SIAM J. SCI. COMPUT.
Vol. 24, No. 2, pp. 619–644

THE WIENER–ASKEY POLYNOMIAL CHAOS FOR STOCHASTIC DIFFERENTIAL EQUATIONS*

DONGBIN XIU† AND GEORGE EM KARNIADAKIS†

Abstract. We present a new method for solving stochastic differential equations based on Galerkin projections and extensions of Wiener's polynomial chaos. Specifically, we represent the stochastic processes with an optimum trial basis from the Askey family of orthogonal polynomials that reduces the dimensionality of the system and leads to exponential convergence of the error. Several continuous and discrete processes are treated, and numerical examples show substantial speed-up compared to Monte Carlo simulations for low dimensional stochastic inputs.

Key words. polynomial chaos, Askey scheme, orthogonal polynomials, stochastic differential equations, spectral methods, Galerkin projection

AMS subject classifications. 65C20, 65C30

PII. S1064827501387826

1. Introduction.

Wiener first defined "homogeneous chaos" as the span of Hermite polynomial functionals of a Gaussian process [19]; polynomial chaos is defined as the member of that set. According to the Cameron–Martin theorem [3], the Fourier–Hermite series converge to any L_2 functional in the L_2 sense. In the context of stochastic processes, this implies that the homogeneous chaos expansion converges to any processes with *finite* second-order moments. Therefore, such an expansion provides a means of representing a stochastic process with Hermite orthogonal polynomials. Other names such as "Wiener chaos," "Wiener–Hermite chaos," etc., have also been used in the literature. In this paper, we will use the term Hermite-chaos.

While Hermite-chaos is useful in the analysis of stochastic processes, efforts have also been made to apply it to model uncertainty in physical applications. In this case, the continuous integral form of the Hermite-chaos is written in the discrete form of infinite summation, which is further truncated. Ghanem and Spanos [9] combined the Hermite-chaos expansion with a finite element method to model uncertainty encountered in various problems of solid mechanics, e.g., [7], [8], [9], etc. In [20], the polynomial chaos was applied to modeling uncertainty in fluid dynamics applications. The algorithm was implemented in the context of the spectral/*hp* element method, and various benchmark tests were conducted to demonstrate convergence in prototype flows.

Although for any arbitrary random process with finite second-order moments the Hermite-chaos expansion converges in accord with the Cameron–Martin theorem [3], it has been demonstrated that the convergence rate is optimal for Gaussian processes; in fact the rate is exponential [15]. This can be understood from the fact that the weighting function of Hermite polynomials is the *same* as the probability density function of the Gaussian random variables. For other types of processes the convergence rate may be substantially slower. In this case, other types of orthogonal polynomials,

*Received by the editors April 11, 2001; accepted for publication (in revised form) April 12, 2002; published electronically October 16, 2002. This work was supported by the DOE and ONR. Computations were performed at Brown's TCASCV and at the facilities of the NCSA (University of Illinois) and NPACI (UCSD).

http://www.siam.org/journals/sisc/24-2/38782.html

†Division of Applied Mathematics, Brown University, Providence, RI 02912 (xiu@cfm.brown.edu, gk@cfm.brown.edu).

instead of Hermite polynomials, could be used to construct the chaos expansion. In an early work by Ogura [16], a chaos expansion based on Charlier polynomials was proposed to represent the Poisson processes, following the theory of "discrete chaos" by Wiener [19].

An important class of orthogonal polynomials are the members of the so-called Askey scheme of polynomials [1]. This scheme classifies the hypergeometric orthogonal polynomials that satisfy some type of differential or difference equation and indicates the limit relations between them. Hermite polynomials are a subset of the Askey scheme. Each subset of the orthogonal polynomials in the Askey scheme has a different weighting function in its orthogonality relationship. It has been realized that some of these weighting functions are identical to the probability function of certain random distributions. For example:

- Hermite polynomials are associated with the Gaussian distribution,
- Laguerre polynomials with the gamma distribution,
- Jacobi polynomials with the beta distribution,
- Charlier polynomials with the Poisson distribution,
- Meixner polynomials with the negative binomial distribution,
- Krawtchouk polynomials with the binomial distribution, and
- Hahn polynomials with the hypergeometric distribution.

This finding opens the possibility of representing stochastic processes with different orthogonal polynomials according to the property of the processes.

The close connection between stochastic processes and orthogonal polynomials has long been recognized. Despite the role of Hermite polynomials in the integration theory of Brownian motion (see [19] and [11]), many birth-and-death models were related to specific orthogonal polynomials. The so-called Karlin–McGregor representation of the transition probabilities of a birth-and-death process is in terms of orthogonal polynomials [12]. In [16] and [5], the integral relation between the Poisson process and the Charlier polynomials was found. In [17], the role of the orthogonal polynomials from the Askey scheme in the theory of Markov processes was studied, and the connection between the Krawtchouk polynomials and the binomial process was established.

In this paper, we extend the work by Ghanem and Spanos for Hermite-chaos expansion [9] and Ogura for Charlier-chaos expansion [16]. We propose an Askey scheme-based polynomial chaos expansion for stochastic processes, which includes all the orthogonal polynomials in the above list. We numerically demonstrate the optimal (exponential) convergence rate of each Wiener–Askey polynomial chaos expansion for its corresponding stochastic processes by solving a stochastic ordinary differential equation, for which the exact solutions can be obtained. It is also shown that if for a certain process the optimal Wiener–Askey polynomial chaos expansion is not employed, the solution also converges but the rate is clearly slower. This approach will provide a guideline for representing stochastic processes in physical applications properly.

In practical applications, one often does not know the analytical form of the distribution of the process, or, if known, it may not be one of the basic distributions, e.g., Gaussian, Poisson, etc. In this case, one can choose a set of Wiener–Askey polynomial chaos expansions and conduct a numerical projection procedure to represent the process. This issue will be addressed in the present paper as well.

This paper is organized as follows: In the next section we review the theory of the Askey scheme of hypergeometric orthogonal polynomials, and in section 3 we review the theory of the original Wiener polynomial chaos. In section 4 we present the framework of Wiener–Askey polynomial chaos expansion for stochastic processes. In section 5 we present numerical solutions of a stochastic ordinary differential equation with different Wiener–Askey chaos expansions. The choice of the particular Wiener–Askey chaos is based on the distribution of the random input, and we demonstrate the exponential convergence rate with the appropriately chosen Wiener–Askey basis. In section 6 we address the issue of representing an arbitrary random distribution, and we show that, although the Wiener–Askey polynomial chaos converges in general, the exponential convergence is not realized if the optimal type of Wiener–Askey chaos is not chosen. We conclude the paper with a discussion on possible extensions and applications to more complicated problems. An appendix of the definitions and properties of the orthogonal polynomials discussed in this paper is included for completeness.

2. The Askey scheme of hypergeometric orthogonal polynomials. The theory of orthogonal polynomials is relatively mature and several books have been devoted to its study (e.g., [18], [2], [4]). However, more recent work has shown that an important class of orthogonal polynomials belong to the Askey scheme of hypergeometric polynomials [1]. In this section, we briefly review the theory of hypergeometric orthogonal polynomials. We adopt the notation of [14] and [17].

2.1. The generalized hypergeometric series. We first introduce the *Pochhammer symbol* $(a)_n$ defined by

$$(a)_n = \begin{cases} 1 & \text{if } n = 0, \\ a(a+1)\cdots(a+n-1) & \text{if } n = 1, 2, 3, \dots. \end{cases} \tag{2.1}$$

In terms of gamma function, we have

$$(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)}, \qquad n > 0. \tag{2.2}$$

The *generalized hypergeometric series* ${}_rF_s$ is defined by

$${}_rF_s(a_1, \dots, a_r; b_1, \dots, b_s; z) = \sum_{k=0}^{\infty} \frac{(a_1)_k \cdots (a_r)_k}{(b_1)_k \cdots (b_s)_k} \frac{z^k}{k!}, \tag{2.3}$$

where $b_i \neq 0, -1, -2, \dots$ for $i = \{1, \dots, s\}$ to ensure that the denominator factors in the terms of the series are never zero. Clearly, the ordering of the numerator parameters and of the denominator parameters is immaterial. The radius of convergence ρ of the hypergeometric series is

$$\rho = \begin{cases} \infty & \text{if } r < s+1, \\ 1 & \text{if } r = s+1, \\ 0 & \text{if } r > s+1. \end{cases} \tag{2.4}$$

Some elementary cases of the hypergeometric series are the following:

- exponential series ${}_0F_0$,
- binomial series ${}_1F_0$,
- Gauss hypergeometric series ${}_2F_1$.

If one of the numerator parameters a_i, $i = 1, \dots, r$, is a negative integer, say $a_1 = -n$, the hypergeometric series (2.3) terminates at the nth term and becomes a polynomial in z,

$${}_rF_s(-n, \dots, a_r; b_1, \dots, b_s; z) = \sum_{k=0}^{n} \frac{(-n)_k \cdots (a_r)_k}{(b_1)_k \cdots (b_s)_k} \frac{z^k}{k!}. \tag{2.5}$$

2.2. Properties of the orthogonal polynomials. A system of polynomials $\{Q_n(x), n \in \mathcal{N}\}$, where $Q_n(x)$ is a polynomial of exact degree n and $\mathcal{N} = \{0, 1, 2, \dots\}$ or $\mathcal{N} = \{0, 1, \dots, N\}$ for a finite nonnegative integer N, is an orthogonal system of polynomials with respect to some real positive measure ϕ if the following orthogonality relations are satisfied:

$$\int_S Q_n(x) Q_m(x) d\phi(x) = h_n^2 \delta_{nm}, \qquad n, m \in \mathcal{N}, \tag{2.6}$$

where S is the support of the measure ϕ and the h_n are nonzero constants. The system is called orthonormal if $h_n = 1$.

