 - 1,\ H_3^1 = X^3 - 3X,\ \ldots \tag{2.2}$$

In any case, for an M-th order PC expansion with N stochastic dimensions, the total number of terms $P + 1$ with order less or equal to M is given by

$$P + 1 = \frac{(M+N)!}{M!N!}. \tag{2.3}$$

For the sake of brevity, the composition $H_k^N(\boldsymbol{\xi})$, divided by the highest order coefficient of H_k^N, is called the k^{th} *N-dimensional Polynomial Chaos*, denoted Ψ_k (to avoid heavy notations, the superscript N vanishes: the considered dimension will be known from the context).

Using the orthogonality of the HERMITE polynomials with respect to the Gaussian-weighted expectation

$$\langle f \rangle = \frac{1}{(2\pi)^{N/2}} \int_{\mathbb{R}^N} f(\eta_1, \eta_2, \ldots, \eta_N) \exp\left[-\frac{\sum_{i=1}^N \eta_i^2}{2}\right] \mathrm{d}\eta_1 \mathrm{d}\eta_2 \cdots \mathrm{d}\eta_N \tag{2.4}$$

the coefficients a_k can be calculated by a GALERKIN projection operation onto the PC basis:

$$(\forall k \in \{0, ..., P\}) \quad a_k = \frac{< a\Psi_k >}{< \Psi_k^2 >} \tag{2.5}$$

Note that the expectations $< \Psi_k >= 0$ for $k > 0$. The 0^{th}-order PC coefficient for each variable is the mean, whereas the higher order coefficients represent stochastic variability around this mean.

For the sake of simplicity, we will use the term *PC variable* to denote the truncated PC expansion of a random variable. Also, for any random variable a, the mapping $(\cdot)_k$ returns the k^{th} PC coefficient of a. When giving specific examples of PC expansions, the shorthand notation $a(a_0, a_1, a_2, \ldots, a_P)$ will be used to list the PC coefficients of a, defined as follows:

$$a = \sum_{i=0}^{P} a_i \Psi_i = a(a_0, a_1, a_2, \ldots, a_P) \tag{2.6}$$

2.2. Elementary Operations on PC variables. The most basic operations on PC variables are additions and subtractions, which are performed by adding/subtracting the corresponding PC coefficients of the variables being added/subtracted. Multiplications of PC variables, however, are a little less straightforward. Consider two random variables, a and b, with their respective PC approximations:

$$\widehat{a} = \sum_{i=0}^{P} a_i \Psi_i \tag{2.7}$$

$$\widehat{b} = \sum_{j=0}^{P} b_j \Psi_j \tag{2.8}$$

Note that no assumption has been made about a and b being independent. We need to determine the coefficients c_k in the PC representation of $c = ab$. Since there is no way to directly compute $\widehat{a\,b}$, we assume $\widehat{c} = \widehat{a}\widehat{b}$, which is a reasonable assumption as long as the PC expansions for a and b are sufficiently high order to properly represent those random variables. Substituting the appropriate PC expansions into $\widehat{c} = \widehat{a}\widehat{b}$ gives

$$\widehat{c} = \sum_{k=0}^{P} c_k \Psi_k \tag{2.9}$$

$$= \sum_{i=0}^{P} a_i \Psi_i \sum_{j=0}^{P} b_j \Psi_j. \tag{2.10}$$

Note that c is expressed using a PC expansion of the same order P as a and b, even though the right hand side product in Eq. 2.10 has twice the order. The c_k coefficients are therefore obtained with a GALERKIN projection, which minimizes the error of the resulting PC representation within the space spanned by the basis functions up to order P. First, (2.10) is multiplied with Ψ_k. After taking the expectation of both the left and right hand side terms, invoking the orthogonality property of the Ψ's, and rearranging terms, one obtains:

$$(\forall k \in \{0, ..., P\}) \quad c_k = \sum_{i=0}^{P} \sum_{j=0}^{P} C_{ijk} a_i b_j \tag{2.11}$$

with

$$\left(\forall(i,j,k)\in\{0,...,P\}^3\right)\quad C_{ijk}\equiv\frac{\langle\Psi_i\Psi_j\Psi_k\rangle}{\langle\Psi_k^2\rangle}\tag{2.12}$$

Since the 3rd-order tensor C_{ijk} is only a function of the Ψ_i's, it needs to be calculated only once during a preprocessing step and can be stored for use throughout the computations. The implementation of (2.11) also takes advantage of the fact that this tensor is sparse, reducing the amount of storage and CPU time needed.

A similar procedure could also be used to determine the PC expansion for the product of three stochastic variables $d = abc$. This would give the spectral coefficients d_k as

$$(\forall l\in\{0,...,P\})\quad d_l=\sum_{i=0}^{P}\sum_{j=0}^{P}\sum_{k=0}^{P}D_{ijkl}a_ib_jc_k\tag{2.13}$$

where

$$\left(\forall(i,j,k,l)\in\{0,...,P\}^4\right)\quad D_{ijkl}\equiv\frac{\langle\Psi_i\Psi_j\Psi_k\Psi_l\rangle}{\langle\Psi_l^2\rangle}\tag{2.14}$$

Instead of this fully spectral approach, however, we use a pseudo-spectral construction to calculate products such as $d = abc$ by repeated use of the two-term product function. First the product ab is calculated with (2.11), and the (P-truncated) result of this multiplication is multiplied similarly with c to give the PC expansion for d. The advantage of this pseudo-spectral approach is that it does not require the evaluation and storage of the 4th-order tensor D_{ijkl}, it is more efficient, and is easy to generalize to products of any number of variables.

At this point, it is important to emphasize that both in the single but especially the repeated multiplications, the Galerkin projections onto a $P + 1$ term PC expansion are essentially truncations, which introduce additional approximation errors. As will be shown in section 3.2, those truncation errors are negligible if the order of the PC expansions is chosen sufficiently high to properly represent the result of the multiplication. However, when performing repeated multiplications such as for the calculation of high powers of PC variables, those truncation errors need to be taken into account.

Another frequently used operation is the division of two random variables. A robust and efficient algorithm to compute divisions was constructed as follows. Consider again three stochastic variables, a, b, and c, with their respective PC expansions given by (2.7–2.9). If we wish to evaluate $a = {}^{c}/_{b}$, then $c = ab$, which is given by (2.11). This equation, assuming the coefficients c_k and b_j are known, is a system of $P + 1$ linear equations in the unknown coefficients a_i. Since it is a sparse system of equations, we solve it efficiently with a GMRES iterative solver, from the SLATEC library [2, 25]. This algorithm can also be used to calculate the inverse $a = {}^{1}/_{b}$ of a stochastic quantity by setting c_0 to 1 and all higher order coefficients to zero for c.

In a similar way, we can compute the square root of a PC variable. Considering the PC variables a and b, $b = \sqrt{a}$ implies $a = b^2$, which is given by

$$(\forall k\in\{0,...,P\})\quad a_k=\sum_{i=0}^{P}\sum_{j=0}^{P}C_{ijk}b_ib_j\tag{2.15}$$

Given the coefficients a_k, this corresponds to a system of $P+1$ non-linear equations in the unknown PC coefficients of b. Starting from an intial guess $\tilde{b} = \sqrt{a_0}$, this system of equations can be solved efficiently using Newton's method. Note however that caution needs to be used with this algorithm, as it does not necessarily converge to quantities that are strictly positive. In situations where this is an issue, other algorithms that will be given in section 2.4 can be used.

