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REVIEW ARTICLE

Fast Numerical Methods for Stochastic Computations: A Review

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Abstract. This paper presents a review of the current state-of-the-art of numerical methods for stochastic computations. The focus is on efficient high-order methods suitable for practical applications, with a particular emphasis on those based on generalized polynomial chaos (gPC) methodology. The framework of gPC is reviewed, along with its Galerkin and collocation approaches for solving stochastic equations. Properties of these methods are summarized by using results from literature. This paper also attempts to present the gPC based methods in a unified framework based on an extension of the classical spectral methods into multi-dimensional random spaces.

AMS subject classifications: 41A10, 60H35, 65C30, 65C50

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Contents

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1 Introduction

The purpose of this paper is to present an overview of the recent development of numerical methods for stochastic computations, with a focus on fast algorithms suitable for large-scale complex problems. This field has received an increasing amount of attention recently and is developing at a fast pace with new results emerging as the paper is under writing. Therefore this paper is not an attempt to present an exhaustive review of all available results, which is a goal almost impossible to achieve. The focus is rather on the popular methods based generalized polynomial chaos (gPC) methodology. We will present the framework and properties of the methods by using (almost) exclusively published work and demonstrate that the methods can be considered as a natural extension of deterministic spectral methods into random spaces.

1.1 Uncertainty quantification

The ultimate objective of numerical simulations is to predict physical events or the behaviors of engineered systems. Extensive efforts have been devoted to the development of accurate numerical algorithms so that simulation predictions are reliable in the sense that numerical errors are well under control and understood. This has been the primary goal of numerical analysis, which remains an active research branch. What has been considered much less in the classical numerical analysis is the understanding of impacts of errors, or uncertainty, in "data" such as parameter values, initial and boundary conditions.

The goal of uncertainty quantification (UQ) is to investigate the impact of such errors in data and subsequently to provide more reliable predictions for practical problems. This topic has received an increasing amount of attention in the past years, especially in the context of complex systems where mathematical models can serve only as simplified and reduced representations of the true physics. Although many models have been successful in revealing quantitative connections between predictions and observations, their usage is constrained by our ability of assigning accurate numerical values to various parameters in the governing equations. Uncertainty represents such variability in data and is ubiquitous because of our incomplete knowledge of the underlying physics and/or inevitable measurement errors. Hence in order to fully understand simulation results and subsequently the true physics, it is imperative to incorporate uncertainty from the beginning of the simulations and not as an afterthought.

1.1.1 Burgers' equation: An illustrative example

Instead of engaging in an extensive discussion on the significance of UQ, which there are many, let us demonstrate the impact of uncertainty via a simple example of the viscous Burgers' equation,

$$\begin{cases} u_t + uu_x = \nu u_{xx}, & x \in [-1,1], \\ u(-1) = 1, \quad u(1) = -1, \end{cases} \tag{1.1}$$

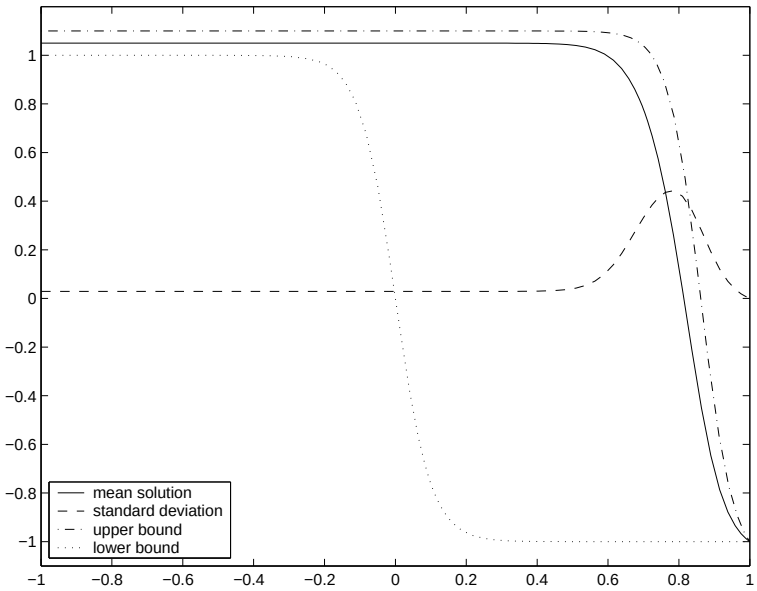

Figure 1: Stochastic solutions of Burgers' equation (1.1) with $u(-1,t)=1+\delta$ where δ is a uniformly distributed random variable in $(0,0.1)$ and $\nu=0.05$. The solid line is the average steady-state solution, with the dotted lines denoting the bounds of the random solutions. The dashed line is the standard deviation of the solution. (Details are in [94].)

where u is the solution field and $\nu>0$ is the viscosity. This is a well-known nonlinear partial differential equation (PDE) for which extensive results exist. The presence of viscosity smooths out the shock discontinuity which will develop otherwise. Thus, the solution has a transition layer, which is a region of rapid variation and extends over a distance $\mathcal{O}(\nu)$ as $\nu\downarrow 0$. The location of the transition layer z, defined as the zero of the solution profile $u(t,z)=0$, is at zero when the solution reaches steady-state. If a small amount of (positive) uncertainty exists in the value of the left boundary condition (possibly due some bias measurement or estimation errors), i.e.,

$$u(-1)=1+\delta,$$

where $0<\delta\ll 1$, then the location of the transition can change significantly. For example, if δ is a uniformly distributed random variable in the range of $(0,0.1)$, then the average steady-state solution with $\nu=0.05$ is the solid line in Fig. 1. It is clear that a small uncertainty of 10% can cause significant changes in the final steady-state solution whose average location is approximated at $z\approx 0.8$, resulting in an $\mathcal{O}(1)$ difference from the solution with idealized boundary condition containing no uncertainty. (Details of the computations can be found in [94].)

The Burgers' equation example demonstrates that for some problems, especially the nonlinear ones, small uncertainty in data may cause non-negligible changes in the system output. Such changes can not be captured by increasing resolution of the classical

numerical algorithms, if the uncertainty is not incorporated at the beginning of the computations.

1.2 Overview of techniques

The importance of understanding uncertainty has been realized by many for a long time, in disciplines such as civil engineering, hydrology, control, etc. Subsequently many methods have been devised to tackle the issue. Due to the "uncertain" nature of the uncertainty, the most dominant approach is to treat data uncertainty as random variables or random processes and recast the original deterministic systems as stochastic systems.

We remark that this type of stochastic systems are different from the classical "stochastic differential equations" (SDE) where the random inputs are some idealized processes such as Wiener processes, Poisson processes, etc., and tools such as stochastic calculus have been developed extensively and are still under active research; see, e.g., [21, 37, 39, 58].

1.2.1 Monte Carlo and sampling based methods

One of the most commonly used methods is Monte Carlo sampling (MCS), or one of its variants. In MCS, one generates (independent) realizations of random inputs based on their prescribed probability distribution. For each realization the data is fixed and the problem becomes deterministic. Upon solving the deterministic realizations of the problem, one collects an ensemble of solutions, i.e., realizations of the random solutions. From this ensemble, statistical information can be extracted, e.g., mean, variance, etc. Although MCS is straightforward to apply as it only requires repetitive executions of deterministic simulations, typically a large number of executions are needed, for the solution statistics converge relatively slowly. For example, the mean value typically converges as $1/\sqrt{K}$ where K is the number of realizations (e.g., [17]). The need for large number of realizations for accurate results can incur excessive computational burden, especially for systems that are already computationally intensive in their deterministic settings.