The measure ϕ often has a density $w(x)$ or weights $w(i)$ at points x_i in the discrete case. The relations (2.6) then become

$$\int_S Q_n(x) Q_m(x) w(x) dx = h_n^2 \delta_{nm}, \qquad n, m \in \mathcal{N}, \tag{2.7}$$

in the continuous case, or

$$\sum_{i=0}^{M} Q_n(x_i) Q_m(x_i) w(x_i) = h_n^2 \delta_{nm}, \qquad n, m \in \mathcal{N}, \tag{2.8}$$

in the discrete case, where it is possible that $M = \infty$.

The density $w(x)$ or weights $w(i)$ in the discrete case are also commonly referred to as the *weighting function* in the theory of orthogonal polynomials. It will be shown later that the weighting functions for some orthogonal polynomials are identical to certain probability functions. For example, the weighting function for the Hermite polynomials is the same as the probability density function (PDF) of the Gaussian random variables. This fact plays an important role in representing stochastic processes with orthogonal polynomials.

All orthogonal polynomials $\{Q_n(x)\}$ satisfy a *three-term recurrence relation*

$$-x Q_n(x) = A_n Q_{n+1}(x) - (A_n + C_n) Q_n(x) + C_n Q_{n-1}(x), \qquad n \geq 1, \tag{2.9}$$

where $A_n, C_n \neq 0$ and $C_n / A_{n-1} > 0$. Together with $Q_{-1}(x) = 0$ and $Q_0(x) = 1$, all $Q_n(x)$ can be determined by the recurrence relation.

It is well known that continuous orthogonal polynomials satisfy the second-order differential equation

$$s(x) y'' + \tau(x) y' + \lambda y = 0, \tag{2.10}$$

where $s(x)$ and $\tau(x)$ are polynomials of at most second and first degree, respectively, and

$$\lambda = \lambda_n = -n\tau' - \frac{1}{2} n(n-1) s'' \tag{2.11}$$

are the eigenvalues of the differential equation; the orthogonal polynomials $y(x) = y_n(x)$ are the eigenfunctions.

In the discrete case, we introduce the forward and backward difference operator, respectively

$$\Delta f(x) = f(x+1) - f(x) \qquad \text{and} \qquad \nabla f(x) = f(x) - f(x-1). \tag{2.12}$$

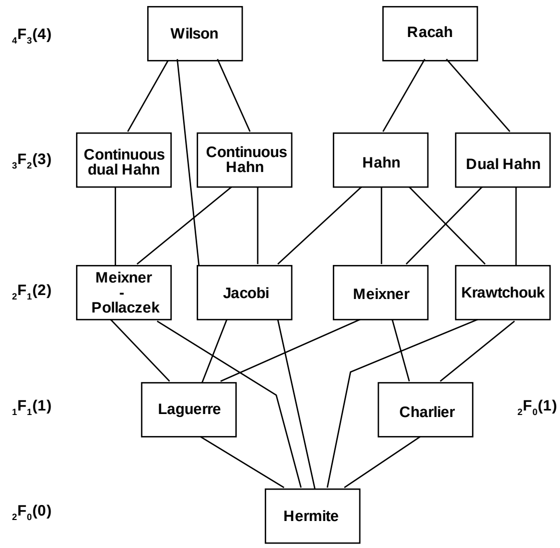

FIG. 2.1. *The Askey scheme of orthogonal polynomials.*

The *difference equation* corresponding to the differential equation (2.10) is

$$s(x)\Delta\nabla y(x) + \tau(x)\Delta y(x) + \lambda y(x) = 0. \tag{2.13}$$

Again $s(x)$ and $\tau(x)$ are polynomials of at most second and first degree, respectively; $\lambda = \lambda_n$ are eigenvalues of the difference equation; and the orthogonal polynomials $y(x) = y_n(x)$ are the eigenfunctions.

All orthogonal polynomials can be obtained by repeatedly applying the differential operator as follows:

$$Q_n(x) = \frac{1}{w(x)} \frac{d^n}{dx^n} \left[w(x) s^n(x) \right]. \tag{2.14}$$

In the discrete case, the differential operator (d/dx) is replaced by the backward difference operator ∇. A constant factor can be introduced for normalization. Equation (2.14) is referred to as the *generalized Rodriguez formula*, named after J. Rodriguez who first discovered the specific formula for Legendre polynomials (see [2]).

2.3. The Askey scheme. The Askey scheme, which can be represented as a tree structure as shown in Figure 2.1, classifies the hypergeometric orthogonal polynomials and indicates the limit relations between them. The "tree" starts with the Wilson polynomials and the Racah polynomials on the top. They both belong to the class $_4F_3$ of the hypergeometric orthogonal polynomials (2.5). The Wilson polynomials are continuous polynomials, and the Racah polynomials are discrete. The lines connecting different polynomials denote the limit transition relationships between them, which imply that polynomials at the lower end of the lines can be obtained by taking the limit of one parameter from their counterparts on the upper end. For example, the limit relation between Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ and Hermite polynomials $H_n(x)$ is

$$\lim_{\alpha\to\infty} \alpha^{-\frac{1}{2}n} P_n^{(\alpha,\alpha)}\left(\frac{x}{\sqrt{\alpha}}\right) = \frac{H_n(x)}{2^n n!},$$

and between Meixner polynomials $M_n(x;\beta,c)$ and Charlier polynomials $C_n(x;a)$ is

$$\lim_{\beta\to\infty} M_n\left(x;\beta,\frac{a}{a+\beta}\right) = C_n(x;a).$$

For a detailed account of the limit relations of the Askey scheme, the interested reader should consult [14] and [17].

The orthogonal polynomials associated with the Wiener–Askey polynomials chaos include Hermite, Laguerre, Jacobi, Charlier, Meixner, Krawtchouk, and Hahn polynomials. A survey with their definitions and properties can be found in the appendix of this paper.

3. The original Wiener polynomial chaos. The homogeneous chaos expansion was first proposed by Wiener [19]; it employs the Hermite polynomials in terms of Gaussian random variables. According to the theorem of Cameron and Martin [3], it can approximate any functionals in $L_2(C)$ and converges in the $L_2(C)$ sense. Therefore, Hermite-chaos provides a means for expanding second-order random processes in terms of orthogonal polynomials. Second-order random processes are processes with finite variance, and this applies to most physical processes. Thus, a general second-order random process $X(\theta)$, viewed as a function of θ as the random event, can be represented in the form

$$\begin{aligned} X(\theta) &= a_0 H_0 \\ &+ \sum_{i_1=1}^{\infty} a_{i_1} H_1(\xi_{i_1}(\theta)) \\ &+ \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1} a_{i_1 i_2} H_2(\xi_{i_1}(\theta),\xi_{i_2}(\theta)) \\ &+ \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2} a_{i_1 i_2 i_3} H_3(\xi_{i_1}(\theta),\xi_{i_2}(\theta),\xi_{i_3}(\theta)) \\ &+ \cdots, \end{aligned} \tag{3.1}$$

where $H_n(\xi_{i_1},\dots,\xi_{i_n})$ denotes the Hermite-chaos of order n in the variables $(\xi_{i_1},\dots,\xi_{i_n})$, where the H_n are Hermite polynomials in terms of the standard Gaussian variables $\boldsymbol{\xi}$ with *zero mean* and *unit variance*. Here $\boldsymbol{\xi}$ denotes the vector consisting of n independent Gaussian variables $(\xi_{i_1},\dots,\xi_{i_n})$. The above equation is the discrete version of the original Wiener polynomial chaos expansion, where the continuous integrals are replaced by summations. The general expression of the polynomials is given by

$$H_n(\xi_{i_1},\dots,\xi_{i_n}) = e^{\frac{1}{2}\boldsymbol{\xi}^T\boldsymbol{\xi}}(-1)^n \frac{\partial^n}{\partial\xi_{i_1}\cdots\partial\xi_{i_n}} e^{-\frac{1}{2}\boldsymbol{\xi}^T\boldsymbol{\xi}}. \tag{3.2}$$

For notational convenience, (3.1) can be rewritten as

$$X(\theta) = \sum_{j=0}^{\infty} \hat{a}_j \Psi_j(\boldsymbol{\xi}), \tag{3.3}$$

where there is a one-to-one correspondence between the functions $H_n(\xi_{i_1},\dots,\xi_{i_n})$ and $\Psi_j(\boldsymbol{\xi})$. The polynomial basis $\{\Psi_j\}$ of Hermite-chaos forms a complete orthogonal basis, i.e.,

$$\langle \Psi_i \Psi_j \rangle = \langle \Psi_i^2 \rangle \delta_{ij}, \tag{3.4}$$

where δ_{ij} is the Kronecker delta and $\langle \cdot, \cdot \rangle$ denotes the ensemble average. This is the inner product in the Hilbert space determined by the support of the Gaussian variables

$$\langle f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) \rangle = \int f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) W(\boldsymbol{\xi}) d\boldsymbol{\xi}, \tag{3.5}$$

with weighting function

$$W(\boldsymbol{\xi}) = \frac{1}{\sqrt{(2\pi)^n}} e^{-\frac{1}{2}\boldsymbol{\xi}^T \boldsymbol{\xi}}. \tag{3.6}$$

What distinguishes the Hermite-chaos expansion from other possible expansions is that the basis polynomials are Hermite polynomials in terms of Gaussian variables and are orthogonal with respect to the weighting function $W(\boldsymbol{\xi})$, which has the form of an n-dimensional independent Gaussian probability density function.

4. The Wiener–Askey polynomial chaos. The Hermite-chaos expansion has been proved to be effective in solving stochastic differential equations with Gaussian inputs as well as certain types of non-Gaussian inputs [9], [8], [7], [20]; this can be justified by the Cameron–Martin theorem [3]. However, for general non-Gaussian random inputs, the optimal exponential convergence rate will not be realized. In some cases the convergence rate is in fact severely deteriorated.