2.3. Taylor Series Approach for non-Polynomial Function Evalutations. Using the algorithms described in the previous section, all polynomial functions of PC variables, as well as divisions, can be readily evaluated. More challenging however is the evaluation of non-polynomial functions of random variables such as the exponential or the logarithm. One way to evaluate these functions is to expand them in Taylor series around the mean of the argument.

For example, the exponential of a random variable a, with a PC expansion given by (2.7), is computed as

$$e^{\widehat{a}} = e^{a_0} \left(1 + \sum_{n=1}^{N_{\text{Tay}}} \frac{d^n}{n!} \right) \tag{2.16}$$

where

$$d = \widehat{a} - a_0 = \sum_{i=1}^{P} a_i \Psi_i \tag{2.17}$$

is the stochastic part of $\widehat{a}$. This Taylor series (2.16) theoretically converges for all values of a. Similarly, the natural logarithm of a random variable a can be computed as

$$\ln \widehat{a} = \ln a_0 + \sum_{n=1}^{N_{\text{Tay}}} \frac{d^n}{n a_0^n} (-1)^{n+1} \tag{2.18}$$

with a theoretical convergence range of $|\widehat{a} - a_0| < |a_0|$. The powers d^n are calculated in a pseudo-spectral way with the product formula (2.11) as $d^n = d\, d^{n-1}$, with d^{n-1} known from the previous term in the Taylor series. For all operations, the number of terms N_{Tay} in the truncated series is chosen adaptively. Terms are added until the maximum PC coefficient in the added term, divided by the mean of the function result (PC coefficient 0) is less than a specified tolerance level in absolute value. For the results shown in this work, a tolerance level of 10^{-15} was chosen.

As will be shown in the results section, the Taylor series approach works reasonably well as long as the uncertainties in the field variables are moderate and the probability density functions (PDFs) of those variables are not too skewed. For highly skewed PDFs, however, high order PC expansions are required to capture this stochastic information, and the evaluation of high power terms d^n in the Taylor series can become inaccurate. Also, if the uncertainty is so large that realizations of a have a non-zero probability of falling outside the range of convergence for the Taylor series, then the series will diverge as well. Note that since the PDF of a Gaussian variable has tails that extend all the way to infinity, there is always a non-zero probability that realizations of a Gaussian variable will fall outside the range of convergence of a Taylor series. In theory, this would imply that only Taylor series with an infinite range of convergence would converge for such random variables. In practice however, if the probability of falling outside the convergence range is sufficiently small, the numerical evaluation of the Taylor series will still give accurate results.

2.4. Integration Approach for Non-Polynomial Function Evaluations. To avoid the possible inaccuracies and divergence of TAYLOR series for non-polynomial function evaluations of PC variables, a new approach has been developed in this work, based on the integration of the derivative of the function to be evaluated.

For example, consider a deterministic $x \in \mathbb{R}$ and a function $u : x \mapsto u(x)$, with $u(x) \in \mathbb{R}$, which has the derivative $g : x \mapsto g(x)$ By definition of the derivative operator, this means that the function u is a solution of the ordinary differential equation

$$\frac{\mathrm{d}u}{\mathrm{d}x} = g \tag{2.19}$$

Therefore, the value of $u(x)$ for an argument $x = a$ can be obtained by integrating

$$\mathrm{d}u = g\,\mathrm{d}x \tag{2.20}$$

from $\tilde{a}$ to a (where $\tilde{a}$ is an arbitrary starting point for the integration, with a known function value $u(\tilde{a})$), resulting in

$$u(a) - u(\tilde{a}) = \int_{\tilde{a}}^{a} g\,\mathrm{d}x \tag{2.21}$$

Now consider the case where x, $u(x)$, and $g(x)$ are random variables with the following PC expansions:

$$x = \sum_{j=0}^{P} x_j \Psi_j \tag{2.22}$$

$$u(x) = \sum_{i=0}^{P} u_i \Psi_i \tag{2.23}$$

$$g(x) = \sum_{i=0}^{P} g_i \Psi_i \tag{2.24}$$

We could intuitively use the same procedure as in the deterministic case above to evaluate $u(x)$, however, differential operators do not readily extend to the case where x is a random variable Need a reference . To deal with this issue, we explicitly write x, u, and g as random processes, *i.e.*,

$$x = x(s,\theta) = \sum_{j=0}^{P} x_j(s)\Psi_j(\theta) \tag{2.25}$$

$$u = u(s,\theta) = \sum_{i=0}^{P} u_i(s)\Psi_i(\theta) \tag{2.26}$$

$$g = f(s,\theta) = \sum_{i=0}^{P} g_i(s)\Psi_i(\theta) \tag{2.27}$$

where $s : \mathbb{R} \to \mathbb{R}^4$ parameterizes the path across the deterministic space of PC coefficients and θ denotes the dependence on the underlying random process. In particular, if s, x, u and g are assumed to be smooth enough (namely, analytical),

then the integration becomes path-independent and we can integrate from s_1 to s_2 with

$$\int_{s_1}^{s_2} \frac{\partial u}{\partial s} \mathrm{d}s = \int_{s_1}^{s_2} g \frac{\partial x}{\partial s} \mathrm{d}s. \tag{2.28}$$

Substituting the PC expansions for u, g and

$$\frac{\partial x}{\partial s} = \sum_{j=0}^{P} \frac{\mathrm{d}x_j}{\mathrm{d}s} \Psi_j \tag{2.29}$$

leads to,

$$\sum_{i=0}^{P} \Psi_i \int_{s_1}^{s_2} \frac{\mathrm{d}u_i}{\mathrm{d}s} \mathrm{d}s = \int_{s_1}^{s_2} \sum_{i=0}^{P} g_i \Psi_i \sum_{j=0}^{P} \frac{\mathrm{d}x_j}{\mathrm{d}s} \Psi_j \, \mathrm{d}s \tag{2.30}$$

or

$$\sum_{i=0}^{P} \Psi_i (u_i(s_2) - u_i(s_1)) = \sum_{j=0}^{P} \int_{s_1}^{s_2} \sum_{i=0}^{P} \Psi_i \Psi_j g_i \frac{\mathrm{d}x_j}{\mathrm{d}s} \, \mathrm{d}s. \tag{2.31}$$

Then, multiplying by Ψ_k, taking expectations, and dividing by $< \Psi_k^2 >$, we obtain

$$u_k(s_2) - u_k(s_1) = \sum_{j=0}^{P} \int_{s_1}^{s_2} \sum_{i=0}^{P} C_{ijk} g_i \frac{\mathrm{d}x_j}{\mathrm{d}s} \, \mathrm{d}s. \tag{2.32}$$

Finally, consider the integral defined for any given $(j,k) \in \{0,...,P\}^2$ as follows:

$$I_{jk} = \int_{s_1}^{s_2} \sum_{i=0}^{P} C_{ijk} g_i \frac{\mathrm{d}x_j}{\mathrm{d}s} \, \mathrm{d}s. \tag{2.33}$$