Techniques have been developed to accelerate the convergence of the brute-force MCS, e.g., Latin hypercube sampling (cf. [50, 74]), quasi Monte Carlo (cf. [18, 54, 55]), to name a few. However, additional restrictions are posed based on the design of these methods, and their applicability is often limited.

1.2.2 Perturbation methods

The most popular non-sampling methods is perturbation methods, where random fields are expanded via Taylor series around their mean and truncated at certain order. Typically, at most second-order expansion is employed because the resulting system of equations becomes extremely complicated beyond second-order. This approach has been used extensively in various engineering fields [38, 47, 48]. An inherent limitation of perturbation methods is that the magnitude of uncertainties, both at the inputs and outputs,

Table 1: The mean location of the transition layer ($\bar{z}$) and its standard deviation (σ_z) by Monte Carlo simulations. n is the number of realizations, $\delta \sim U(0,0.1)$ and $\nu = 0.05$. Also shown are the converged gPC solutions.

	$n=100$	$n=1{,}000$	$n=2{,}000$	$n=5{,}000$	$n=10{,}000$	gPC
$\bar{z}$	0.819	0.814	0.815	0.814	0.814	0.814
σ_z	0.387	0.418	0.417	0.417	0.414	0.414

cannot be too large (typically less than 10%), and the methods do not perform well otherwise.

1.2.3 Moment equations

In this approach one attempts to compute the moments of the random solution *directly*. The unknowns are the moments of the solution and their equations are derived by taking averages of the original stochastic governing equations. For example, the mean field is determined by the mean of the governing equations. The difficulty lies in the fact that the derivation of a moment almost always, except in some rare occasions, requires the information of higher moments. This brings out the so-called "closure" problem, which is often dealt with by utilizing some *ad hoc* arguments on the properties of the higher moments. More detailed presentations of the moment equation approach, in the context of hydrology, can be found in [105].

1.2.4 Operator based methods

These kinds of approaches are based on manipulation of the stochastic operators in the governing equations. They include Neumann expansion, which expresses the inverse of the stochastic operator in a Neumann series [69, 104], and the weighted integral method [14,15]. Similar to perturbation methods, these operator based methods are also restricted to small uncertainties. Their applicability is often strongly dependent on the underlying operator and is typically limited to static problems.

1.2.5 Generalized polynomial chaos (gPC)

A recently developed method, generalized polynomial chaos (gPC) [91], a generalization of the classical polynomial chaos [29], has become one of the most widely used methods. With gPC, stochastic solutions are expressed as orthogonal polynomials of the input random parameters, and different types of orthogonal polynomials can be chosen to achieve better convergence. It is essentially a spectral representation in random space, and exhibits fast convergence when the solution depends smoothly on the random parameters. GPC based methods will be the focus of this paper.

1.2.6 Burgers' equation revisited

Let us return to the viscous Burgers' example (1.1), with the same parameter settings that produced the Fig. 1. Let us examine the location of the averaged transition layer and the standard deviation of the solution at this location, obtained by different methods. Table

Table 2: The mean location of the transition layer ($\bar{z}$) and its standard deviation (σ_z) obtained by perturbation methods. k is the order of the perturbation expansion, $\delta \sim U(0,0.1)$ and $\nu = 0.05$. Also shown are the converged gPC solutions.

	$k=1$	$k=2$	$k=3$	$k=4$	gPC
$\bar{z}$	0.823	0.824	0.824	0.824	0.814
σ_z	0.349	0.349	0.328	0.328	0.414

1 shows the results by Monte Carlo simulations, and Table 2 by a perturbation method at different orders. The converged solutions by gPC (up to three significant digits) are obtained by a fourth-order expansion and are tabulated for comparison. It can be seen that the MCS achieves same accuracy with $\mathcal{O}(10^4)$ realizations. On the other hand, the computational cost of the fourth-order gPC is approximately equivalent to five deterministic simulations. The perturbation methods have similar low computational cost as that of gPC. However, the accuracy of the perturbation methods is much less desirable, as shown in Table 2. In fact, by increasing the perturbation orders, no clear convergence can be observed. This is caused by the relatively large uncertainty at the output, which can be as high as 40%, even though the input uncertainty is small.

This example demonstrates the accuracy and efficiency of gPC method. It should be remarked that although gPC shows significant advantage here, the conclusion can not be trivially generalized to other problems, as the strength and weakness of gPC, or any methods for this matter, are problem dependent.

1.3 Development of gPC

The development of gPC started with the seminal work on PC (polynomial chaos) by R. Ghanem and co-workers. Inspired by the theory of Wiener-Hermite homogeneous chaos ([85]), Ghanem employed Hermite polynomials as orthogonal basis to represent random processes and applied the technique to solutions of many engineering problems with success, cf., [25–27,73]. An overview can be found in [29].

The use of Hermite polynomials, albeit mathematically sound, presents difficulties in some applications, particularly in term of convergence and probability approximations for non-Gaussian problems [12, 59]. Subsequently, the generalized polynomial chaos (gPC) was proposed in [91] to alleviate the difficulty. In gPC, different kinds of orthogonal polynomials are chosen as basis depending on the probability distribution of random inputs. Optimal convergence can be achieved by choosing the proper basis. In a series of paper, the strength of gPC is demonstrated for a variety of PDEs [90, 92].

The work of gPC was further generalized by not requiring the basis polynomials to be globally smooth. In fact in principle any set of complete basis can be a viable choice, just like in finite element method, depending on the given problem. Such generalization includes the piecewise polynomial basis [5, 66], wavelet basis [42, 43], and multi-element gPC [80, 82].

When applied to differential equations with random inputs, the quantities to be solved

are the expansion coefficients of the gPC expansion. A typical approach is to conduct a Galerkin projection to minimize the error of the finite-order gPC expansion, and the resulting set of equations for the expansion coefficients are deterministic and can be solved via conventional numerical techniques. This is the stochastic Galerkin approach and has been applied from the early work of PC and proved to be effective. However, stochastic Galerkin (SG) procedure can be challenging when the governing stochastic equations take complicated forms. In this case, the derivation of explicit equations for the gPC coefficients can be very difficult, sometime even impossible.

Very recently, there is a surge of interests in high-order stochastic collocation (SC) approach, following the work of [89]. This is in some way a re-discovery of the old technique of "deterministic sampling method", which has been used as a numerical integration method in lower dimensions for a long time. Earlier work of stochastic collocation methods includes [52,77] and uses tensor products of one-dimensional quadrature points as "sampling pints". Although it was shown that this approach can achieve high orders, see [4], its applicability is restricted to smaller number of random variables as the number of sampling points grows exponentially fast otherwise. The work of [89] introduced the "sparse grid" technique from multivariate interpolation analysis and can significantly reduce the number of sampling points in higher random dimensions. In this way SC combines the advantages of both Monte Carlo sampling and gPC-Galerkin method. The implementation of a SC algorithm is similar to that of MCS, i.e., only repetitive realizations of a deterministic solver is required; and by choosing a proper set of sampling points such as the sparse grid, it retains the high accuracy and fast convergence of gPC Galerkin approach. In the original high-order stochastic collocation formulation, the basis functions are Lagrange polynomials defined by the nodes, either sparse grid [89] or tensor grid [4]. A more practical "pseudo-spectral" approach that can recast the collocation solutions in terms of the gPC polynomial basis was proposed in [86]. The pseudo-spectral gPC method is easier to manipulate in practice than the Lagrange interpolation approach.

The major challenge in stochastic computations is high dimensionality, i.e., how to deal with the large number of random variables. One approach to alleviate the computational cost is to use adaptivity. The current work includes adaptive choice of polynomial basis [19,79], adaptive element selection in multi-element gPC [80], and adaptive sparse grid collocation [20,78].