In order to deal with more general random inputs, we introduce the Wiener–Askey polynomial chaos expansion as a generalization of the original Wiener-chaos expansion. The expansion basis is the complete polynomial basis from the Askey scheme (see section 2.3). As in section 3, we represent the general second-order random process $X(\theta)$ as

$$\begin{aligned} X(\theta) = a_0 I_0 & \\ &+ \sum_{i_1=1}^{\infty} c_{i_1} I_1(\zeta_{i_1}(\theta)) \\ &+ \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} c_{i_1 i_2} I_2(\zeta_{i_1}(\theta), \zeta_{i_2}(\theta)) \\ &+ \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} \sum_{i_3=1}^{i_2} c_{i_1 i_2 i_3} I_3(\zeta_{i_1}(\theta), \zeta_{i_2}(\theta), \zeta_{i_3}(\theta)) \\ &+ \cdots, \end{aligned} \tag{4.1}$$

where $I_n(\zeta_{i_1}, \ldots, \zeta_{i_n})$ denotes the Wiener–Askey polynomial chaos of order n in terms of the random vector $\boldsymbol{\zeta} = (\zeta_{i_1}, \ldots, \zeta_{i_n})$. In the Wiener–Askey chaos expansion, the polynomials I_n are not restricted to Hermite polynomials but rather can be all types of orthogonal polynomials from the Askey scheme in Figure 2.1. Again for notational convenience, we rewrite (4.1) as

$$X(\theta) = \sum_{j=0}^{\infty} \hat{c}_j \Phi_j(\boldsymbol{\zeta}), \tag{4.2}$$

TABLE 4.1
The correspondence of the types of Wiener–Askey polynomial chaos and their underlying random variables ($N \geq 0$ is a finite integer).

	Random variables $\boldsymbol{\zeta}$	Wiener–Askey chaos $\{\Phi(\boldsymbol{\zeta})\}$	Support
Continuous	Gaussian	Hermite-chaos	$(-\infty, \infty)$
	gamma	Laguerre-chaos	$[0, \infty)$
	beta	Jacobi-chaos	$[a, b]$
	uniform	Legendre-chaos	$[a, b]$
Discrete	Poisson	Charlier-chaos	$\{0, 1, 2, \dots\}$
	binomial	Krawtchouk-chaos	$\{0, 1, \dots, N\}$
	negative binomial	Meixner-chaos	$\{0, 1, 2, \dots\}$
	hypergeometric	Hahn-chaos	$\{0, 1, \dots, N\}$

where there is a one-to-one correspondence between the functions $I_n(\zeta_{i_1}, \dots, \zeta_{i_n})$ and $\Phi_j(\boldsymbol{\zeta})$. Since each type of polynomial from the Askey scheme forms a complete basis in the Hilbert space determined by its corresponding support, we can expect each type of Wiener–Askey expansion to converge to any L_2 functional in the L_2 sense in the corresponding Hilbert functional space as a generalized result of the Cameron–Martin theorem (see [3] and [16]). The orthogonality relation of the Wiener–Askey polynomial chaos takes the form

$$\langle \Phi_i \Phi_j \rangle = \langle \Phi_i^2 \rangle \delta_{ij}, \tag{4.3}$$

where δ_{ij} is the Kronecker delta and $\langle \cdot, \cdot \rangle$ denotes the ensemble average, which is the inner product in the Hilbert space of the variables $\boldsymbol{\zeta}$,

$$\langle f(\boldsymbol{\zeta}) g(\boldsymbol{\zeta}) \rangle = \int f(\boldsymbol{\zeta}) g(\boldsymbol{\zeta}) W(\boldsymbol{\zeta}) d\boldsymbol{\zeta} \tag{4.4}$$

or

$$\langle f(\boldsymbol{\zeta}) g(\boldsymbol{\zeta}) \rangle = \sum_{\boldsymbol{\zeta}} f(\boldsymbol{\zeta}) g(\boldsymbol{\zeta}) W(\boldsymbol{\zeta}), \tag{4.5}$$

in the discrete case. Here $W(\boldsymbol{\zeta})$ is the weighting function corresponding to the Wiener–Askey polynomial chaos basis $\{\Phi_i\}$; see the appendix for detailed formulas.

As pointed out in the appendix, some types of orthogonal polynomials from the Askey scheme have weighting functions the same as the probability function of certain types of random distributions. In practice, we then choose the type of independent variables $\boldsymbol{\zeta}$ in the polynomials $\{\Phi_i(\boldsymbol{\zeta})\}$ according to the type of random distribution, as shown in Table 4.1. It is clear that the original Wiener polynomial chaos corresponds to the Hermite-chaos and is a subset of the Wiener–Askey polynomial chaos. The Hermite-, Laguerre-, and Jacobi-chaos are continuous chaos, while Charlier-, Meixner-, Krawtchouk-, and Hahn-chaos are discrete chaos. It is worthy mentioning that the Legendre polynomials, which are a special case of the Jacobi polynomials with parameters $\alpha = \beta = 0$ (section A.1.3), correspond to an important distribution—the *uniform distribution*. Due to the importance of the uniform distribution, we list it separately in the table and term the corresponding chaos expansion as the Legendre-chaos.

5. Applications of Wiener–Askey polynomial chaos. In this section we apply the Wiener–Askey polynomial chaos to solution of stochastic differential equations. We first introduce the general procedure of applying the Wiener–Askey polynomial chaos, and then we solve a specific stochastic ordinary differential equation with different types of random inputs. We demonstrate the convergence rates of Wiener–Askey expansion by comparing the numerical results with the corresponding exact solution.

5.1. General procedure. Let us consider the stochastic differential equation

$$\mathcal{L}(\mathbf{x}, t, \theta; u) = f(\mathbf{x}, t; \theta), \tag{5.1}$$

where $u := u(\mathbf{x}, t; \theta)$ is the solution and $f(\mathbf{x}, t; \theta)$ is the source term. Operator $\mathcal{L}$ generally involves differentiations in space/time and can be nonlinear. Appropriate initial and boundary conditions are assumed. The existence of the random parameter θ is due to the introduction of uncertainty into the system via boundary conditions, initial conditions, material properties, etc. The solution u, which is regarded as a random process, can be expanded by the Wiener–Askey polynomial chaos as

$$u(\mathbf{x}, t; \theta) = \sum_{i=0}^{P} u_i(\mathbf{x}, t)\Phi_i(\boldsymbol{\zeta}(\theta)). \tag{5.2}$$

Note that here the infinite summation has been truncated at the finite term P. The above representation can be considered as a spectral expansion in the random dimension θ, and the random trial basis $\{\Phi_i\}$ is the Askey scheme-based orthogonal polynomials discussed in section 4. The total number of expansion terms is $(P + 1)$ and is determined by the dimension (n) of random variable $\boldsymbol{\zeta}$ and the highest order (p) of the polynomials $\{\Phi_i\}$:

$$(P + 1) = \frac{(n + p)!}{n!p!}. \tag{5.3}$$

Upon substituting (5.2) into the governing equation (5.1), we obtain

$$\mathcal{L}\left(\mathbf{x}, t, \theta; \sum_{i=0}^{P} u_i\Phi_i\right) = f(\mathbf{x}, t; \theta). \tag{5.4}$$

A Galerkin projection of the above equation onto each polynomial basis $\{\Phi_i\}$ is then conducted in order to ensure that the error is orthogonal to the functional space spanned by the finite dimensional basis $\{\Phi_i\}$,

$$\left\langle \mathcal{L}\left(\mathbf{x}, t, \theta; \sum_{i=0}^{P} u_i\Phi_i\right), \Phi_k \right\rangle = \langle f, \Phi_k\rangle, \qquad k = 0, 1, \ldots, P. \tag{5.5}$$

By using the orthogonality of the polynomial basis, we can obtain a set of $(P+1)$ coupled equations for each random mode $u_i(\mathbf{x}, t)$, where $i = \{0, 1, \ldots, P\}$. It should be noted that by utilizing the Wiener–Askey polynomial chaos expansion (5.2), the randomness is effectively transferred into the basis polynomials. Thus, the governing equations for the expansion coefficients u_i resulting from (5.5) are *deterministic*. Discretizations in space $\mathbf{x}$ and time t can be carried out by any conventional deterministic techniques, e.g., Runge–Kutta solvers in time and the spectral/*hp* element method in space for highly accurate solution in complex geometry [13].

5.2. Stochastic ordinary differential equation. We consider the ordinary differential equation

$$\frac{dy(t)}{dt} = -ky, \qquad y(0) = \hat{y}, \tag{5.6}$$

where the decay rate coefficient k is considered to be a random variable $k(\theta)$ with certain distribution and mean value $\bar{k}$. The probability function is $f(k)$ for the continuous case or $f(k_i)$ for the discrete case. The *deterministic* solution is

$$y(t) = y_0 e^{-\bar{k}t}, \tag{5.7}$$

and the *mean* of the *stochastic* solution is

$$\bar{y}(t) = \hat{y} \int_S e^{-kt} f(k) dk \qquad \text{or} \qquad \bar{y}(t) = \hat{y} \sum_i e^{-k_i t} f(k_i), \tag{5.8}$$

corresponding to the continuous and discrete distributions, respectively. The integration and summation are taken within the support defined by the corresponding distribution.

By applying the Wiener–Askey polynomial chaos expansion (4.2) to the solution y and random input k

$$y(t) = \sum_{i=0}^{P} y_i(t)\Phi_i, \qquad k = \sum_{i=0}^{P} k_i \Phi_i \tag{5.9}$$

and substituting the expansions into the governing equation, we obtain

$$\sum_{i=0}^{P} \frac{dy_i(t)}{dt}\Phi_i = -\sum_{i=0}^{P}\sum_{j=0}^{P} \Phi_i \Phi_j k_i y_j(t). \tag{5.10}$$

We then project the above equation onto the random space spanned by the orthogonal polynomial basis $\{\Phi_i\}$ by taking the inner product of the equation with each basis. By taking $\langle ., \Phi_l \rangle$ and utilizing the orthogonality condition (4.3), we obtain the following set of equations:

$$\frac{dy_l(t)}{dt} = -\frac{1}{\langle \Phi_l^2 \rangle} \sum_{i=0}^{P}\sum_{j=0}^{P} e_{ijl} k_i y_j(t), \qquad l = 0, 1, \dots, P, \tag{5.11}$$

where $e_{ijl} = \langle \Phi_i \Phi_j \Phi_l \rangle$. Note that the coefficients are smooth and thus any standard ordinary differential equation solver can be employed here. In the following, the standard second-order Runge–Kutta scheme is used.