Since $g = g(x)$, then $g_i = g_i(x) = g_i(x_0, x_1, \cdots, x_P)$. In the evaluation of I_{jk}, only one x-coefficient, x_j is varied, while $x_{r \neq j}$ are kept constant. Thus, in this context, $g_i = g_i(x_j; x_{r \neq j}) = g_i(x_j)$, such that

$$\left(\forall (j,k) \in \{0,...,P\}^2\right) \quad I_{jk} = \int_{x_j(s_1)}^{x_j(s_2)} \sum_{i=0}^{P} C_{ijk} g_i \mathrm{d}x_j \tag{2.34}$$

and

$$(\forall k \in \{0,...,P\}) \quad u_k(s_2) - u_k(s_1) = \sum_{j=0}^{P} \int_{x_j(s_1)}^{x_j(s_2)} \sum_{i=0}^{P} C_{ijk} g_i \mathrm{d}x_j. \tag{2.35}$$

Thus, to evaluate $u(x)$ for a given argument $x = a$, with a given PC expansion $a = \sum_{i=0}^{P} a_i \Psi_i$, we choose a suitable $\tilde{a} = \sum_{i=0}^{P} \tilde{a}_i \Psi_i$ where $u(\tilde{a})$ is known. Then choosing $x_j(s_1) = \tilde{a}_j$, and $x_j(s_2) = a_j$ for $j = 0, \ldots, P$, we have that each coefficient u_k of the function result $u(a)$ is found as a summation of $P+1$ coupled integrals

$$(\forall k \in \{0,...,P\}) \quad (u(a))_k = u_k = (u(\tilde{a}))_k + \sum_{j=0}^{P} \int_{\tilde{a}_j}^{a_j} \sum_{i=0}^{P} C_{ijk} \, g_i \, \mathrm{d}x_j. \tag{2.36}$$

The feasibility of this integration approach for evaluating $u(a)$ depends, of course, on two conditions. First, we need to be able to evaluate $u(\tilde{a})$ and second, we need to be able to evaluate $g(x)$ at all points along the integration path. The first condition is met most easily by taking a_0, the mean coefficient of a, as the starting point $\tilde{a}$ for the integration. This way, $u(a_0)$ is a regular operation on a deterministic scalar a_0, and $u(a)$ is obtained by integrating (2.36), with all $\tilde{a}_{j\neq 0} = 0$.

The second condition puts restrictions on the derivative function g. As discussed in the previous sections, we can readily evaluate polynomials, as well as divisions and square roots of PC variables. Therefore, g can be evaluated if it can be written in terms of these elementary operations applied to x as well as u, since u is known at the current point from the integration along the preceding part of the integration path. For example, this algorithm is applicable to the evaluation of the functions $u = e^x$, $u = e^{-x^2}$, and $u = \ln(x)$ as follows:

$$e^a - e^{\tilde{a}} = \int_{\tilde{a}}^{a} u \, \mathrm{d}x \tag{2.37}$$

$$e^{-a^2} - e^{-\tilde{a}^2} = \int_{\tilde{a}}^{a} -2xu \, \mathrm{d}x \tag{2.38}$$

$$\ln(a) - \ln(\tilde{a}) = \int_{\tilde{a}}^{a} \frac{\mathrm{d}x}{x} \tag{2.39}$$

Also, an alternative way to evaluate the square root function is

$$\sqrt{a} - \sqrt{\tilde{a}} = \int_{\tilde{a}}^{a} \frac{\mathrm{d}x}{2u} \tag{2.40}$$

By extension, arbitrary powers of PC variables can be obtained as:

$$u = x^y = e^{y \ln(x)} \tag{2.41}$$

where both x and y can be PC variables.

For the implementation in the current work, a straight line path from $\tilde{a}$ to a has been chosen for the integrals (2.36). In this way, the distance along the integration path for all stochastic coefficients can be parameterized using a single variable s:

$$x_j = (a_j - \tilde{a}_j)s + \tilde{a}_j \tag{2.42}$$

with s evolving from 0 to 1. The integrals (2.36) can therefore be reformulated as a system of (P+1) ordinary differential equations (ODEs) in the integration variable s. This system of ODEs is solved efficiently using the DVODE [1,17] package.

The examples given in the results section below show the accuracy of this integration approach, even for situations where the Taylor series approach breaks down. A drawback, however, is the relatively high cost of integration. Besides making the ODE integration routines more efficient, another way to speed up this approach is to choose the starting point for the integration intelligently. As mentioned above, for a one–time evaluation of a non–polynomial function, the starting point for the integration is typically the mean coefficient of the PC variable, as this facilitates the evaluation of the function at the starting point. However, for subsequent evaluations of the same function for slightly different arguments, previous function evaluations may supply better starting points. Consider for example the calculation of the pH of a buffer solution in a temporally evolving microfluidic system. At each time step, this

requires the evaluation of pH$= -\log[\mathrm{H}^+]$, with $[\mathrm{H}^+]$ the hydrogen ion concentration represented as a PC variable. If this concentration does not change very rapidly in time, then the $[\mathrm{H}^+]$ from the previous time step will be very close in stochastic space to $[\mathrm{H}^+]$ at the current time step. Therefore, this concentration from the previous time step, with its corresponding value of $\log[\mathrm{H}^+]$, may be a better starting point for the integration (2.36) than the mean coefficient of $[\mathrm{H}^+]$ at the current time step.

2.5. Sampling Approach for Non-Polynomial Function Evaluations. An alternative approach for evaluating non-polynomial functions of PC variables involves the use of sampling. In this context, the evaluation of the spectral modes (u_k) of $u = \sum_{k=0}^{P} u_k \Psi_k = f(x)$, where $x = \sum_{k=0}^{P} x_k \Psi_k$, and the x_k's are known, can be done as follows.

- Sample values of $\boldsymbol{\xi} = (\xi_1, \xi_2, \cdots, \xi_N)$, based on the known random variable distributions of the ξ_i's.
- For each sample $\boldsymbol{\xi}^j$, evaluate $\Psi_k = H_k^N(\boldsymbol{\xi}^j)$, x^j, and $u^j = f(x^j)$.
- Summing over all samples, evaluate the expectations required for the GALERKIN-projection

$$(\forall k \in \{0, ..., P\}) \quad u_k = \frac{< u\Psi_k >}{< \Psi_k^2 >} \tag{2.43}$$

  where the best means of evaluation of the expectation depends on the sampling strategy.
- With the u_k's thus computed, assemble the PC expansion for u.

We have used this Non-Intrusive Spectral Projection (NISP) approach in previous works [15,19,22]. It is *non-intrusive* in the sense that it does not require reformulation of the function f, or more generally of the governing equations of a given model. One key aspect of this algorithm is the sampling, or *quadrature*, strategy. Recall that these expectations $< f >$ are given by (2.4), and therefore involve primarily numerical quadrature formulae. Straightforward Monte Carlo (MC) approaches to quadrature are optimal when the random processes at hand have a uniform distribution, and the number of stochastic dimensions is large. However, we are not dealing with uniformly distributed quantities. Given this, the simplest construction involves the use of Latin Hypercube (LH) sampling of the vector of Normal random variables ξ. In this case, $< f >$ is simply evaluated as the arithmetic mean of the set of realizations of f [22]. On the other hand, a more efficient quadrature construction, for small N ($\sim< 5$), uses GAUSS-HERMITE (GH) quadrature, $\sum_i w_i f_i$, for the evaluation of the integrals in $< f >$ [19]. Based on the degree of polynomial exactness of these quadrature rules, $M + 1$ sample points in each stochastic dimensions are sufficient to correctly integrate the expectations in (2.43) provided u is represented well with an PC expansion of order M. Therefore, this methodology is very useful to generate accurate PC representations of $f(x)$. However, while efficient for small N, the dense tensor product implementation of GH in multiple dimensions leads to an exponential increase in the number of samples such that its performance for $N > 10$ is worse than LH. In the present work, we exclusively employ $N = 1$, and therefore will use GH for the NISP evaluations of PC expansions.