1.4 Outline

The paper is organized as follows. In Section 2, the probabilistic formulation of a deterministic system with random inputs is discussed in a general setting. The gPC framework is presented in Section 3. Its Galerkin application is discussed in Section 4 and collocation application in Section 5, where examples and details of the approaches are presented. Discussions on some general properties of Galerkin versus collocation and more recent advances are in Section 6. A brief review on how to deal problems with random geometry is included in Section 7, before we conclude the paper.

2 Formulations

In this section, we present the mathematical framework of the kind of stochastic computations we are interested in. For notational convenience, the exposition is restricted to boundary value problems. The framework is nevertheless applicable to general time dependent problems.

2.1 Governing equations

Let $D\subset\mathbb{R}^d$, $d=1,2,3$, be a fixed physical domain with boundary ∂D, and $x=(x_1,\cdots,x_d)$ be the coordinates. Let us consider a partial differential equations (PDE),

$$\begin{aligned} &L(x,u;y)=0, \quad \text{in } D,\\ &B(x,u;y)=0, \quad \text{on } \partial D, \end{aligned} \tag{2.1}$$

where L is a differential operator and B is a boundary operator. The operator B can take various forms on different boundary segments, e.g., $B\triangleq I$, where I is the identity operator, on Dirichlet segments and $B\triangleq n\cdot\nabla$ on Neumann segments whose outward unit normal vector is n. Here $y=(y_1,\cdots,y_N)\in\mathbb{R}^N, N\geq 1$, are *parameters* of interests. We assume that these parameters $(y_1,\cdots,y_N)$ are mutually independent of each other. In another word, there may exist additional parameters that either are functions of y, or are not of our interests in studying. Note in practice one may also be interested a set of quantities

$$g=(g_1,\cdots,g_K)\in\mathbb{R}^K=G(u), \tag{2.2}$$

called *observables* here, that are functions of the solution u of (2.1), in addition to the solution itself.

2.2 Probabilistic framework

In what follows, we will adopt a probabilistic framework and model $y=(y_1,\cdots,y_N)$ as a N-variate random vector with independent components in a properly defined probability space $(\Omega,\mathcal{A},\mathcal{P})$, whose event space is Ω and is equipped with σ-algebra $\mathcal{A}$ and probability measure $\mathcal{P}$. The following exposition will primarily focus on continuous random variables, although the framework works equally well for discrete random variables (see [91]).

Let $\rho_i:\Gamma_i\to\mathbb{R}^+$ be the probability density function (PDF) of the random variable $y_i(\omega)$, $\omega\in\Omega$, whose image is $\Gamma_i\triangleq y_i(\Omega)\subset\mathbb{R}$ for $i=1,\cdots,N$. Then

$$\rho(y)=\prod_{i=1}^{N}\rho_i(y_i), \tag{2.3}$$

is the joint probability density of the random vector $y=(y_1,\cdots,y_N)$ with the support

$$\Gamma\triangleq\prod_{i=1}^{N}\Gamma_i\subset\mathbb{R}^N. \tag{2.4}$$

This allows us to conduct numerical formulations in the finite dimensional (N-dimensional) random space Γ, in replacement of the infinite dimensional space Ω. And the governing equation (4.7) should be valid for all $y\in\Gamma$. Naturally, we seek a solution $u(x,y):\bar{D}\times\Gamma\to\mathbb{R}$ such that (2.1) is satisfied for all $x\in\bar{D}$ and $y\in\Gamma$.

Finally, it is convenient to consider "standard" random variables, similar to the standard elements in FEM, and this can always be achieved by proper scaling. To this end, there are three kinds of supports Γ_i for the random variables $y_i, i=1,\cdots,N$, i.e., the bounded support in $(-1,1)$ (occasionally $(0,1)$ is employed), the half space $(0,+\infty)$, and the whole space $(-\infty,+\infty)$. If all random variables y_i have the same support, which is not required but often assumed in practice, then the finite dimensional probability space Γ is

$$\text{hypercube: } (-1,1)^N, \quad (0,+\infty)^N, \quad \text{or } \mathbb{R}^N, \tag{2.5}$$

respectively.

2.3 Parameterizing random inputs

One of the most important step before carrying out numerical simulations of stochastic systems such as (2.1), regardless the form of numerical methods, is to properly identify the random variables y so that the input data uncertainty is accurately modeled.

The key issue is to parameterize the input uncertainty by a set of finite number (N) independent random variables.

This task is often easy to accomplish when the uncertainty inputs are the physical parameters of the system, for example, reaction constants of a bio-chemical network. In this case it is relatively straightforward to identify the independent parameters and model them as random variables with proper distribution based on measurements, experience, or intuition.

It is less obvious when the random inputs include continuous random processes, e.g., boundary conditions along a segment of the boundary, initial condition in the computational domain. For Gaussian processes, the parameterization is relatively easier as Gaussian processes can be completely determined by their first two moments – mean and covariance. The most popular methods include spectral series [103] and Karhunen-Loève (KL) expansion [49], or in a slightly more general framework in term of orthogonal series [106]. These methods seek to represent a Gaussian process by a linear series of Gaussian random variables, where the expansion coefficients are determined by matching the spectrum (as in the spectral series [103]) or the covariance function (as in the KL expansion [49]) of the underlying process. The number of expansion terms is determined by controlling the errors of the series. In principle the error diminishes as the number of terms is increased. However, each term introduces an independent random variable (Gaussian) and hence an additional dimension of $\Gamma\subset\mathbb{R}^N$. Therefore in practice the number of random variables is to be minimized. Convergence properties for the KL expansion was examined numerically in [35] and more rigorously in [67].

For non-Gaussian processes things are much more involved, as the two quantities, mean and covariance, are far from sufficient to completely specify a given process. Many techniques have been investigated, with most seeking to match (numerically) mean, covariance, and marginal distributions at some given physical locations. This remains an active research, see, for example, [32, 60, 61, 63, 70, 102].

The independence requirement in the parameterization of input random processes is essential in stochastic computations as mathematically it allows us to define the subsequent functional spaces via tensor product rule. This is a rather general requirement for practically all numerical methods – for example, any sampling methods would employ a pseudo random number generator which generates independent series of random numbers. It should be noted that it is possible to construct multi-dimensional functional spaces based on finite number of *dependent* random variables [72]. However, such a construction does not, in its current form, allow straightforward numerical implementations.

A very common approach for non-Gaussian processes is to employ the Karhunen-Loève expansion and further assume the resulting set of *uncorrelated* random variables are mutually independent. The reconstructed process obviously can not match the given process from distribution point of view, but it does retain its approximation of the mean and covariance functions. This approach is often adopted when the focus is on the ensuing numerical procedure and not on the parameterization of the input processes. We remark that it is possible to transform a set of dependent random variables into independent ones, via, for example, the Rosenblatt transformation [62]. Such procedures, however, are of little practical use as they usually require the knowledge of all the joint distribution functions among all the random variables at all the physical locations.

In this paper, we will assume that the random inputs are already characterized by a set of mutually independent random variables via a given procedure and with satisfactory accuracy and focus on the following numerical approach for (2.1).

3 Generalized polynomial chaos

In the finite dimensional random space Γ defined in (2.4), the gPC expansion seeks to approximate a random function via orthogonal polynomials of random variables.