5.3. Numerical results. In this section we present numerical results of the stochastic ordinary differential equation by the Wiener–Askey polynomial chaos expansion. For the purpose of benchmarking, we will arbitrarily assume the type of distributions of the decay parameter k and employ the corresponding Wiener–Askey chaos expansion, although in practice there are certainly more favorable assumptions about k depending on the specific physical background. We define the two error measures for the mean and variance of the solution,

$$\varepsilon_{\text{mean}}(t) = \left| \frac{\bar{y}(t) - \bar{y}_{\text{exact}}(t)}{\bar{y}_{\text{exact}}(t)} \right|, \qquad \varepsilon_{\text{var}}(t) = \left| \frac{\sigma(t) - \sigma_{\text{exact}}(t)}{\sigma_{\text{exact}}(t)} \right|, \tag{5.12}$$

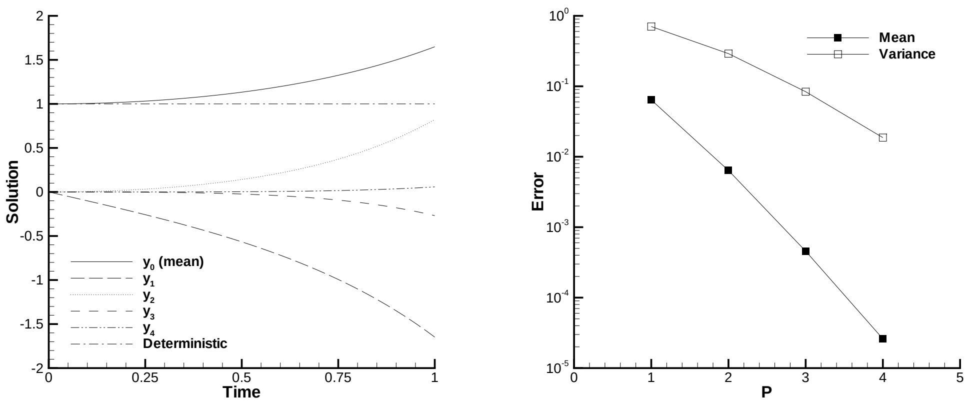

FIG. 5.1. *Solution with Gaussian random input by fourth-order Hermite-chaos. Left: Solution of each random mode; Right: Error convergence of the mean and the variance.*

where $\bar{y}(t) = E[y(t)]$ is the mean value of $y(t)$, and $\sigma(t) = E[(y(t) - \bar{y}(t))^2]$ is the variance of the solution. The initial condition is fixed to be $\hat{y} = 1$, and the integration is performed up to $t = 1$ (nondimensional time units).

5.3.1. Gaussian distribution and Hermite-chaos. In this section k is assumed to be a Gaussian random variable with PDF

$$f(k) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}, \tag{5.13}$$

which has zero mean value ($\bar{k} = 0$) and unit variance ($\sigma_k^2 = 1$). The exact stochastic mean solution is

$$\bar{y}(t) = \hat{y} e^{t^2/2}. \tag{5.14}$$

The Hermite-chaos from the Wiener–Askey polynomial chaos family is employed as a natural choice due to the fact that the random input is Gaussian. Figure 5.1 shows the solution by the Hermite-chaos expansion. The convergence of errors of the mean and variance as the number of expansion terms increases is shown on a semilog plot, and it is seen that the *exponential* convergence rate is achieved. It is also noticed that the *deterministic* solution remains constant as the mean value of k is zero; however, the mean of the stochastic solution (random mode with index 0, y_0) is nonzero and grows with time.

5.3.2. Gamma distribution and Laguerre-chaos. In this section we assume that the distribution of the decay parameter k is the gamma distribution with PDF of the form

$$f(k) = \frac{e^{-k} k^{\alpha}}{\Gamma(\alpha + 1)}, \qquad 0 \le k < \infty, \ \alpha > -1. \tag{5.15}$$

The mean and variance of k are $\mu_k = \bar{k} = \alpha + 1$ and $\sigma_k^2 = \alpha + 1$, respectively. The mean of the stochastic solution is

$$\bar{y}(t) = \hat{y} \frac{1}{(1 + t)^{\alpha+1}}. \tag{5.16}$$

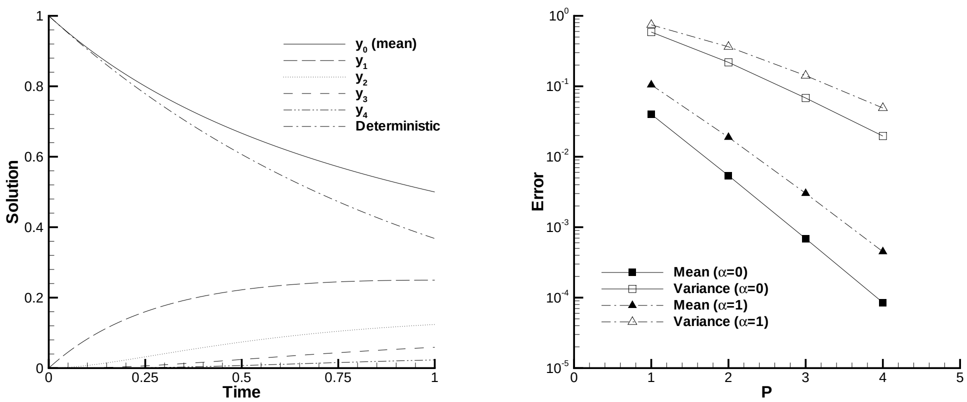

FIG. 5.2. *Solution with gamma random input by fourth-order Laguerre-chaos. Left: Solution of each mode ($\alpha = 0$: exponential distribution); Right: Error convergence of the mean and the variance with different α.*

The special case of $\alpha = 0$ corresponds to another important distribution: the *exponential* distribution. Because the random input has a gamma distribution, we employ the Laguerre-chaos as the specific Wiener–Askey chaos (see Table 4.1). Figure 5.2 shows the evolution of each solution mode over time, together with the convergence of the errors of the mean and the variance with different values of parameter α. The special case of exponential distribution ($\alpha = 0$) is included. Again the mean of the stochastic solution and deterministic solution show significant difference. As α becomes larger, the spread of the gamma distribution is larger, and this leads to larger errors with fixed number of Laguerre-chaos expansion. However, the exponential convergence rate is still realized.

5.3.3. Beta distribution and Jacobi-chaos. We now assume the distribution of the random variable k to be the beta distribution with PDF of the form

$$f(k; \alpha, \beta) = \frac{(1-k)^\alpha (1+k)^\beta}{2^{\alpha+\beta+1} B(\alpha+1, \beta+1)}, \qquad -1 < k < 1, \ \alpha, \beta > -1, \tag{5.17}$$

where $B(\alpha, \beta)$ is the beta function defined as $B(p, q) = \Gamma(p)\Gamma(q)/\Gamma(p+q)$. We then employ the Jacobi-chaos expansion, which has the weighting function in the form of the beta distribution. An important special case is $\alpha = \beta = 0$, in which the distribution becomes the uniform distribution and the corresponding Jacobi-chaos becomes the Legendre-chaos.

Figure 5.3 shows the solution by the Jacobi-chaos. On the left is the evolution of all random modes of the Legendre-chaos ($\alpha = \beta = 0$) with uniformly distributed random input. In this case, k has zero mean value and the deterministic solution remains constant, but the mean of the stochastic solution grows over time. The convergence of errors of the mean and the variance of the solution with respect to the order of Jacobi-chaos expansion is shown on the semilog scale, and the exponential convergence rate is obtained with different sets of parameter values α and β.

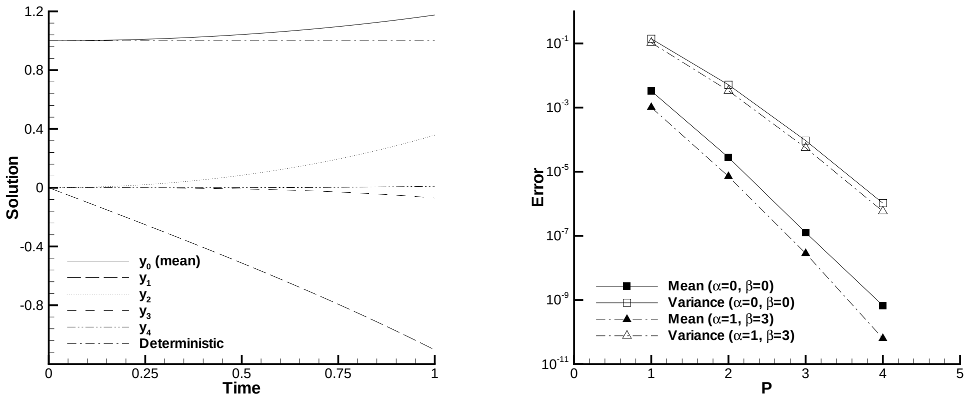

FIG. 5.3. *Solution with beta random input by fourth-order Jacobi-chaos. Left: Solution of each mode ($\alpha = \beta = 0$: Legendre-chaos); Right: Error convergence of the mean and the variance with different α and β.*