2.6. Uncertainty Quantification Toolkit. As part of the current work, all the operations described above, among many others, have been implemented in a UQ toolkit library. This UQ toolkit greatly facilitates the development of new source code

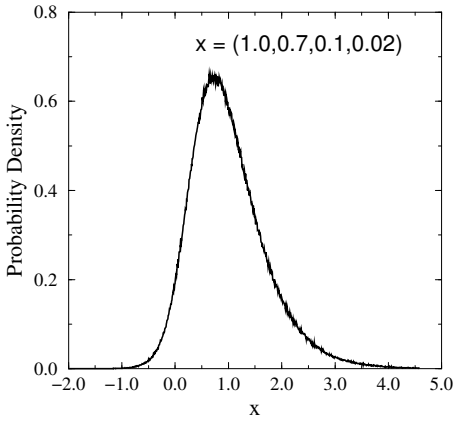

FIG. 3.1. *PDF of the variable x with the PC expansion $x(1.0, 0.7, 0.1, 0.02)$*

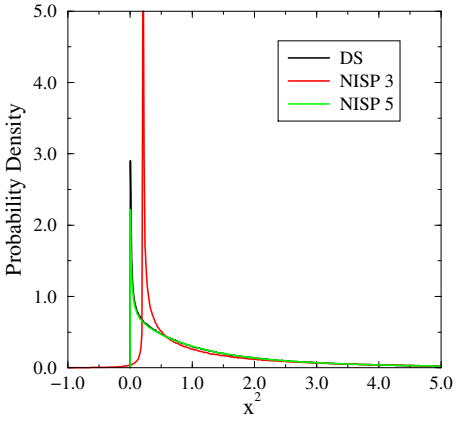

FIG. 3.2. *PDF of x^2 as obtained from direct sampling (DS), as well as from NISP/GH with both 3^{rd} and 5^{th} order PC. The 5^{th} order PC expansion represents the exact PDF well.*

for stochastic operations, as well as the conversion of existing deterministic routines into stochastic ones. Essentially, existing deterministic routines can be converted by replacing deterministic variables with PC variables where necessary, and replacing the mathematical operators that act on those variables with the appropriate stochastic equivalents from the UQ toolkit library.

3. Numerical Results.

3.1. Accuracy of PC Representations with Gaussian basis functions. In performing operations on PC variables, it is important to take into account the accuracy of the PC representation itself. To represent a random variable with a Gaussian PDF, a first order PC representation is sufficient (mean + standard deviation) when using Gaussian basis functions. However, variables with a highly skewed PDF can require considerably higher order terms in order to be properly represented with a PC expansion. For example, Fig. 3.1 shows the PDF of a variable x given by a third order PC expansion $x(1.0, 0.7, 0.1, 0.02)$ (see Eqn. (2.6) for the definition of this notation). This variable has a mean of 1.0 with a coefficient of variation of about 70 %, and higher order terms that cause the PDF to be asymmetric. Figure 3.2 shows the PDFs of the square of this variable, as obtained with various sampling methods. With the "direct sampling" (DS) approach, the PDF of x^2 is obtained by sampling the PDF of x, calculating x^2 for each sample, and compiling the PDF of the results through binning and normalizing. With the NISP/GH approach, the PC representation of x^2 is generated using GAUSS-HERMITE quadrature (see section 2.5) and the PDF of x^2 is then obtained by sampling the resulting PC expansion. Since the NISP/GH approach, with a sufficient number of sample points, gives an exact projection onto the PC basis functions, the resulting PDFs highlight the accuracy of PC expansions with a given order to represent random variables. As can be seen in Fig. 3.2, the 3^{rd} order PC expansion is not accurate enough to represent the PDF of x^2. However, a 5^{th} order expansion is of high enough order as the associated PDF coincides with the directly sampled PDF.

3.2. Truncation Errors. As explained in section 2.2, integer powers x^n of PC variables can be obtained through repeated multiplications in a pseudo-spectral approach. For example, x^4 is conceptually obtained as

$$x^4 = ((x * x) * x) * x \tag{3.1}$$

where each multiplication is performed using (2.11). As mentioned in section 2.2, each one of those stochastic multiplications involves a truncation via a GALERKIN projection of a quantity up to order $2M$ onto a PC basis up to order M. This implies that information in x^n of order higher than M will get lost. In this section, we show that this procedure may affect the accuracy of the lower order coefficients in x^n as well and investigate the importance of these truncation errors.

To evaluate the accuracy of the integer power x^n of a PC variable x with a specified order M, comparisons were made between the $(P+1)$ coefficients of x^n as obtained with the pseudo-spectral approach and the corresponding $(P+1)$ coefficients of x^n as obtained with higher order NISP/GH calculations. The errors in the PC coefficients obtained from the pseudo-spectral approach were quantified using a root-mean-square (RMS) measure, calculated as:

$$E_{rms} = \sqrt{\sum_{i=0}^{P} \left[(y_{\text{NISP/GH}})_i - (y_{\text{PS}})_i\right]^2 < \Psi_i^2 >} \tag{3.2}$$

where $y_{\text{NISP/GH}}$ is the NISP/GH approximation and y_{PS} is the pseudo-spectral approximation of the quantity y considered. Note that this RMS measure only considers the $(P+1)$ lowest order modes, even though the NISP/GH approximations in this section were calculated with a higher order PC representation for accuracy. In this way, the RMS measure (3.2) evaluates the accuracy of the PC representation of x^n within the space covered by the basis functions up to order P. Considering $x = x(1.0, 0.2)$, with its PDF shown in Fig. 3.3, the RMS error in the pseudo–spectral PC coefficients of x^n is shown in Fig. 3.4 x^n as a function of n for two different orders of the PC representation. For low values of n, the RMS error in the PC coefficients of x^n is negligible, indicating that the $(P+1)$ coefficients of x^n are properly calculated with the pseudo-spectral construction. For n larger than $M+1$, however, the RMS error increases dramatically. Apparently, the order of the PC representation becomes too low for these high powers of x and the absence of the higher order coefficients required to properly represent x^n affects the lower order coefficients. Note that the errors in the PC coefficients are still fairly small. For example, the PS approximation of x^5 with third order PC and the NISP/GH approximation with fifth order PC are respectively:

$$x^5_{\text{PS}} = (1.4240, 1.2448, 4.4800 \times 10^{-1}, 8.1920 \times 10^{-2}) \tag{3.3}$$

$$x^5_{\text{NISP/GH}} = (1.4240, 1.2448, 4.4800 \times 10^{-1}, 8.3200 \times 10^{-2}, 8.0000 \times 10^{-3}, 3.2000 \times 10^{-4}) \tag{3.4}$$

The error in the modes of x^5_{PS} shows up only in the second significant digit of the third order term. However, as shown in Fig. 3.5, there is a rather large difference between the PDF sampled from the x^5_{PS} PC expansion and the directly sampled PDF. The PDF sampled from x^5_{PS} does agree with the PDF sampled from the $x^5_{\text{NISP/GH}}$ PC expansion that has been truncated after the 3$^{\text{rd}}$ order terms, i.e.