3.1 Univariate gPC basis

Let us define one-dimensional orthogonal polynomial spaces with respect to the measure $\rho_i(y_i)dy$ in Γ_i,

$$W^{i,d_i} \equiv \left\{ v : \Gamma_i \to \mathbb{R} : v \in \text{span}\{\phi_m(y_i)\}_{m=0}^{d_i} \right\}, \qquad i = 1, \cdots, N, \tag{3.1}$$

where $\{\phi_m(y_i)\}$ are a set of orthogonal polynomials satisfying the orthogonality conditions

$$\int_{\Gamma_i} \rho_i(y_i)\phi_m(y_i)\phi_n(y_i)dy_i = h_m^2 \delta_{mn}, \tag{3.2}$$

Table 3: Correspondence between the type of gPC polynomial basis and probability distribution ($N \geq 0$ is a finite integer).

	Distribution	gPC basis polynomials	Support
Continuous	Gaussian	Hermite	$(-\infty,\infty)$
	Gamma	Laguerre	$[0,\infty)$
	Beta	Jacobi	$[a,b]$
	Uniform	Legendre	$[a,b]$
Discrete	Poisson	Charlier	$\{0,1,2,\cdots\}$
	Binomial	Krawtchouk	$\{0,1,\cdots,N\}$
	Negative Binomial	Meixner	$\{0,1,2,\cdots\}$
	Hypergeometric	Hahn	$\{0,1,\cdots,N\}$

where δ_{mn} is the Kronecker delta function and

$$h_m^2 = \int_{\Gamma_i} \rho_i \phi_m^2 dy_i$$

is normalization factor. With proper scaling, one can always normalize the bases such that $h_m^2 \equiv 1, \forall m$, and this shall be adopted throughout this paper.

The probability density function $\rho_i(y_i)$ in the above orthogonality relation (3.2) serves as a role of integration weight, which in turn defines the type of orthogonal polynomials $\{\phi_n\}$. For example, if y_i is a uniformly distributed random variable in $(-1,1)$, its PDF is a constant and (3.2) defines Legendre polynomials. For Gaussian distributed random variable y_i, its PDF defines Hermite polynomials and this is the classical polynomial chaos method [29]. In fact, for most well known probability distribution, there exists a corresponding known orthogonal polynomials. The well known correspondences are listed in Table 3. (See [90, 91] for more detailed discussions.)

The correspondence between the probability distribution of random variables and the type of orthogonal polynomials offers an efficient means of representing general random variables. Fig. 2 shows an example of approximating a uniform random variable. With Hermite polynomials, the uniform distribution can be approximated more accurately by using higher-order polynomials, although Gibb's oscillations are clearly visible. If one employs the corresponding gPC basis — the Legendre polynomials in this case — then the first order polynomials can represent this distribution *exactly*.

3.2 Multivariate gPC basis

The corresponding N-variate orthogonal polynomial space in Γ is defined as

$$W_N^P \equiv \bigotimes_{|\mathbf{d}| \leq P} W^{i,d_i}, \tag{3.3}$$

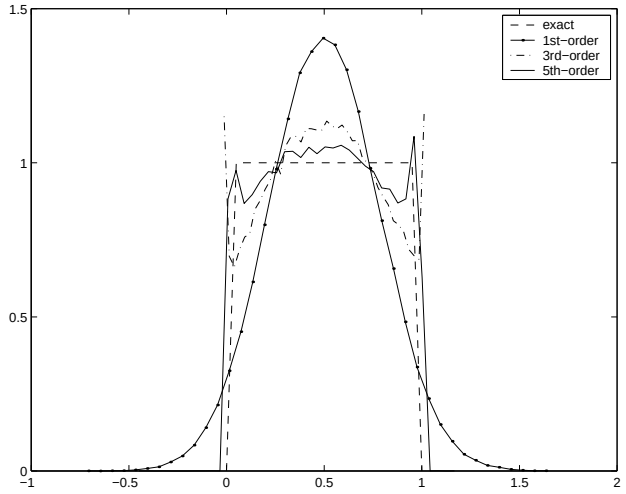

Figure 2: gPC approximation of a uniform random distribution by Hermite basis. (Legendre basis can represent the distribution exactly with first-order.)

where the tensor product is over all possible combinations of the multi-index $\mathbf{d}=(d_1,\cdots,d_N)\in\mathbb{N}_0^N$ satisfying $|\mathbf{d}|=\sum_{i=1}^N d_i\leq P$. Thus, W_N^P is the space of N-variate orthonormal polynomials of total degree at most P. Let $\{\Phi_m(y)\}$ be the N-variate orthonormal polynomials from W_N^P. They are constructed as products of a sequence of univariate polynomials in each directions of $y_i, i=1,\cdots,N$, i.e.,

$$\Phi_m(y)=\phi_{m_1}(y_1)\cdots\phi_{m_N}(y_N),\qquad m_1+\cdots+m_N\leq P, \tag{3.4}$$

where m_i is the order of the univariate polynomials of $\phi(y_i)$ in the y_i direction for $1\leq i\leq N$. Obviously, we have

$$\mathbb{E}[\Phi_m(y)\Phi_n(y)]\triangleq\int\Phi_m(y)\Phi_n(y)\rho(y)dy=\delta_{mn},\quad\forall 1\leq m,n\leq\dim(W_N^P), \tag{3.5}$$

where $\mathbb{E}$ is the expectation operator and δ_{mn} is again the Kronecker delta function. The number of basis functions is

$$\dim(W_N^P)=\binom{N+P}{N}. \tag{3.6}$$

It should be noted that sometimes the full tensor product polynomial space where the polynomial order in each dimension is at most P is also employed. This is done primarily for the convenience of analysis (for example, [5]), and is not desirable in practical computations as the number of basis functions is $(P+1)^N$ and grows too fast in large dimensions N. From now on we will focus on the space (3.3), which is used in most stochastic computations with gPC, cf. [29,90,92].

3.3 GPC approximation

The P^{th}-order, gPC approximations of the solution $u(x,y)$ of (2.1) can be obtained by projecting u onto the space W_N^P, i.e., $\forall x \in D$,

$$\mathbb{P}_N^P u \triangleq u_N^P(x,y) = \sum_{m=1}^{M} \hat{u}_m(x)\Phi_m(y), \quad M = \binom{N+P}{N}, \tag{3.7}$$

where $\mathbb{P}_N^P$ denotes the orthogonal projection operator from $L_\rho^2(\Gamma)$ onto W_N^P and $\{\hat{u}_m\}$ are the Fourier coefficients defined as

$$\hat{u}_m(x) = \int u(x,y)\Phi_m(y)\rho(y)dy = \mathbb{E}[u(x,y)\Phi_m(y)], \quad 1 \le m \le M. \tag{3.8}$$

The classical approximation theory guarantees that this is the best approximation in $\mathcal{P}_N^P$, the linear polynomial space of N-variate polynomials of degree up to P, i.e., for any $x \in D$ and $u \in L_\rho^2(\Gamma)$,

$$\|u - \mathbb{P}_N^P u\|_{L_\rho^2(\Gamma)} = \inf_{\Psi \in \mathcal{P}_N^P} \|u - \Psi\|_{L_\rho^2(\Gamma)}. \tag{3.9}$$

The error of this finite-order projection can be defined as

$$\begin{aligned} \epsilon_G(x) &\triangleq \|u - \mathbb{P}_N^P u\|_{L_\rho^2(\Gamma)} \\ &= \left(\mathbb{E}[(u(x,y) - u_N^P(x,y))^2]\right)^{1/2}, \quad \forall x \in D, \end{aligned} \tag{3.10}$$

and will converge to zero as the order of approximation P is increased.