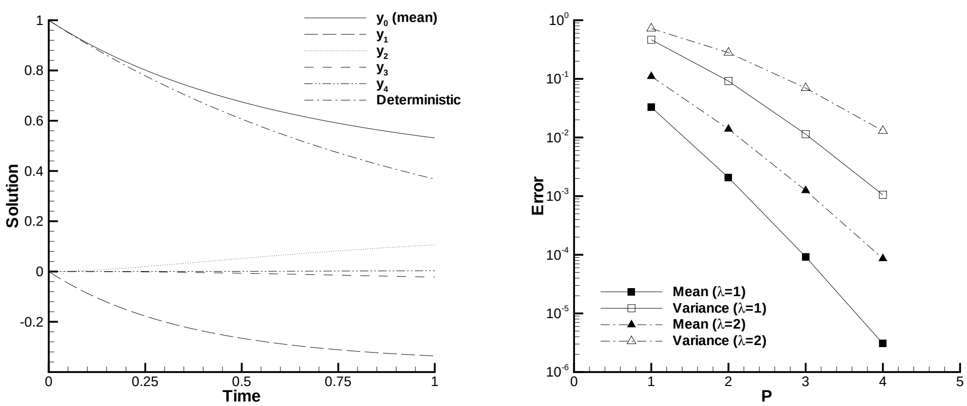

FIG. 5.4. *Solution with Poisson random input by fourth-order Charlier-chaos. Left: Solution of each mode ($\lambda = 1$); Right: Error convergence of the mean and the variance with different λ.*

5.3.4. Poisson distribution and Charlier-chaos. We now assume the distribution of the decay parameter k to be Poisson of the form

$$f(k;\lambda) = e^{-\lambda}\frac{\lambda^k}{k!}, \qquad k = 0, 1, 2, \dots,\ \lambda > 0. \tag{5.18}$$

The mean and variance of k are $\mu_k = \bar{k} = \lambda$ and $\sigma_k^2 = \lambda$, respectively. The analytic solution of the mean stochastic solution is

$$\bar{y}(t) = \hat{y}e^{-\lambda + \lambda e^{-t}}. \tag{5.19}$$

The Charlier-chaos expansion is employed to represent the solution process, and the results with a fourth-order expansion are shown in Figure 5.4. Once again we see the

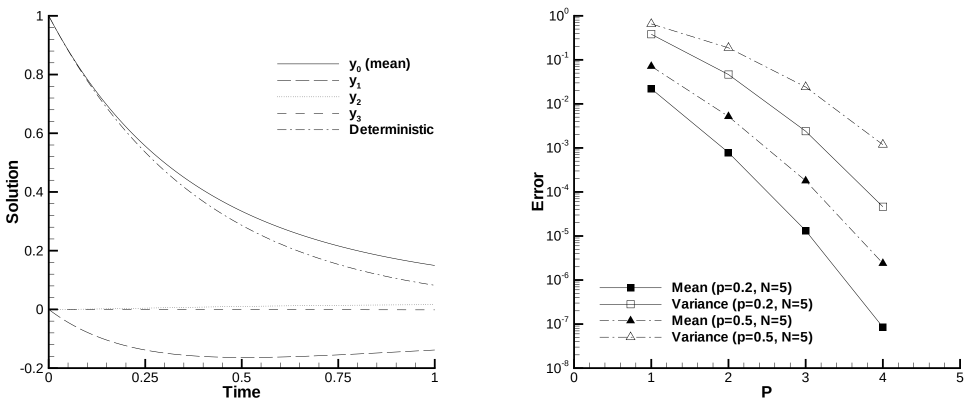

FIG. 5.5. *Solution with binomial random input by fourth-order Krawtchouk-chaos. Left: Solution of each mode ($p = 0.5$, $N = 5$); Right: Error convergence of the mean and the variance with different p and N.*

noticeable difference between the deterministic solution and the mean of the stochastic solution. An exponential convergence rate is obtained for different values of the parameter λ.

5.3.5. Binomial distribution and Krawtchouk-chaos. In this section the distribution of the random input k is assumed to be binomial:

$$f(k; p, N) = \binom{N}{k} p^k (1-p)^{N-k}, \qquad 0 \le p \le 1,\ k = 0, 1, \ldots, N. \tag{5.20}$$

The exact mean solution of (5.6) is

$$\bar{y}(t) = \hat{y} \left[1 - \left(1 - e^{-t}\right) p\right]^N. \tag{5.21}$$

Figure 5.5 shows the solution with fourth-order Krawtchouk-chaos. With different parameter sets, Krawtchouk-chaos expansion correctly approximates the exact solution, and the convergence rate with respect to the order of expansion is exponential.

5.3.6. Negative binomial distribution and Meixner-chaos. In this section we assume that the distribution of the random input of k is the negative binomial distribution

$$f(k; \beta, c) = \frac{(\beta)_k}{k!} (1-c)^\beta c^k, \qquad 0 \le c \le 1,\ \beta > 0,\ k = 0, 1, \ldots. \tag{5.22}$$

In case of β being integer, this is often called the Pascal distribution. The exact mean solution of (5.6) is

$$\bar{y}(t) = \hat{y} \left(\frac{1 - ce^{-t}}{1 - c}\right)^{-\beta}. \tag{5.23}$$

The Meixner-chaos is chosen since the random input is negative binomial (see Table 4.1). Figure 5.6 shows the solution with fourth-order Meixner-chaos. Exponential convergence rate is observed by the Meixner-chaos approximation with different sets of parameter values.

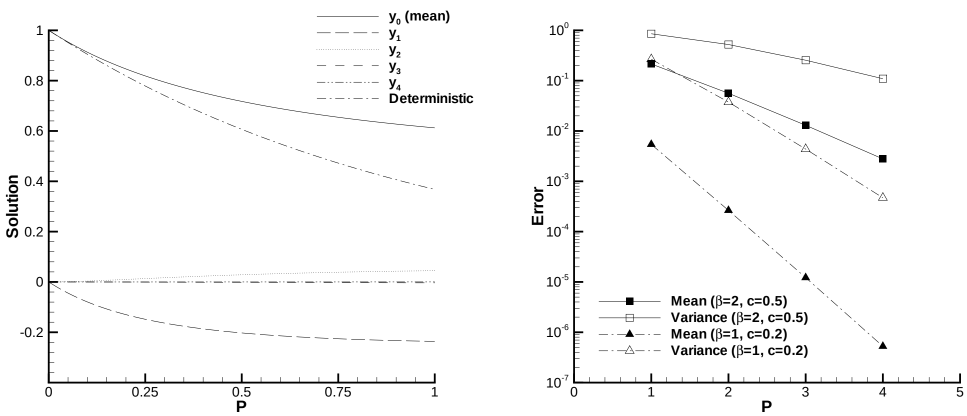

FIG. 5.6. *Solution with negative binomial random input by fourth-order Meixner-chaos. Left: Solution of each mode ($\beta = 1$, $c = 0.5$); Right: Error convergence of the mean and the variance with different β and c.*

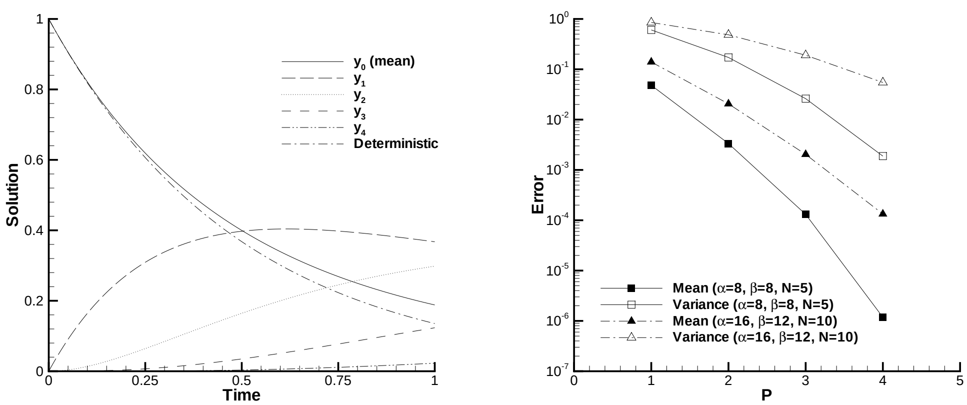

FIG. 5.7. *Solution with hypergeometric random input by fourth-order Hahn-chaos. Left: Solution of each mode ($\alpha = \beta = 5$, $N = 4$); Right: Error convergence of the mean and the variance with different α, β, and N.*

5.3.7. Hypergeometric distribution and Hahn-chaos. We now assume that the distribution of the random input k is hypergeometric:

$$f(k;\alpha,\beta,N) = \frac{\binom{\alpha}{k}\binom{\beta}{N-k}}{\binom{\alpha+\beta}{N}}, \qquad k = 0, 1, \dots, N, \ \alpha, \beta > N. \tag{5.24}$$

In this case, the optimal Wiener–Askey polynomial chaos is the Hahn-chaos (Table 4.1). Figure 5.7 shows the solution by fourth-order Hahn-chaos. It can be seen from the semilog plot of the errors of the mean and variance of the solution that an exponential convergence rate is obtained with respect to the order of Hahn-chaos expansion for different sets of parameter values.

TABLE 5.1
Error convergence of the mean solution by Monte Carlo simulation: N is the number of realizations and $\varepsilon_{\text{mean}}$ is the error of mean solution defined in (5.12)*; random input has exponential distribution.*

N	1×10^2	1×10^3	1×10^4	1×10^5
$\varepsilon_{\text{mean}}$	4.0×10^{-2}	1.1×10^{-2}	5.1×10^{-3}	6.5×10^{-4}

5.4. Efficiency of Wiener–Askey chaos expansion. We have demonstrated the exponential convergence of the Wiener–Askey polynomial chaos expansion. From the results above, we notice that it normally takes an expansion order $P = 2 \sim 4$ for the error of the mean solution to reach the order of $O(10^{-3})$. Equation (5.11) shows that the Wiener–Askey chaos expansion with highest order of P results in a set of $(P + 1)$ coupled ordinary differential equations. Thus, the computational cost is slightly more than $(P + 1)$ times that of a single realization of the deterministic integration. On the other hand, if the Monte Carlo simulation is used, it normally requires $O(10^4) \sim O(10^5)$ realizations to reduce the error of the *mean* solution to $O(10^{-3})$. For example, if k is an exponentially distributed random variable, the error convergence of the mean solution of the Monte Carlo simulation is shown in Table 5.1.