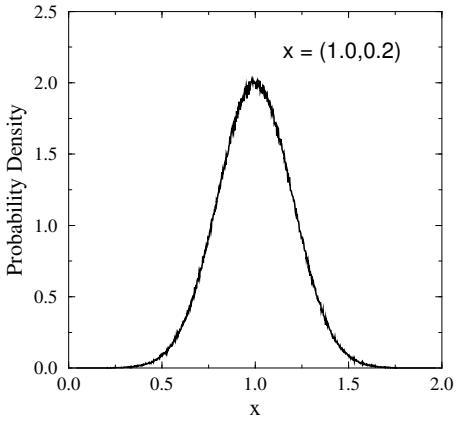

FIG. 3.3. *PDF of the variable x given by the PC expansion $x(1.0, 0.2)$*

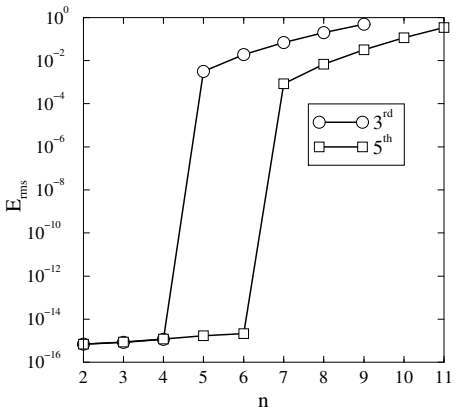

FIG. 3.4. *Root-mean-squared error in the PC coefficients of x^n obtained with a 3^{rd} and a 5^{th} order PC pseudo-spectral method. The error increases dramatically for powers of x that are more than one larger than the order of the PC expansions.*

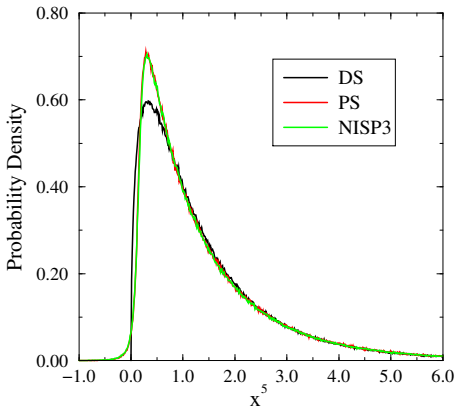

FIG. 3.5. *PDF of x^5 as obtained by direct sampling (DS), pseudo-spectral (PS) calculation with 3^{rd} order PC, as well as the sampling of the NISP/GH result truncated after the 3^{rd}. The low order PC expansion results in finite probabilities for negative values of x^5.*

$(1.4240, 1.2448, 4.4800 \times 10^{-1}, 8.3200 \times 10^{-2})$. This indicates that the small error in the resolved coefficients is less important than the absence of the higher order terms in the PC expansion.

The observations above seem to suggest that PC expansions with a given order M can represent powers x^n with n not larger than $M+1$. However, in general, x may have significant higher order information to begin with, instead of the Gaussian x that was used in this specific example. The more higher order information is present in x, the higher the order of the PC expansions will need to be in order to properly represent x^n. Therefore, the representation of x^n may break down for powers of x that are smaller than $M + 1$. To make sure that a sufficiently high order PC has been used in a calculation, it is therefore recommended to repeat the calculations

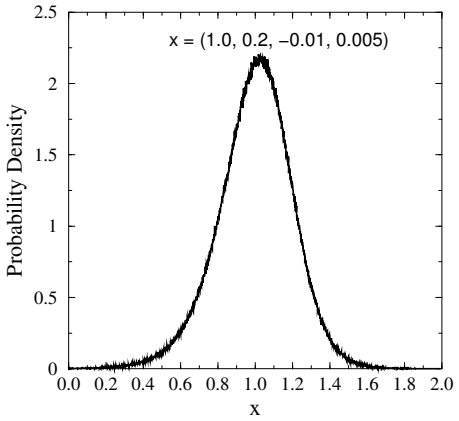

FIG. 3.6. *PDF of the variable x given by the PC expansion $x(1.0, 0.2, -0.01, 0.005)$*

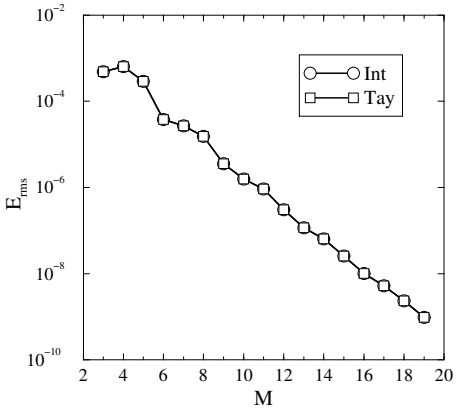

FIG. 3.7. *Root-mean-squared difference between the PC coefficients of* $\exp(x)$ *for the* TAYLOR *series and integration approaches compared to the NISP/GH method, as a function of the order M of the expansion used. Both* TAYLOR *series and the integration approach give the same results.*

with increasingly higher order PC representations, until the results do not change any more.

As will be shown in the following section, the inability of low order PC expansions to represent high powers of PC variables will affect the accuracy of TAYLOR series approximations for non-polynomial function evaluations of PC variabiles when many terms are required to reach convergence.

3.3. Non-Polynomial Function Evaluations. In this section, the evaluation of non-polynomial functions of PC variables is studied. Comparisons are made between the NISP/GH, TAYLOR series and integration approaches for both the evaluation of exponentials and logarithms.

3.3.1. Exponentials. First, consider a PC variable x, given by the PC expansion $x(1.0, 0.2, -0.01, 0.005)$. This variable has a moderate uncertainty of about 20 % and a slightly skewed PDF, as shown in Fig. 3.6. The PC expansion representing $\exp(x)$ was calculated using both the TAYLOR series and integration approaches for increasing orders M of the PC expansions. Each time, the root-mean-squared (RMS) difference was calculated between the resulting PC coefficients and the result of a NISP/GH evaluation of $\exp(x)$ with the same order PC representation. As shown in Fig. 3.7, both the TAYLOR series and integration approaches give the same results at each order M. Also, except for the fourth order calculation, the RMS difference with the NISP/GH approach decreases monotonically with the order of the PC representation. To properly interpret these results, it is important to note that contrary to the analysis in section 3.2, the NISP/GH results here are not necessarily the exact solution. In section 3.2, a sufficiently high order PC representation and excess quadrature points were used in order to get an exact evaluation of the integrals in (2.43). In this section, however, the same order PC expansion is used in the TAYLOR series, integration, as well as the NISP/GH method. For random variables with very high order information, this means that the quadrature integrations in (2.43) will not be exact. In practice though, the NISP/GH method generally gives very accurate results,