3.4 Statistical information

When a sufficiently accurate gPC approximation (3.7) is available, one has in fact an *analytical* representation of u in term of the random inputs y. Therefore, practically all statistical information can be retrieved in a straightforward manner. For example, the *mean* solution is

$$\mathbb{E}[u] \approx \mathbb{E}[u_N^P] = \int \left(\sum_{m=1}^{M} \hat{u}_m \Phi_m(y) \right) \rho(y)dy = \hat{u}_1, \tag{3.11}$$

following the orthogonality (3.5). The *second-moment*, i.e., the *covariance function*, can be estimated by

$$\begin{aligned} R_{uu}(x_1,x_2) &\triangleq \mathbb{E}\left[\left(u(x_1,y) - \mathbb{E}[u(x_1,y)]\right) \left(u(x_2,y) - \mathbb{E}[u(x_2,y)]\right) \right] \\ &\approx \mathbb{E}\left[\left(u_N^P(x_1,y) - \mathbb{E}[u_N^P(x_1,y)]\right) \left(u_N^P(x_2,y) - \mathbb{E}[u_N^P(x_2,y)]\right) \right] \\ &= \sum_{m=2}^{M} [\hat{u}_m(x_1)\hat{u}_m(x_2)]. \end{aligned} \tag{3.12}$$

The *variance* of the solution can be obviously approximated as

$$Var(u(x)) = \mathbb{E}\left[(u(x,y) - \mathbb{E}[u(x,y))^2\right] \approx \sum_{m=2}^{M} \left[\hat{u}_m^2(x)\right]. \tag{3.13}$$

Other statistical quantities such as sensitivity coefficients can also be evaluated. For example, the global sensitivity coefficients can be approximated as

$$S_j(x) \triangleq \mathbb{E}\left[\frac{\partial u}{\partial y_j}\right] \approx \sum_{m=1}^{M} \left(\hat{u}_m(x) \int \frac{\partial \Phi_m(y)}{\partial y_j} \rho(y) dy\right), \qquad j = 1, \cdots, N, \tag{3.14}$$

where the integrals of the derivatives of the orthogonal polynomials can be readily evaluated analytically prior to any computations.

4 Stochastic Galerkin method

The key in using the gPC expansion (3.7) is to evaluate the expansion coefficients $\{\hat{u}_m\}$. To this end the definition (3.8) is of little use as it involves the unknown solution $u(x,y)$, and one needs to devise alternative strategies to estimate these coefficients.

4.1 Formulation

A typical approach to obtain gPC solution in the form of (3.7) is to employ a stochastic Galerkin approach. Here we again seek an approximate gPC solution in the form of

$$v_N^P(x,y) = \sum_{m=1}^{M} \hat{v}_m(x) \Phi_m(y), \quad M = \binom{N+P}{N}. \tag{4.1}$$

The expansion coefficients $\{\hat{v}_m\}$ are obtained by satisfying (2.1) in the following weak form, for all $w(y) \in W_N^P$,

$$\begin{aligned} &\int L(x, v_N^P; y) w(y) \rho(y) dy = 0, \qquad \text{in } D, \\ &\int B(x, v_N^P; y) w(y) \rho(y) dy = 0, \qquad \text{on } \partial D. \end{aligned} \tag{4.2}$$

The resulting equations are a set of (coupled) *deterministic* PDEs for $\{\hat{v}_m\}$, and standard numerical techniques can be applied. Such a Galerkin procedure has been used extensively in the literature [5, 19, 29, 42, 90–92]. However, one should keep in mind that when the governing equation (2.1) takes a complicated form, the derivation of Galerkin equations for $\{\hat{v}_m\}$ via (4.2) can become highly nontrivial, sometimes impossible.

4.2 Examples of gPC Galerkin

Here we demonstrate the details of the gPC Galerkin method by two illustrative examples.

4.2.1 Ordinary differential equation

Let us consider an ordinary differential equation

$$\begin{aligned} &\frac{du(t)}{dt} = -\alpha(y)u, \quad t>0, \\ &u(0) = u_0, \end{aligned} \tag{4.3}$$

where the decay rate coefficient α is assumed to be a random variable with certain distribution, and u_0 is the initial condition.

By applying the generalized polynomial chaos expansion (3.7) to the solution u and the random parameter α

$$u(t,y) = \sum_{i=1}^{M} \hat{v}_i(t)\Phi_i(y), \qquad \alpha(y) = \sum_{i=1}^{M} \hat{\alpha}_i \Phi_i(y) \tag{4.4}$$

and substituting the expansions into the governing equation, we obtain

$$\sum_{i=1}^{M} \frac{d\hat{v}_i(t)}{dt}\Phi_i = -\sum_{i=1}^{M}\sum_{j=1}^{M} \Phi_i\Phi_j\hat{\alpha}_i\hat{v}_j(t). \tag{4.5}$$

A Galerkin projection onto each polynomial basis results in a set of coupled ordinary differential equations for each expansion coefficients:

$$\frac{d\hat{v}_k(t)}{dt} = \sum_{i=1}^{M}\sum_{j=1}^{M} e_{ijk}\hat{\alpha}_i\hat{v}_j(t), \qquad k=1,\cdots,M, \tag{4.6}$$

where $e_{ijk} = \mathbb{E}[\Phi_i\Phi_j\Phi_k]$. This is a system of couple ODEs and standard integration techniques such as Runge-Kutta schemes can be employed. This is the first example considered in [91], where exponentially fast convergence of gPC Galerkin was reported and the impact on accuracy with non-optimal gPC basis was studied.

4.2.2 Stochastic diffusion equation

Let us consider a time-dependent stochastic diffusion equation

$$\begin{aligned} &\frac{\partial u(t,x,y)}{\partial t} = \nabla_x\cdot(\kappa(x,y)\nabla_x u(t,x,y)) + f(t,x,y), \quad x\in D, t\in(0,T]; \\ &u(0,x,y) = u_0(x,y), \quad u(t,\cdot,y)|_{\partial D} = 0, \end{aligned} \tag{4.7}$$

and its steady-state counterpart

$$-\nabla_x\cdot(\kappa(x,y)\nabla_x u(x,y))=f(x,y),\quad x\in D;\qquad u(\cdot,y)|_{\partial D}=0. \tag{4.8}$$

We assume that the random diffusivity field takes a form

$$\kappa(x,y)=\hat{\kappa}_0(x)+\sum_{i=1}^{N}\hat{\kappa}_i(x)y_i, \tag{4.9}$$

where $\{\hat{\kappa}_i(x)\}_{i=0}^N$ are fixed functions with $\hat{\kappa}_0(x)>0,\forall x$, obtained by following some parameterization procedure (e.g., the KL expansion) of the random diffusivity field. Alternatively (4.9) can be written as

$$\kappa(x,y)=\sum_{i=0}^{N}\hat{\kappa}_i(x)y_i, \tag{4.10}$$

where $y_0=1$. For well posedness we require

$$\kappa(x,y)\geq\kappa_{\min}>0,\qquad \forall x,y. \tag{4.11}$$

Such a requirement obviously excludes random vector y which can take negative values with non-zero probability, e.g., Gaussian distribution.