Monte Carlo simulations with other types of random inputs as discussed in this paper have also been conducted and the results are similar. The actual numerical values of the errors with a given number of realizations may vary depending on the property of the random number generators used, but the order of magnitude should be the same. Techniques such as variance reduction are not used. Although such techniques, if applicable, can speed up Monte Carlo simulation by an order or more, depending on the specific problem, the advantage of Wiener–Askey polynomial chaos expansion is obvious. For the ordinary differential equation discussed in this paper, speed-up of order $O(10^3) \sim O(10^4)$ compared with straight Monte Carlo simulations can be expected. However, for more complicated problems where there exist multidimensional random inputs, the multidimensional Wiener–Askey chaos is needed. The total number of expansion terms increases quickly for large dimensional problems (see (5.3)). Thus the efficiency of the chaos expansion will be reduced.

6. Representation of arbitrary random inputs. As demonstrated above, with appropriately chosen Wiener–Askey polynomial chaos expansion according to the type of the random input, optimal exponential convergence rate of the chaos expansion can be realized. In practice, we often encounter distributions of random inputs not belonging to the basic types of distributions listed in Table 4.1, or even when they do belong to certain basic types, the correspondence may not be explicitly known. In such cases, we need to project the input process onto the Wiener–Askey polynomial chaos basis directly in order to solve the differential equation.

Let us assume in the stochastic ordinary differential equation of (5.6) that the distribution of the decay parameter k is known in the form of probability function $f(k)$. The representation of k by the Wiener–Askey polynomial chaos expansion takes the form

$$k = \sum_{i=0}^{P} k_i \Phi_i, \qquad k_i = \frac{\langle k \Phi_i \rangle}{\langle \Phi_i^2 \rangle}, \tag{6.1}$$

where the operation $\langle \cdot, \cdot \rangle$ denotes the inner product in the Hilbert space spanned by the Wiener–Askey chaos basis $\{\Phi_i\}$, i.e.,

$$k_i = \frac{1}{\langle\Phi_i^2\rangle}\int k\Phi_i(\zeta)g(\zeta)d\zeta \qquad \text{or} \qquad k_i = \frac{1}{\langle\Phi_i^2\rangle}\sum_j k\Phi_i(\zeta_j)g(\zeta_j), \tag{6.2}$$

where $g(x)$ and $g(x_i)$ are the probability functions of the random variable ζ in the Wiener–Askey polynomial chaos for continuous and discrete cases, respectively. The underlying assumption here is that the random variable ζ is fully dependent on the target random variable k. We notice that the above equations are mathematically *meaningless* due to the fact that the support of k and ζ are likely to be different. In other words, the random variables k and ζ could belong to two different probability spaces $(\Omega, \mathcal{A}, P)$ with different event space Ω, σ-algebra $\mathcal{A}$ and probability measure P.

6.1. Analytical approach. In order to conduct the above projection, we need to transform the fully correlated random variables k and ζ to the same probability space. Under the theory of probability, this is always possible. In practice, it is convenient to transform them to the uniformly distributed probability space $u \in U(0,1)$. In fact, the inverse procedure is an important technique for random number generation, where one first generates the uniformly distributed numbers as the seeds and then performs the inverse transformation according to the desired distribution function. Without loss of generality, we discuss in detail the case in which k and ζ are continuous random variables.

Let us assume that the random variable u is uniformly distributed in $(0,1)$ and the PDFs for k and ζ are $f(k)$ and $g(\zeta)$, respectively. A transformation of variables in probability space shows that

$$du = f(k)dk = dF(k), \qquad du = g(\zeta)d\zeta = dG(\zeta), \tag{6.3}$$

where F and G are the distribution function of k and ζ, respectively,

$$F(k) = \int_{-\infty}^{k} f(t)dt, \qquad G(\zeta) = \int_{-\infty}^{\zeta} g(t)dt. \tag{6.4}$$

If we require the random variables k and ζ to be transformed to the *same* uniformly distributed random variable u, we obtain

$$u = F(k) = G(\zeta). \tag{6.5}$$

After inverting the above equations, we obtain

$$k = F^{-1}(u) \equiv h(u), \qquad \zeta = G^{-1}(u) \equiv l(u). \tag{6.6}$$

Now that we have effectively transformed the two different random variables k and ζ to the same probability space defined by $u \in U(0,1)$, the projection (6.2) can be performed, i.e.,

$$\begin{aligned} k_i &= \frac{1}{\langle\Phi_i^2\rangle}\int k\Phi_i(\zeta)g(\zeta)d\zeta \\ &= \frac{1}{\langle\Phi_i^2\rangle}\int_0^1 h(u)\Phi_i(l(u))du. \end{aligned} \tag{6.7}$$

In general, the above integral cannot be integrated analytically. However, it can be efficiently evaluated with the Gauss quadrature in the closed domain $[0,1]$ with sufficient accuracy. The analytical forms of the inversion relations (6.6) are known for some basic distributions: Gaussian, exponential, beta, etc. (see [6]).

The above procedure works equally well for the discrete distributions, where the inversion procedure is slightly modified and the integral in (6.7) is replaced by summation.

6.2. Numerical approach. The procedure described above requires that the distribution functions $F(k)$ and $G(\zeta)$ be known and the inverse functions F^{-1} and G^{-1} exist and be known as well. In practice, these conditions are not always satisfied. Often we know only the probability function $f(k)$ for a specific problem. The probability function $g(\zeta)$ is known from the choice of Wiener–Askey polynomial chaos, but the inversion is not always known either. In this case, we can perform the projection (6.2) directly by Monte Carlo integration, where a large ensemble of random numbers k and ζ are generated. The requirement that k and ζ be transformed to the same probability space $u \in U(0,1)$ by (6.5) implies that each pair of k and ζ has to be generated from the *same* seed of uniformly generated random number $u \in U(0,1)$.

6.3. Results. In this section we present numerical examples of representing an arbitrarily given random distribution. More specifically, we present results of using Hermite-chaos expansion for some non-Gaussian random variables. Although in theory, Hermite-chaos converges and it has been successfully applied to some non-Gaussian processes [8], [20], we demonstrate numerically that an optimal exponential convergence rate is not realized.

6.3.1. Approximation of gamma distribution by Hermite-chaos. Let us assume that the decay parameter k in the ordinary differential equation (5.6) is a random variable with gamma distribution (5.15). We consider the specific case of $\alpha = 0$. In this case k is a random variable with exponential distribution and with PDF of the form

$$f(k) = e^{-k}, \qquad k > 0. \tag{6.8}$$

The inverse of its distribution function $F(k)$ (equation (6.6)) is known as

$$h(u) \equiv F^{-1}(u) = -\ln(1-u), \qquad u \in U(0,1). \tag{6.9}$$

We then use Hermite-chaos to represent k instead of the optimal Laguerre-chaos. The random variable ζ in (6.7) is a standard Gaussian variable with PDF $g(\zeta) = (1/\sqrt{2\pi})e^{-\zeta^2/2}$. The inverse of the Gaussian distribution $G(\zeta)$ is known as

$$l(u) \equiv G^{-1}(u) = sign\left(u - \frac{1}{2}\right)\left(t - \frac{c_0 + c_1 t + c_2 t^2}{1 + d_1 t + d_2 t^2 + d_3 t^3}\right), \tag{6.10}$$

where

$$t = \sqrt{-\ln\left[\min(u, 1-u)\right]^2}$$

and

$$\begin{aligned} c_0 &= 2.515517, \quad c_1 = 0.802853, \quad c_2 = 0.010328, \\ d_1 &= 1.432788, \quad d_2 = 0.189269, \quad d_3 = 0.001308. \end{aligned}$$

The formula is from Hastings [10], and the numeric values of the constants have absolute error less than 4.5×10^{-4} (also see [6]).

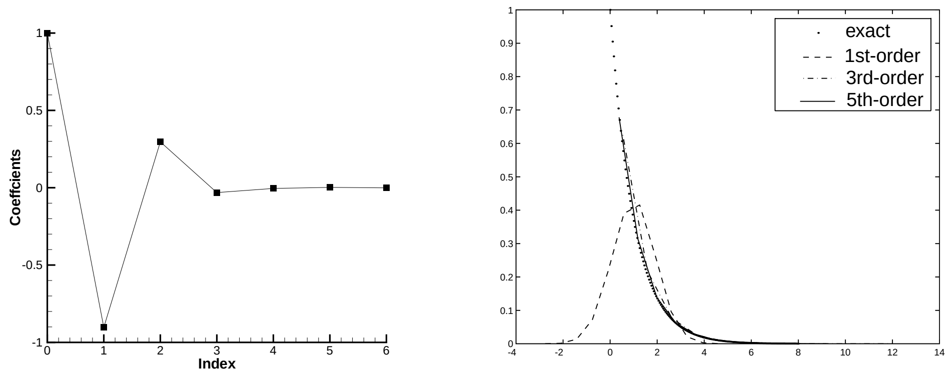

FIG. 6.1. *Approximation of exponential distribution with Hermite-chaos. Left: The expansion coefficients; Right: The PDF of different orders of approximations.*

In Figure 6.1 we show the result of the approximation of the exponential distribution by the Hermite-chaos. The expansion coefficients k_i are shown on the left, and we see that the major contributions of the Hermite-chaos approximation are from the first three terms. The PDFs of different orders of the approximations are shown on the right, together with the exact PDF of the exponential distribution. We notice that the third-order approximation gives fairly good results, and fifth-order Hermite-chaos is very close to the exact distribution. The Hermite-chaos does not approximate the PDF well at $x \sim 0$, where the PDF reaches its peak at 1. In order to capture this rather sharp region, more Hermite-chaos terms are needed.

The above result is the representation of the random input k for the ordinary differential equation of (5.6). If the optimal Wiener–Askey chaos is chosen, in this case the Laguerre-chaos, only one term is needed to represent k *exactly*. We can expect that if the Hermite-chaos is used to solve the differential equation in this case, the solution would not retain the exponential convergence as realized by the Laguerre-chaos.

In Figure 6.2 the errors of the mean solution defined by (5.12) with Laguerre-chaos and Hermite-chaos to the ordinary differential equation of (5.6) are shown. The random input of k has exponential distribution, which implies that the Laguerre-chaos is the optimal Wiener–Askey polynomial chaos. It is seen from the result that the exponential convergence rate is not obtained by the Hermite-chaos as opposed to the Laguerre-chaos.