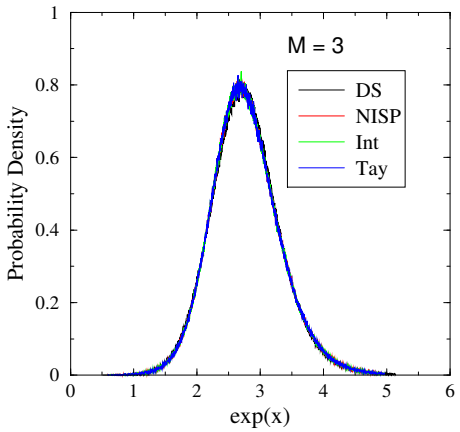

FIG. 3.8. *Comparison of the PDF of* $\exp(x)$ *as generated with the different methods using* 3^{rd} *order PC representations. All methods give the same result.*

especially when the uncertainties and non-linearities are moderate. For the current example, all three approaches are very accurate, even for low order PC approximations. Figure 3.8 compares the PDFs generated by sampling the PC representations from the NISP/GH, integration and TAYLOR series approaches with the directly sampled PDF of $\exp(x)$. Even with the low, third order PC approximation, all PDFs are indistinguishable from the directly sampled PDF.

The evaluation of $\exp(x)$ becomes more challenging when the uncertainty in x increases and higher order modes create a more skewed PDF. Consider for example the PC variable $x(1.4, 1.1, -0.22, 0.04, -0.009, 0.004, -0.001)$ with its PDF shown in Fig. 3.9. Similar to the previous example, the PC representations of $\exp(x)$ obtained with the integration and TAYLOR series approaches are compared for increasing order M in the PC expansions to the NISP/GH evaluations of $\exp(x)$ generated with the same order PC expansions. For both the integration and TAYLOR series methods, the RMS differences with the NISP/GH results are shown in Fig. 3.10. A first observation regarding these RMS differences is that they are considerably larger than in the previous example (Fig. 3.7), indicating that the evaluation of $\exp(x)$ is indeed more challenging. Second, for orders M higher than 9, the TAYLOR series breaks down due to the large number of terms, and consequently high powers of x required to reach sufficient accuracy in the TAYLOR series approximation. For the 9^{th} order PC representation, 130 terms are required for the TAYLOR series to reach sufficient accuracy in this case. Given the limitations in the representation of x^n with a given order PC expansion, it is actually surprising that the TAYLOR series in this case holds up so well. For higher order representations of $\exp(x)$, however, the terms in the TAYLOR series start to grow above a certain power of x and the series does not converge any longer. The integration approach, on the other hand, is able to evaluate $\exp(x)$, even for large orders M in the PC representations. As M increases, the RMS difference between the integration approach and NISP/GH decreases in a general sense, although not monotonically. Again, it is important to realize that the NISP/GH approach does not necessarily represent the exact result, especially since the random variable $\exp(x)$ in this case requires a very high order PC expansion in order to be properly represented. Figure 3.11 illustrates this by plotting the PDF of $\exp(x)$ obtained by direct sampling, and comparing this to the PDFs obtained by sampling the PC rep-

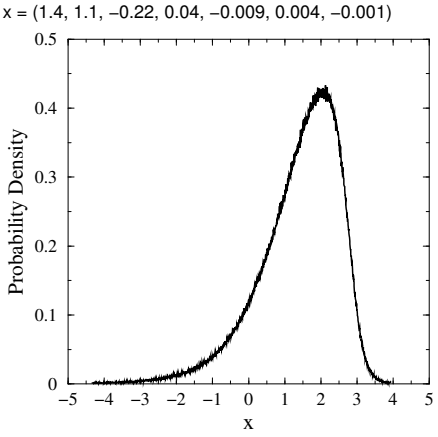

FIG. 3.9. *PDF of the variable* $x(1.4, 1.1, -0.22, 0.04, -0.009, 0.004, -0.001)$

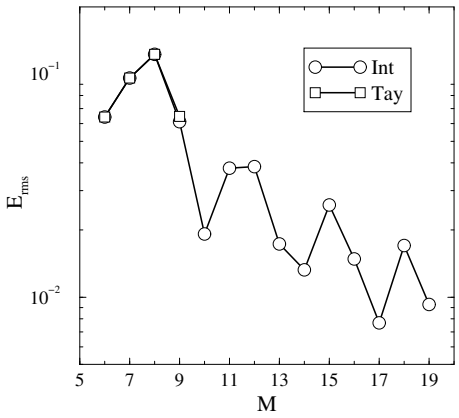

FIG. 3.10. *Root-mean-squared difference between the PC coefficients of* $\exp(x)$ *for the* TAYLOR *series and integration approaches compared to the NISP/GH method, as a function of the order* M *of the expansion used. The* TAYLOR *series breaks down for* $M > 9$ *whereas the integration approach gets closer to the NISP/GH results for increasing* M*.*

resentations generated with the other methods. As the directly sampled PDF shows in this figure, the PDF of $\exp(x)$ has a long and smooth tail on the right side, but has a very steep drop-off near zero, which is caused by the long tail towards negative values in the PDF of x. This steep drop-off near zero requires a very high order PC expansion to resolve. While the 6^{th} order approximations with NISP/GH as well as the integration and the TAYLOR series approach look fairly good overall in Fig. 3.11a, zooming in on the origin in Fig. 3.11b reveals several discrepancies with the directly sampled PDF. The NISP/GH result does not reproduce the steep drop-off near zero and has a relatively large probability for (unphysical) negative values for $\exp(x)$. The TAYLOR series and integration approach resolve the steep gradient near zero fairly well, but have a large overshoot between 0 and 0.5. Increasing the order of the PC expansions slowly improves the accuracy of the representation of $\exp(x)$. The PDFs from the 19^{th} order PC expansions, as shown in Fig. 3.11c and d, are in much better agreement with the directly sampled PDF, although not perfect. An even higher order PC expansion would be required to perfectly represent the random variable $\exp(x)$. As explained above, the TAYLOR series approach is not able to generate these high order representations, but the integration approach still works well. An alternative way to compare the accuracy of the different methods is to look at the cumulative distribution functions (CDFs) of the generated random variables. Figure 3.12 plots the probability that $\exp(x)$ is smaller than a given value X, as a function of X, on a logarithmic scale so that the left tail is emphasized. Even though there were some differences in the PDFs for $\exp(x)$ between the different methods using 6^{th} order PC expansions, this figure shows that there is actually quite a good agreement between all methods when looking at the CDFs. Apparently the differences get leveled out in the integration of the PDF to get the CDF. The right tail of the PDF is harder to