Upon substituting (4.9) and the gPC approximation (4.1) into the governing equation (4.7) and projecting the resulting equation onto the subspace spanned by the first M gPC basis polynomials, we obtain for all $k=1,\cdots,M$,

$$\begin{aligned}\frac{\partial\hat{v}_k}{\partial t}(t,x)&=\sum_{i=0}^{N}\sum_{j=1}^{M}\nabla_x\cdot(\hat{\kappa}_i(x)\nabla_x\hat{v}_j)e_{ijk}+\hat{f}_k(t,x)\\&=\sum_{j=1}^{M}\nabla_x\cdot\left(a_{jk}(x)\nabla_x\hat{v}_j\right)+\hat{f}_k(t,x),\end{aligned} \tag{4.12}$$

where

$$\begin{aligned}&e_{ijk}=\mathbb{E}[y_i\Phi_j\Phi_k]=\int y_i\Phi_j(y)\Phi_k(y)\rho(y)dy,\quad 0\leq i\leq N,\ 1\leq j,k\leq M,\\&a_{jk}(x)=\sum_{i=0}^{N}\hat{\kappa}_i(x)e_{ijk},\quad 1\leq j,k\leq M.\end{aligned} \tag{4.13}$$

Let us denote $\mathbf{v}=(\hat{v}_1,\cdots,\hat{v}_M)^T$, $\mathbf{f}=(\hat{f}_1,\cdots,\hat{f}_M)^T$ and $\mathbf{A}(x)=(a_{jk})_{1\leq j,k\leq M}$. By definition, $\mathbf{A}=\mathbf{A}^T$ is symmetric. The gPC Galerkin equations (4.12) can be written as

$$\begin{aligned}&\frac{\partial\mathbf{v}}{\partial t}(t,x)=\nabla_x\cdot[\mathbf{A}(x)\nabla_x\mathbf{v}]+\mathbf{f},\quad (t,x)\in(0,T]\times D,\\&\mathbf{v}(0,x)=\mathbf{v}_0(x),\quad \mathbf{v}|_{\partial D}=0.\end{aligned} \tag{4.14}$$

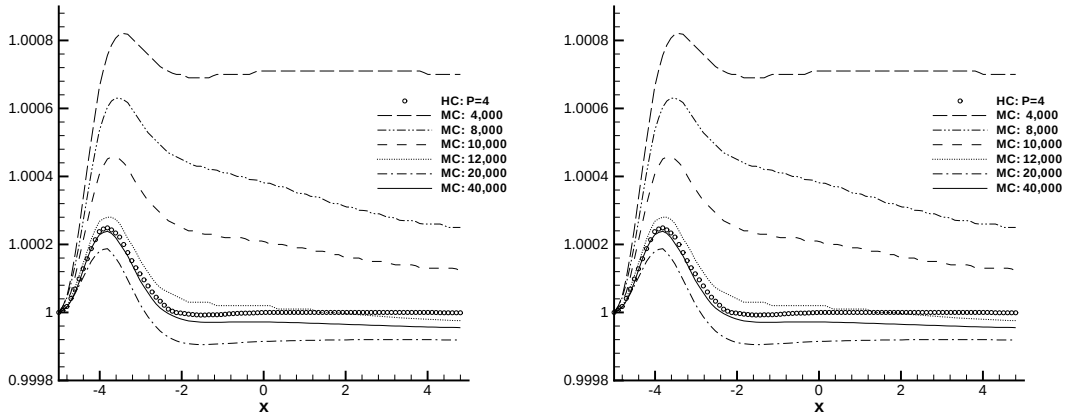

Figure 3: Monte Carlo (MC) simulations and gPC with Hermite basis (HC) solutions of the mean velocities along the centerline of the incompressible channel flow; Left: horizontal velocity component, Right: vertical velocity component. (Details are in [92].)

This is a coupled system of diffusion equations, where $\mathbf{v}_0(x)$ is the gPC expansion coefficient vector of the initial condition of (4.7)

Similarly, by removing the time variable t from the above discussion, we find that the gPC Galerkin approximation to (4.8) is:

$$-\nabla_x \cdot [\mathbf{A}(x)\nabla_x \mathbf{v}] = \mathbf{f}, \quad x \in D; \qquad \mathbf{v}|_{\partial D} = 0. \tag{4.15}$$

This is a coupled system of elliptic equations.

4.2.3 Stochastic Navier-Stokes equations

While applications of the stochastic Galerkin method are abundant, we here illustrate its advantage via an nonlinear system of equations – the incompressible stochastic Navier-Stokes equations,

$$\begin{aligned} &\nabla_x \cdot \mathbf{v}(t,x,y) = 0, \\ &\frac{\partial \mathbf{v}}{\partial t}(t,x,y) + (\mathbf{v}\cdot\nabla_x)\mathbf{v} = -\nabla_x p + \nu \nabla_x^2 \mathbf{v}, \end{aligned} \tag{4.16}$$

where $\mathbf{v}$ is the velocity vector field, p is the pressure field and ν is the viscosity.

The first numerical studies can be found in [41,44], in the context of classical Hermite PC; and in [92] in the context of gPC. In [92], detailed numerical convergence studies were conducted via a pressure driven channel flow problem. The channel is of nondimensional length 10 and height 2 and with random boundary conditions at the bottom wall which are characterized by a four-dimensional random vector, i.e., $y \in \mathbb{R}^4$. Fig. 3 shows the average velocity profiles along the center line of the channel at steady-state. Here "HC" stands for gPC with Hermite-chaos basis, as the random boundary condition is modeled

as a Gaussian process, and "MC" is Monte Carlo results with different numbers of realizations. One clearly observes the convergence of MC results towards the converged (at order $P=3$) gPC solution, as the number of MC realizations is increased. The gPC solution requires only $M=35$ coupled Navier-Stokes systems and achieves significant computational speed-up compared to MC. More details of the computations including other types of random boundary conditions as well as numerical formulations can be found in [92].

5 Stochastic collocation methods

In collocation methods one seeks to satisfy the governing equation (2.1) at a discrete set of points, called "nodes", in the corresponding random space. From this point of view, all classical sampling methods like Monte Carlo sampling are collocation methods. However our focus here is on the approaches that utilize polynomial approximation theory to strategically locate the nodes to gain accuracy. Therefore the traditional sampling approaches based on random or quasi-random nodes are not discussed. Two of the major approaches of high-order stochastic collocation methods are the Lagrange interpolation approach, first presented in [89] and later (independently) in [4], and the pseudo-spectral gPC approach from [86].

5.1 Lagrange interpolation approach

Let $\Theta_N=\{y^{(i)}\}_{i=1}^{Q}\in\Gamma$ be a set of (prescribed) nodes in the N-dimensional random space Γ, where Q is the number of nodes. A Lagrange interpolation of the solution $u(x,y)$ of (2.1) can be written as

$$\mathcal{I}u(x,y)=\sum_{k=1}^{Q}\widetilde{u}_k(x)L_k(y),\quad \forall x\in D, \tag{5.1}$$

where

$$L_i(y^{(j)})=\delta_{ij},\quad 1\le i,j\le Q, \tag{5.2}$$

are the Lagrange polynomials and

$$\widetilde{u}_k(x)\triangleq u(x,y^{(k)}),\qquad 1\le k\le Q, \tag{5.3}$$

is the value of the solution u at the given node $y^{(k)}\in\Theta_N$.

By requiring (2.1) to be satisfied at each of the nodes, we immediately obtain: $\forall k=1,\cdots,Q$,

$$\begin{aligned} &L\left(x,\widetilde{u}_k;y^{(k)}\right)=0,\quad \text{in } D,\\ &B\left(x,\widetilde{u}_k;y^{(k)}\right)=0,\quad \text{on } \partial D. \end{aligned} \tag{5.4}$$

Thus, the stochastic collocation method is equivalent to solving Q deterministic problems (2.1) with "realizations" of the random vector $y^{(k)}$ for $k=1,\cdots,Q$. A significant advantage

is that existing deterministic solvers can be readily applied. This is in direct contrast to the stochastic Galerkin approaches, where the resulting expanded equations are in general coupled.

Once the Lagrange interpolation form of the solution (5.1) is obtained, the statistics of random solution can be evaluated, e.g.,

$$\mathbb{E}[u(x,y] \approx \mathbb{E}[\mathcal{I}u(x,y)] = \sum_{k=1}^{Q} \widetilde{u}(x) \int L_k(y)\rho(y)dy. \tag{5.5}$$

Here the quantities $\int L_k(y)\rho(y)dy$ serve as a role of weights in the discrete sum.