6.3.2. Approximation of beta distribution by Hermite-chaos. We now assume that the distribution of k is a beta distribution; see (5.17). We return to the more conventional definition of beta distribution in the domain $[0, 1]$:

$$f(k) = \frac{1}{B(\alpha+1, \beta+1)} k^{\alpha}(1-k)^{\beta}, \qquad \alpha, \beta > -1,\ 0 \le k \le 1. \tag{6.11}$$

Figure 6.3 shows the PDF of first-, third-, and fifth-order Hermite-chaos approximations to the beta random variable. The special case of $\alpha = \beta = 0$ is the important uniform distribution. It can be seen that the Hermite-chaos approximation converges to the exact solution as the number of expansion terms increases. Oscillations are observed near the corners of the square. This is in analogy with the Gibb's phenomenon,

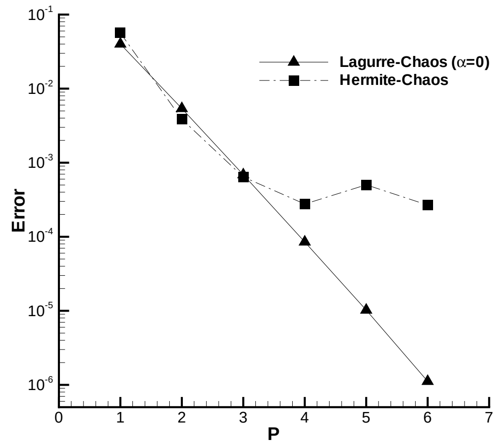

FIG. 6.2. *Error convergence of the mean solution of the Laguerre-chaos and Hermite-chaos to a stochastic ordinary differential equation with random input of the exponential distribution.*

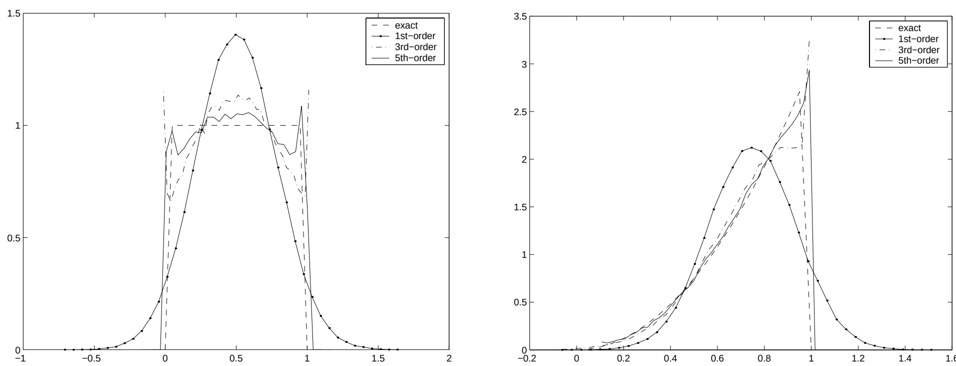

FIG. 6.3. *PDF of approximations of beta distributions by Hermite-chaos. Left:* $\alpha = \beta = 0$*, the uniform distribution; Right:* $\alpha = 2$*,* $\beta = 0$*.*

which occurs when Fourier expansions are used to approximate functions with sharp corners. Since all Wiener–Askey polynomial chaos expansions can be considered as spectral expansions in the random dimension, the oscillations here can be regarded as *stochastic Gibb's phenomena*. For uniform distribution, Hermite-chaos does not work very well due to the stochastic Gibb's phenomenon even when more higher-order terms are added. On the other hand, the first-order Jacobi-chaos expansion is already *exact*. In addition to the exponential convergence, the proper Wiener–Askey basis leads to dramatic lowering of the dimensionality of the problem.

7. Conclusion. We have proposed a Wiener–Askey polynomial chaos expansion to represent stochastic processes and further model the uncertainty in practical applications. The Wiener–Askey polynomial chaos can be regarded as the generalization of the homogeneous chaos first proposed by Wiener in 1938 [19]. The original Wiener expansion employs the Hermite polynomials in terms of Gaussian random variables. In the Wiener–Askey chaos expansion, the basis polynomials are those from the Askey scheme of hypergeometric orthogonal polynomials, and the underlying variables are random variables chosen according to the weighting function of the polynomials. We give a general guideline of choosing the optimal Wiener–Askey polynomial chaos according to the random inputs. By solving a stochastic ordinary differential equation, we demonstrate numerically that the Wiener–Askey polynomial chaos exhibits an exponential convergence rate. For any given type of random input, the Wiener–Askey polynomial chaos converges in general, although the exponential rate is not retained if the optimal chaos is not chosen. The Wiener–Askey polynomial chaos proposed in the present paper can deal with general random inputs more effectively than the original Wiener–Hermite chaos. It can be extended to more complex stochastic systems governed by partial differential equations without any fundamental difficulties.

Appendix A. Some important orthogonal polynomials in the Askey scheme. In this section we briefly review the definitions and properties of some important orthogonal polynomials from the Askey scheme, which are discussed in this paper for Wiener–Askey polynomial chaos.

A.1. Continuous polynomials.

A.1.1. Hermite polynomial $H_n(x)$ and Gaussian distribution.

Definition:

$$H_n(x) = (2x)^n \, {}_2F_0\left(-\frac{n}{2}, -\frac{n-1}{2};\ ; -\frac{1}{x^2}\right). \tag{A.1}$$

Orthogonality:

$$\frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x) dx = 2^n n! \delta_{mn}. \tag{A.2}$$

Recurrence relation:

$$H_{n+1}(x) - 2xH_n(x) + 2nH_{n-1}(x) = 0. \tag{A.3}$$

Rodriguez formula:

$$e^{-x^2} H_n(x) = (-1)^n \frac{d^n}{dx^n}\left(e^{-x^2}\right). \tag{A.4}$$

The weighting function is $w(x) = e^{-x^2}$ from the orthogonality condition (A.2). After rescaling x by $\sqrt{2}$, the weighting function is the same as the PDF of a standard *Gaussian* random variable with zero mean and unit variance.

A.1.2. Laguerre polynomial $L_n^{(\alpha)}(x)$ and gamma distribution.

Definition:

$$L_n^{(\alpha)}(x) = \frac{(\alpha+1)_n}{n!} \, {}_1F_1(-n; \alpha+1; x). \tag{A.5}$$

Orthogonality:

$$\int_0^{\infty} e^{-x} x^{\alpha} L_m^{(\alpha)}(x) L_n^{(\alpha)}(x) dx = \frac{\Gamma(n+\alpha+1)}{n!}\delta_{mn}, \qquad \alpha > -1. \tag{A.6}$$

Recurrence relation:

$$(n+1)L_{n+1}^{(\alpha)}(x) - (2n+\alpha+1-x)L_n^{(\alpha)}(x) + (n+\alpha)L_{n-1}^{(\alpha)}(x) = 0. \tag{A.7}$$

Rodriguez formula:

$$e^{-x}x^{\alpha}L_n^{(\alpha)}(x) = \frac{1}{n!}\frac{d^n}{dx^n}\left(e^{-x}x^{n+\alpha}\right). \tag{A.8}$$

Recall that the *gamma* distribution has the PDF

$$f(x) = \frac{x^{\alpha}e^{-x/\beta}}{\beta^{\alpha+1}\Gamma(\alpha+1)}, \qquad \alpha > -1,\ \beta > 0. \tag{A.9}$$

Despite the scale parameter β and a constant factor $\Gamma(\alpha+1)$, this is the same as the weighting function of the Laguerre polynomial.

A.1.3. Jacobi polynomial $P_n^{(\alpha,\beta)}(x)$ and beta distribution.

Definition:

$$P_n^{(\alpha,\beta)}(x) = \frac{(\alpha+1)_n}{n!}\ {}_2F_1\left(-n, n+\alpha+\beta+1; \alpha+1; \frac{1-x}{2}\right). \tag{A.10}$$

Orthogonality:

$$\int_{-1}^{1}(1-x)^{\alpha}(1+x)^{\beta}P_m^{(\alpha,\beta)}(x)P_n^{(\alpha,\beta)}(x)dx = h_n^2\delta_{mn}, \qquad \alpha > -1,\ \beta > -1, \tag{A.11}$$

where

$$h_n^2 = \frac{2^{\alpha+\beta+1}}{2n+\alpha+\beta+1}\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{\Gamma(n+\alpha+\beta+1)n!}.$$

Recurrence relation:

$$\begin{aligned} xP_n^{(\alpha,\beta)}(x) &= \frac{2(n+1)(n+\alpha+\beta+1)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)}P_{n+1}^{(\alpha,\beta)}(x) \\ &+ \frac{\beta^2-\alpha^2}{(2n+\alpha+\beta)(2n+\alpha+\beta+2)}P_n^{(\alpha,\beta)}(x) \\ &+ \frac{2(n+\alpha)(n+\beta)}{(2n+\alpha+\beta)(2n+\alpha+\beta+1)}P_{n-1}^{(\alpha,\beta)}(x). \end{aligned} \tag{A.12}$$

Rodriguez formula:

$$(1-x)^{\alpha}(1+x)^{\beta}P_n^{(\alpha,\beta)}(x) = \frac{(-1)^n}{2^n n!}\frac{d^n}{dx^n}\left[(1-x)^{n+\alpha}(1+x)^{n+\beta}\right]. \tag{A.13}$$

The *beta* distribution has the PDF

$$f(x) = \frac{(x-a)^{\beta}(b-x)^{\alpha}}{(b-a)^{\alpha+\beta+1}B(\alpha+1,\beta+1)}, \qquad a \le x \le b, \tag{A.14}$$

where $B(p,q)$ is the *beta function* defined as

$$B(p,q) = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)}. \tag{A.15}$$

It is clear that despite the constant factor, the weighting function of the Jacobi polynomial $w(x) = (1-x)^{\alpha}(1+x)^{\beta}$ from (A.11) is the same as the PDF of the beta distribution defined in domain $[-1,1]$. When $\alpha = \beta = 0$, the Jacobi polynomials become the Legendre polynomials, and the weighting function is a constant which corresponds to the important *uniform distribution*.