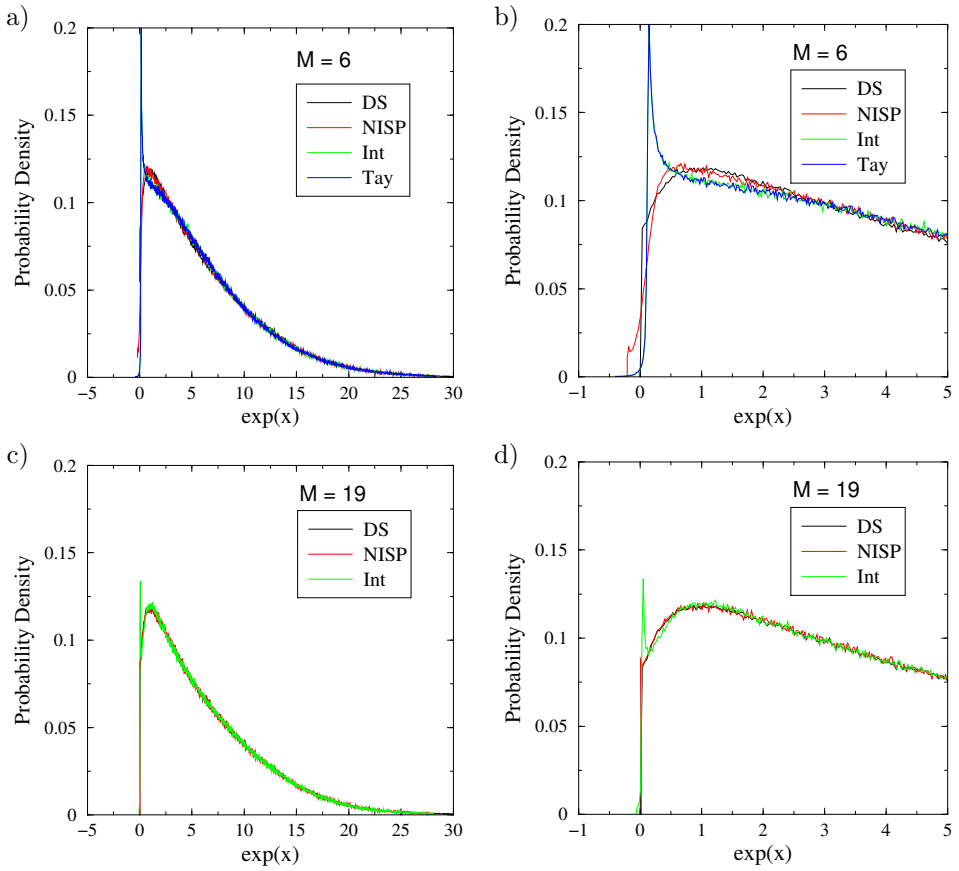

FIG. 3.11. *Comparison of the PDF of* $\exp(x)$ *generated with the* TAYLOR *series, integration and NISP/GH approaches to the directly sampled PDF: a) Approximations with* 6^{th} *order PC expansions; b) Same, but zoomed in on the origin; c) Approximations with* 19^{th} *order PC expansions; d) Same, but zoomed in on the origin.*

match however, as shown in Fig. 3.13, which plots the probability of $\exp(x) > X$ as a function of X. For the 6^{th} order PC expansions in Fig. 3.13a, the results obtained with the integration approach fall on top of the TAYLOR series results, which are very close to the NISP/GH results. All of these methods fail to match the directly sampled results however. With 19^{th} order PC expansions, however, the NISP/GH results fall almost on top of the directly sampled results. The integration approach also gives a very accurate approximation of this tail while, as mentioned before, the TAYLOR series approach fails for this high order.

3.3.2. Logarithms. As a first example of the evaluation of logarithms of PC variables, consider the PC variable $x(1.0, 0.1, 0.01, 0.001)$. The PC coefficients of x have been chosen such that the PDF of x, as shown in Fig. 3.14 has finite probabilities only for values of x that are sufficiently far away from zero and are within the range of convergence of the TAYLOR series (2.18) for $\ln(x)$: $|x - x_0| < |x_0|$. As in the study of the exponential function evaluations, the PC representations for $\ln(x)$ generated with the TAYLOR series and the integration approach are compared to the NISP/GH results for increasing order M of the PC representations, as shown in Fig. 3.15. Up to

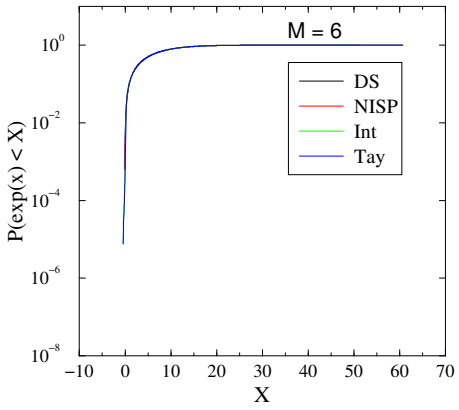

FIG. 3.12. *Comparison of the tails of the CDF $P(\exp(x) < X)$ generated with the* TAYLOR *series, integration and NISP/GH approaches to the directly sampled results.*

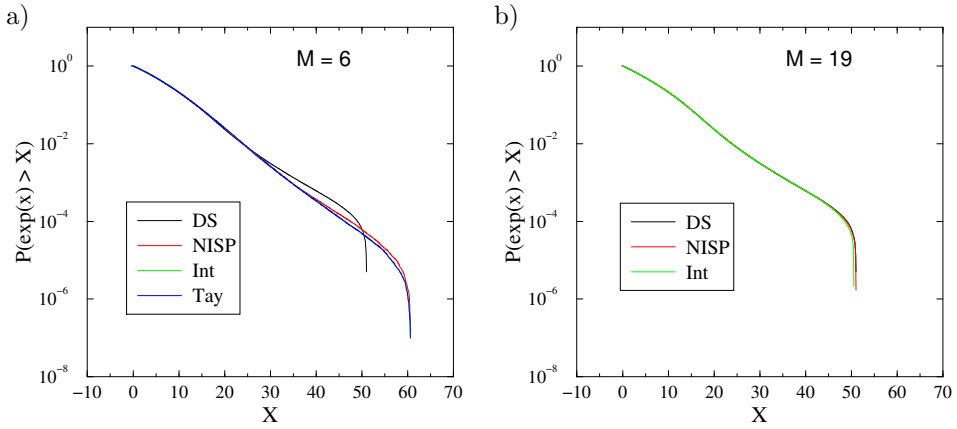

FIG. 3.13. *Comparison of the tails of the CDF $P(\exp(x) > X)$ generated with the* TAYLOR *series, integration and NISP/GH approaches to the directly sampled results: a) Approximations with 6^{th} order PC expansions; b) Approximations with 19^{th} order PC expansions.*

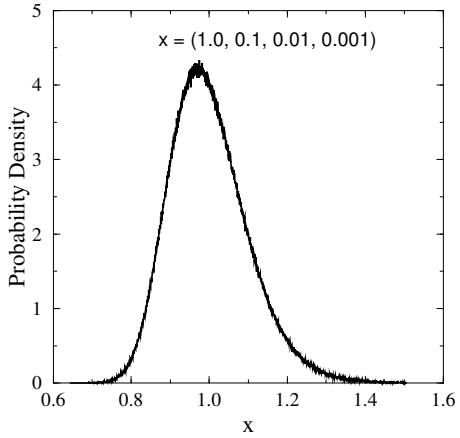

FIG. 3.14. *PDF of the PC variable* $x(1.0, 0.1, 0.01, 0.001)$

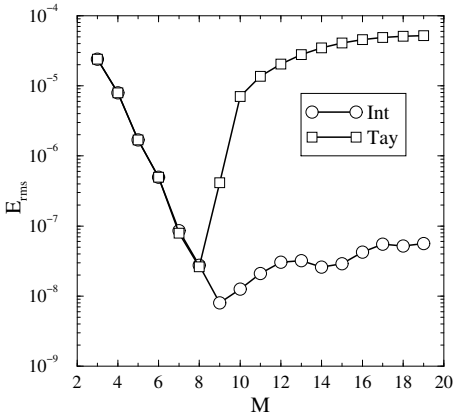

FIG. 3.15. *RMS difference between the PC coefficients of* $\ln(x)$ *for the* TAYLOR *series and integration approaches compared to the NISP/GH method, as a function of the order* M *of the expansion used. The* TAYLOR *series breaks down for* $M > 8$*. The integration approach gets closer to the NISP/GH results up to order 9 but then levels off.*