Although the method is conceptually straightforward and easy to implement, in practice the selection of nodes is a nontrivial problem. This is especially true in multiple dimensional spaces, for many theoretical aspects of Lagrange interpolation are unclear. Although in engineering applications there are some "rules" on how to choose the nodes, most of them are *ad hoc* and have no control over the interpolation errors. Furthermore, manipulation of multivariate Lagrange polynomials is not straightforward. Hence the formula (5.5) is of little use, as the weights in the discrete sum are not readily available. Most, if not all, stochastic collocation methods utilizing this approach (including those of [4,89]) thus choose the nodes to be a set of cubature points. In this way when integrals are replaced by a discrete sum like (5.5) the weights are explicitly known, thus avoiding explicit evaluations of the Lagrange polynomials. To this end, the method becomes nothing but a "deterministic" sampling scheme.

5.2 Pseudo-spectral approach: Discrete expansion

To avoid the cumbersomeness of manipulating Lagrange polynomials, a pseudo-spectral collocation approach is proposed in [86] that allows one to reconstruct a gPC representation of the solution of (2.1). In this approach, we again seek an approximate solution in the form of gPC expansion, similar to (3.7), i.e., for any $x \in D$,

$$\mathbb{I}_N^P u \triangleq w_N^P(x,y) = \sum_{m=1}^{M} \hat{w}_m(x)\Phi_m(y), \qquad M = \binom{N+P}{N}, \tag{5.6}$$

where $\mathbb{I}_N^P$ is another projector from $L^2_\rho(\Gamma)$ to W_N^P and the expansion coefficients are determined as

$$\hat{w}_m(x) = \sum_{j=1}^{Q} u(x,y^{(j)})\Phi_m(y^{(j)})\alpha^{(j)}, \qquad m = 1,\cdots,M. \tag{5.7}$$

where $\{y^{(j)},\alpha^{(j)}\}_{j=1}^{Q}$ are a set of nodes and weights, and $u(x,y^{(j)})$ is again the deterministic solution of (2.1) with fixed $y^{(j)}$. The choice of the nodes and weights should be made such that

$$\mathcal{U}^Q[f] \triangleq \sum_{j=1}^{Q} f(y^{(j)})\alpha^{(j)} \tag{5.8}$$

is an approximation to the integral

$$\mathcal{I}[f] \triangleq \int f(y)\rho(y)dy = \mathbb{E}[f(y)] \tag{5.9}$$

for sufficiently smooth functions $f(y)$, i.e.,

$$\mathcal{U}^Q[f] \approx \mathcal{I}[f]. \tag{5.10}$$

With such a choice of the nodal set, (5.7) approximates (3.8). Subsequently $\mathbb{I}_N^P u$ of (5.6) becomes an approximation of the exact gPC expansion $\mathbb{P}_N^P u$ of (3.7). The difference between the two,

$$\epsilon_Q \triangleq \left\| \mathbb{I}_N^P u - \mathbb{P}_N^P u \right\|_{L^2_\rho(\Gamma)} = \left(\mathbb{E}\left[(\mathbb{I}_N^P - \mathbb{P}_N^P)u \right]^2 \right)^{1/2}, \tag{5.11}$$

is caused by the integration error from (5.10) and is termed as "aliasing error" in [86], following the similar terminology from the classical deterministic spectral methods. (cf. [7, 30]).

The pseudo-spectral gPC method also requires only repetitive deterministic solutions with fixed "realizations" of the random inputs. The evaluation of the gPC coefficients (5.7) and the reconstruction of the gPC expansion (5.6) do not require additional solutions of the original system and can be considered as post-process procedures. Once the approximate gPC expansion (5.6) is available, we again have an analytical expression of the solution in term of the random inputs and solution statistics can be readily obtained, as discussed in Section 3.4. In this respect the pseudo-spectral approach is more advantageous than the Lagrange interpolation approach. The evaluations of the approximate gPC expansion coefficients (5.7) are completely independent. And one can choose to compute only a few coefficients that are important for a given problem without evaluating the other coefficients. This is in contrast to the gPC Galerkin method, where all the gPC coefficients are coupled and solved simultaneously. However, it should be noted that in the pseudo-spectral gPC method the existence of the aliasing error (5.11) can become a dominant source of errors in multi-dimensional random spaces. For more detailed discussions on pseudo-spectral gPC method and its error estimate, see [86].

5.3 Points selection

The selection of nodes is the key ingredient in all stochastic collocation methods. In both Lagrange interpolation and pseudo-spectral gPC methods, it is essential that the nodal set is a good cubature rule such that multiple integrals can be well approximated by a weighted discrete sum in the form of (5.5) or (5.10).

The point selection is straightforward in one-dimensional space (N=1), where numerous studies exist, and the optimal choice is usually the Gauss quadratures. The challenge is in multi-dimensional spaces with $N>1$, especially for large dimensions $N \gg 1$.

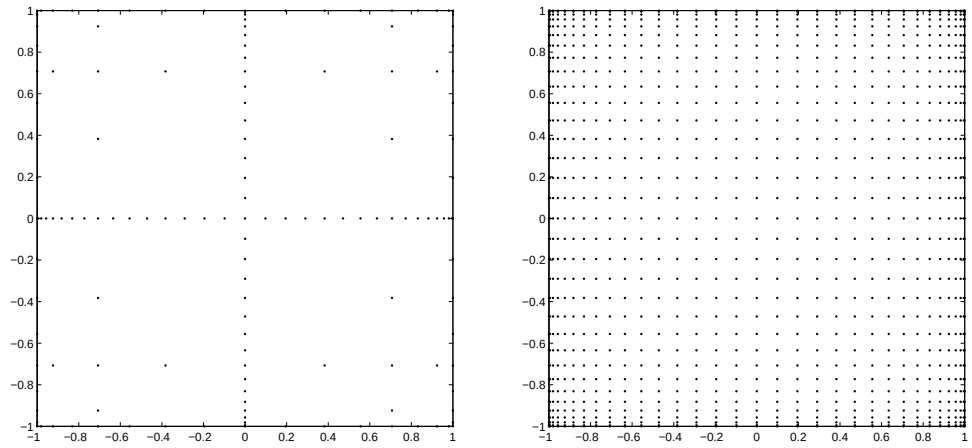

Figure 4: Two-dimensional ($N=2$) nodes based on the same one-dimensional grids. Left: Sparse grids. The total number of points is 145. Right: Tensor product grids. The total number of nodes is 1,089.

5.3.1 Tensor products

One choice is to use the tensor product of the one-dimensional nodes, e.g., Gauss quadratures. In this way the properties of one-dimensional interpolation and integration can be easily generalized. This approach has been used in the early work of deterministic sampling and collocation methods [52, 77], and its errors are analyzed in a recent work [4]. The problem for this approach is that the total number of points grows quickly in high dimensional random spaces. If one uses q points in each dimension, then the total number of points in a N-dimensional space is $Q=q^N$. For a (very) modest approximation with three points ($q=3$) in each dimension, $Q=3^N\gg 1$ for $N\gg 1$ (e.g., for $N=10$, $3^{10}\sim 6\times 10^4$). Because of the rapid growth of the number of nodes in high dimensions, the tensor product approach is mostly used at lower dimensions, e.g., $N\leq 5$.

5.3.2 Sparse grids

Sparse grids were first proposed in [71], and it has been studied in the context of multivariate integration and interpolation ever since ([6,56,57]). In [89] sparse grids were first introduced as an effective choice for high order stochastic collocation methods, and are now widely used.