A.2. Discrete polynomials.

A.2.1. Charlier polynomial $C_n(x;a)$ and Poisson distribution.
Definition:

$$C_n(x;a) = {}_2F_0\left(-n, -x; \ ; -\frac{1}{a}\right). \tag{A.16}$$

Orthogonality:

$$\sum_{x=0}^{\infty} \frac{a^x}{x!} C_m(x;a) C_n(x;a) = a^{-n} e^a n! \delta_{mn}, \qquad a > 0. \tag{A.17}$$

Recurrence relation:

$$-xC_n(x;a) = aC_{n+1}(x;a) - (n+a)C_n(x;a) + nC_{n-1}(x;a). \tag{A.18}$$

Rodriguez formula:

$$\frac{a^x}{x!} C_n(x;a) = \nabla^n \left(\frac{a^x}{x!}\right), \tag{A.19}$$

where ∇ is the backward difference operator (2.12).

The probability function of the *Poisson* distribution is

$$f(x;a) = e^{-a} \frac{a^x}{x!}, \qquad k = 0, 1, 2, \ldots. \tag{A.20}$$

Despite the constant factor e^{-a}, this is the same as the weighting function of Charlier polynomials.

A.2.2. Krawtchouk polynomial $K_n(x;p,N)$ and binomial distribution.
Definition:

$$K_n(x;p,N) = {}_2F_1\left(-n, -x; -N; \frac{1}{p}\right), \quad n = 0, 1, \ldots, N. \tag{A.21}$$

Orthogonality:

$$\sum_{x=0}^{N} \binom{N}{x} p^x (1-p)^{N-x} K_m(x;p,N) K_n(x;p,N) = \frac{(-1)^n n!}{(-N)_n} \left(\frac{1-p}{p}\right)^n \delta_{mn}, \tag{A.22}$$
$$0 < p < 1.$$

Recurrence relation:

$$\begin{aligned} -xK(x;p,N) &= p(N-n)K_{n+1}(x;p,N) - [p(N-n) + n(1-p)]K_n(x;p,N) \\ &\quad + n(1-p)K_{n-1}(x;p,N). \end{aligned} \tag{A.23}$$

Rodriguez formula:

$$\binom{N}{x} \left(\frac{p}{1-p}\right)^x K_n(x;p,N) = \nabla^n \left[\binom{N-n}{x} \left(\frac{p}{1-p}\right)^x\right]. \tag{A.24}$$

Clearly, the weighting function from (A.22) is the probability function of the *binomial* distribution.

A.2.3. Meixner polynomial $M_n(x;\beta,c)$ and negative binomial distribution.

Definition:

$$M_n(x;\beta,c) = {}_2F_1\left(-n,-x;\beta;1-\frac{1}{c}\right). \tag{A.25}$$

Orthogonality:

$$\sum_{x=0}^{\infty}\frac{(\beta)_x}{x!}c^x M_m(x;\beta,c)M_n(x;\beta,c) = \frac{c^{-n}n!}{(\beta)_n(1-c)^\beta}\delta_{mn}, \qquad \beta>0,\ 0<c<1. \tag{A.26}$$

Recurrence relation:

$$\begin{aligned}(c-1)xM_n(x;\beta,c) &= c(n+\beta)M_{n+1}(x;\beta,c) - [n+(n+\beta)c]M_n(x;\beta,c)\\ &\quad + nM_{n-1}(x;\beta,c).\end{aligned} \tag{A.27}$$

Rodriguez formula:

$$\frac{(\beta)_x c^x}{x!}M_n(x;\beta,c) = \nabla^n\left[\frac{(\beta+n)_x c^x}{x!}\right]. \tag{A.28}$$

The weighting function is

$$f(x) = \frac{(\beta)_x}{x!}(1-c)^\beta c^x, \qquad 0<p<1, \quad \beta>0, \quad x=0,1,2,\dots. \tag{A.29}$$

It can verified that it is the probability function of a *negative binomial* distribution. In the case in which β is an integer, it is often called the *Pascal* distribution.

A.2.4. Hahn polynomial $Q_n(x;\alpha,\beta,N)$ and hypergeometric distribution.

Definition:

$$Q_n(x;\alpha,\beta,N) = {}_3F_2(-n,n+\alpha+\beta+1,-x;\alpha+1,-N;1), \qquad n=0,1,\dots,N. \tag{A.30}$$

Orthogonality: For $\alpha>-1$ and $\beta>-1$ or for $\alpha<-N$ and $\beta<-N$,

$$\sum_{x=0}^{N}\binom{\alpha+x}{x}\binom{\beta+N-x}{N-x}Q_m(x;\alpha,\beta,N)Q_n(x;\alpha,\beta,N) = h_n^2\delta_{mn}, \tag{A.31}$$

where

$$h_n^2 = \frac{(-1)^n(n+\alpha+\beta+1)_{N+1}(\beta+1)_n n!}{(2n+\alpha+\beta+1)(\alpha+1)_n(-N)_n N!}.$$

Recurrence relation:

$$-xQ_n(x) = A_nQ_{n+1}(x) - (A_n+C_n)Q_n(x) + C_nQ_{n-1}(x), \tag{A.32}$$

where

$$Q_n(x) := Q_n(x;\alpha,\beta,N)$$

and

$$\begin{cases} A_n = \dfrac{(n+\alpha+\beta+1)(n+\alpha+1)(N-n)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)}, \\ C_n = \dfrac{n(n+\alpha+\beta+N+1)(n+\beta)}{(2n+\alpha+\beta)(2n+\alpha+\beta+1)}. \end{cases}$$

Rodriguez formula:

$$w(x;\alpha,\beta,N)Q_n(x;\alpha,\beta,N) = \frac{(-1)^n(\beta+1)_n}{(-N)_n}\nabla^n[w(x;\alpha+n,\beta+n,N-n)], \tag{A.33}$$

where

$$w(x;\alpha,\beta,N) = \binom{\alpha+x}{x}\binom{\beta+N-x}{N-x}.$$

If we set $\alpha = -\tilde{\alpha}-1$ and $\beta = -\tilde{\beta}-1$, we obtain

$$\tilde{w}(x) = \frac{1}{\binom{N-\tilde{\alpha}-\tilde{\beta}-1}{N}} \frac{\binom{\tilde{\alpha}}{x}\binom{\tilde{\beta}}{N-x}}{\binom{\tilde{\alpha}+\tilde{\beta}}{N}}.$$

Apart from the constant factor $1/\binom{N-\tilde{\alpha}-\tilde{\beta}-1}{N}$, this is the definition of a *hypergeometric* distribution.

REFERENCES

[1] R. Askey and J. Wilson, *Some Basic Hypergeometric Polynomials that Generalize Jacobi Polynomials*, Mem. Amer. Math. Soc. 319, AMS, Providence, RI, 1985.

[2] P. Beckmann, *Orthogonal Polynomials for Engineers and Physicists*, Golem Press, Boulder, CO, 1973.

[3] R. Cameron and W. Martin, *The orthogonal development of nonlinear functionals in series of Fourier-Hermite functionals*, Ann. of Math. (2), 48 (1947), pp. 385–392.

[4] T. Chihara, *An Introduction to Orthogonal Polynomials*, Gordon and Breach, New York, 1978.

[5] D. Engel, *The Multiple Stochastic Integral*, Mem. Amer. Math. Soc. 265, AMS, Providence, RI, 1982.

[6] G. Fishman, *Monte Carlo: Concepts, Algorithms, and Applications*, Springer-Verlag, New York, 1996.

[7] R. Ghanem, *Ingredients for a general purpose stochastic finite element formulation*, Comput. Methods Appl. Mech. Engrg., 168 (1999), pp. 19–34.

[8] R. Ghanem, *Stochastic finite elements for heterogeneous media with multiple random non-Gaussian properties*, ASCE J. Eng. Mech., 125 (1999), pp. 26–40.

[9] R. Ghanem and P. Spanos, *Stochastic Finite Elements: A Spectral Approach*, Springer-Verlag, New York, 1991.

[10] C. Hastings, *Approximations for Digital Computers*, Princeton University Press, Princeton, NJ, 1955.

[11] K. Ito, *Multiple Wiener integral*, J. Math. Soc. Japan, 3 (1951), pp. 157–169.

[12] S. Karlin and J. McGregor, *The differential equations of birth-and-death processes, and the Stieltjes moment problem*, Trans. Amer. Math. Soc., 85 (1957), pp. 489–546.

[13] G. Karniadakis and S. Sherwin, *Spectral/hp Element Methods for CFD*, Oxford University Press, Oxford, UK, 1999.

[14] R. Koekoek and R. Swarttouw, *The Askey-Scheme of Hypergeometric Orthogonal Polynomials and Its q-Analogue*, Tech. report 98-17, Department of Technical Mathematics and Informatics, Delft University of Technology, Delft, The Netherlands, 1998.

[15] D. Lucor, D. Xiu, and G. Karniadakis, *Spectral representations of uncertainty in simulations: Algorithms and applications*, in Proceedings of the International Conference on Spectral and High Order Methods (ICOSAHOM-01), Uppsala, Sweden, 2001.

[16] H. Ogura, *Orthogonal functionals of the Poisson process*, IEEE Trans. Inform. Theory, 18 (1972), pp. 473–481.
[17] W. Schoutens, *Stochastic Processes and Orthogonal Polynomials*, Springer-Verlag, New York, 2000.
[18] G. Szegö, *Orthogonal Polynomials*, American Mathematical Society, Providence, RI, 1939.
[19] N. Wiener, *The homogeneous chaos*, Amer. J. Math., 60 (1938), pp. 897–936.
[20] D. Xiu and G. Karniadakis, *Modeling uncertainty in flow simulations via generalized polynomial chaos*, J. Comput. Phys., to appear.