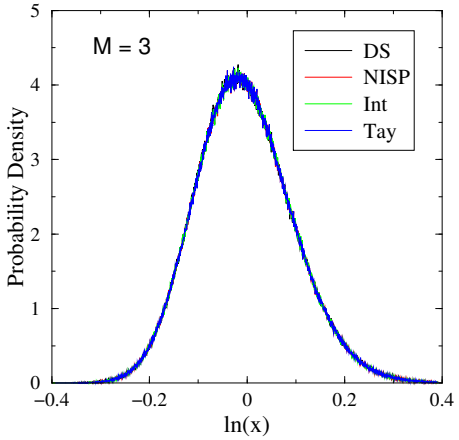

FIG. 3.16. *Comparison of the PDF of* $\ln(x)$ *generated with the* TAYLOR *series, integration and NISP/GH approaches to the directly sampled PDF for* 3^{rd} *order PC representations.*

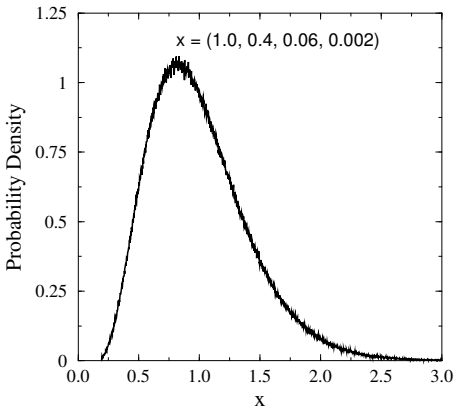

FIG. 3.17. *PDF of the PC variable* $x(1.0, 0.4, 0.06, 0.002)$

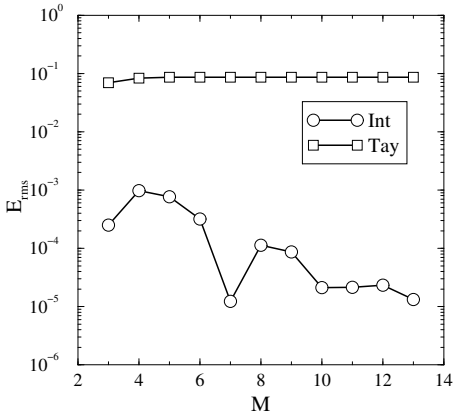

FIG. 3.18. *RMS difference between the PC coefficients of* $\ln(x)$ *for the* TAYLOR *series and integration approaches compared to the NISP/GH method, as a function of the order* M *of the expansion used. The* TAYLOR *series is not convergent for this case but the integration approach gives results that generally improve for increasing* M.

order 8, both the TAYLOR series and the integration approach rapidly get closer to the NISP/GH results. However, above 8^{th} order, the TAYLOR series stops converging as its terms start to grow after a certain power of x. In the TAYLOR series implementation in this work, the series is truncated at the point where its terms start to grow, and therefore, the TAYLOR series data in Fig. 3.15 for $M > 8$ is from this truncated series expansion. The integration approach levels off above 9^{th} order, but in contrast with the TAYLOR series approximations, the error does not grow significantly for higher orders. All methods, however, are able to properly represent $\ln(x)$ with low order PC expansions. As is shown in Fig. 3.16, all methods match the PDF generated by direct sampling of $\ln(x)$. Therefore, the TAYLOR series approach would work fine for this specific case, as long as a low order PC representation is used. The integration approach does not suffer from this limitation though, and gives good results for any order PC expansion.

In the second example of the calculation of $\ln(x)$, the PC coefficients of $x(1.0, 0.4, 0.06, 0.002)$ were chosen so that its PDF, as shown in Fig. 3.17, would stay away from zero but allow values of x that are outside the convergence range of the TAYLOR series for $\ln(x)$. Therefore, the TAYLOR series diverges after only about 4 terms for all orders M and the PC representation truncated at that point is inaccurate, as illustrated in Fig. 3.18. The integration approach on the other hand, returns considerably more accurate PC approximations for $\ln(x)$ and its results generally improve with increasing order M, although not monotonically. As shown in Fig. 3.19, the TAYLOR series, truncated after 4 terms, does not give a good agreement with the exact PDF. The integration approach on the other hand matches the NISP/GH as well as the directly sampled PDF, even for a low, 3^{rd} order PC representation.

4. Conclusions. In this paper, we presented an overview of the use of Polynomial Chaos expansions to represent stochastic processes in computations such as intrusive spectral uncertainty quantifications. Major challenges in the use of those PC

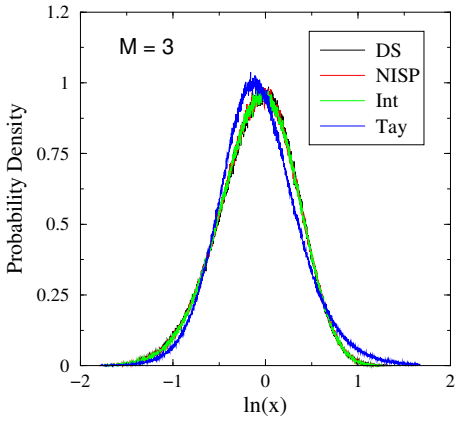

FIG. 3.19. *Comparison of the PDF of* $\ln(x)$ *generated with the* TAYLOR *series, integration and NISP/GH approaches to the directly sampled PDF for* 3^{rd} *order PC representations. The integration approach matches the NISP/GH and directly sampled results, whereas the* TAYLOR *series does not converge.*

representations include the accuracy of the representations as well as the evaluation of polynomial and non-polynomial functions of variables represented by PC expansions.

Several methods were presented to perform "stochastic arithmetic" on PC variables and to evaluate functions of PC variables. Besides TAYLOR series and sampling-based spectral projection methods, a new method was developed for non-polynomial function evaluations. This new method is based on the integration of the derivative of the function to be evaluated and is applicable to all functions $u : x \mapsto u(x)$ where $\frac{\mathrm{d}u}{\mathrm{d}x}$ can be expressed as a rational function of x and/or u.

A rigorous comparison was performed between the TAYLOR series, integration, and sampling-based methods for non-polynomial function evaluations. TAYLOR series work well as long as the required order in the PC expansions to properly represent the results is not too high, and as long as realizations of the PC variable can not fall outside the range of convergence of the TAYLOR series. The integration method on the other hand is a robust and accurate approach to evaluate non-polynomial functions, even when very high order information is present in the PC expansions.

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