The sparse grids, based on the Smolyak algorithm [71], are a subset of the full tensor product grids. The subset is chosen strategically in such a way that the approximation properties for $N=1$ are preserved for $N>1$ as much as possible. Fig. 4 shows the comparison of two-dimensional grids based the same one-dimensional nodes. It is clear that the sparse grids consist of much less number of nodes than that of the full tensor grids. As a result one can conduct stochastic collocation computations in much higher dimensional random spaces. For example, the first sparse grids stochastic collocation computations in [89] went to as high as $N=50$ random spaces.

5.3.3 Cubature rules

Cubature rules are designed to compute multiple integrals by discrete weighted sum, as in (5.10). This has been, and still is, an active research field. See [13, 33] for extensive reviews. Cubature rules are usually characterized by "degree". That is, a rule of degree m indicates (5.10) is exact when the integrand is any multivariate polynomials of degree at most m but not $m+1$. Most cubature rules have a fixed degree and, unlike the sparse grids, the integration accuracy can not be systematically refined. A large collection of cubature rules are available, and they can be good candidates in stochastic collocation computations.

It is worthwhile to point out two particular sets of low-degree cubature rules. One is a set of degree-two rules, which integrate up to second-degree multivariate polynomials exactly. The rules consist of $(N+1)$ equally weighted nodes in N-dimensional space, and the number of nodes is proved to be minimal. The other is a set of degree-three rules and require only $2N$ equally weighted nodes. These rules were first discussed in [75], for integrals in hypercube with constant integration weights, or uniform probability distribution in the context of stochastic computations. Later they were generalized to arbitrary integration domains with arbitrary probability distributions [87]. Due to the extremely small number of nodes, these rules can be highly efficient particularly for large scale problems. Although the integration degrees are relatively low, the results in many instances are surprisingly accurate.

6 General discussions

Since the first introduction of polynomial chaos by R. Ghanem in 1990's ([29]), and particularly the generalization to gPC ([91]), the field of stochastic computations has undergone tremendous growth, with numerous analysis and applications. Although the exposition of gPC here is in the context of boundary value problems (2.1), and the examples are for linear problems, the gPC framework can be readily applied to complex problems including the time-dependent and nonlinear ones, for example, Burgers' equation [34, 94], fluid dynamics [40, 41, 44, 46, 92], flow-structure interactions [96], hyperbolic problems [11, 31], material deformation [1, 2], natural convection [20], Bayesian analysis for inverse problems [51, 83], multibody dynamics [64, 65], biological problems [23, 99], acoustic and electromagnetic scattering [9, 10, 97], multiscale computations [3, 68, 88, 95, 100], model construction and reduction [16, 24, 28], etc.

6.1 Galerkin or collocation?

While the gPC expansion (3.7) provides a solid framework for stochastic computations, a question often asked is whether one should use the Galerkin method or the collocation method to solve for the expansion coefficients.

The advantage of stochastic collocation is clear – it requires only repetitive executions of existing deterministic solvers. Stochastic collocation methods has become very

popular after the introduction of high-order methods by using the sparse grids and cubature in higher dimensional random spaces [89]. Moreover, in addition to solution statistics, one can construct a similar gPC expansion like that of the Galerkin method via the pseudo-spectral approach without incurring more computations [86]. The applicability of stochastic collocations is not affected by the complexity or nonlinearity of the original problem, so long as one can develop a reliable deterministic solver.

The stochastic Galerkin method, on the other hand, is relatively more cumbersome to implement, primarily due to the fact that the equations for the expansion coefficients are almost always coupled. Hence new codes need to be developed to deal with the larger and coupled system of equations. Furthermore, when the original problem (2.1) takes highly complex form, the explicit derivation of the gPC equations may not be possible.

However, an important issue to keep in mind is that at the exact same accuracy (usually measured in term of the degree of gPC expansion), all of the existing collocation methods requires solutions of (much) larger number of equations than that of gPC Galerkin, especially for higher dimensional random spaces. Furthermore, the aliasing errors in stochastic collocation can be significant, especially, again, for higher dimensional random spaces [86]. This indicates that the gPC Galerkin method offers the most accurate solutions involving least number of equations in multi-dimensional random spaces, even though the equations are coupled.

The exact cost comparison between Galerkin and collocation depends on many factors including error analysis for the chosen collocation scheme which is largely unknown for many nodal sets and even coding efforts involved in developing a Galerkin code. However it is fair to state that for large-scale simulations where a single deterministic computation is already time consuming, the gPC Galerkin method should be preferred (because of the less number of equations) whenever (1) the coupling of gPC Galerkin equations does not incur much additional computational cost, for example, for Navier-Stokes equations with random boundary/initial conditions the evaluations of the coupling terms are negligible ([92]); or, (2) efficient solvers can be developed to effectively decouple the gPC system. For example, Galerkin methods for stochastic diffusion equation has been widely studied, see, for example, [5, 19, 36, 53, 90]. It has been shown that the Galerkin system of equations can be decoupled for both steady diffusion [90] and unsteady diffusion [93], and the technique was analyzed rigorously in [98].

Finally we remark the theory of the gPC Galerkin method for hyperbolic equations is much less developed. One important issue is the correspondence between the characteristics of the Galerkin system and those of the original equations. This was studied for a linear wave equation in [31], but much more is still unknown.

6.2 Multi-element basis

In this paper we have focused on gPC basis that are global orthogonal polynomials. In practice the basis does not need to be globally smooth. In fact when the stochastic solutions exhibit discontinuity in random space, gPC basis of piecewise polynomials

should be used to avoid accuracy lost. Such approaches include piecewise polynomial basis [5, 66], wavelet basis [42, 43], and multi-element gPC [80, 82]. When the basis is partitioned properly, gPC approximation can be highly accurate because the Gibb's oscillations are eliminated. The challenge is that for many problems, especially dynamical problems, the location of discontinuity in random space is not known *a priori*. Another potential issue is that whenever the random space is partitioned into elements in certain dimension, the construction of elements in the whole multi-dimensional space is inevitably through tensor product. Hence the number of elements can be too large. Combined with the gPC solution, Galerkin or collocation, inside each element, this can make computations prohibitively time consuming. This issue has been addressed in [80], where adaptive element selection is employed to reduce the total number of elements.

6.3 Long-term integration

Despite the success of PC and gPC in a large variety types of stochastic computations, it has long been recognized that gPC expansion may suffer accuracy loss for problems involving long-term integration. The problem is most noticeable when a stochastic solution takes a form of $\cos(\alpha(y)t)$, or any other oscillating functions, where $\alpha(y)$ represents a random frequency. In such cases when time t increases the convergence of a finite-order gPC expansion can not be retained for long. This is, however, not an inherent deficiency of gPC expansion. It is rather a result of the classical approximation theory. When a polynomial expansion in term of y is employed, as in gPC, the time variable t in such cases serves a role of "wavenumber". A well-known approximation theory states that the larger the "wavenumber" the more basis functions one needs to employ in order to keep a given accuracy (see, for example, [30]). Hence for a fixed accuracy requirement, in such stochastic computations one needs higher and higher order gPC expansions as time evolves. The convergence of gPC for such functions was discussed in [31, 81]. One typical application when the convergence issue may rise is wave propagation with random wave speed. For this problem the convergence of gPC Galerkin is proved and the result clearly shows that the approximation error is proportional to the time variable [31]. Note that such difficulty may very well occur in spatial domain, where a long spatial range x plays a similar role as t in the above example.

The problem of approximating functions with large wavenumber has been long standing. In stochastic computations, it is not clear if there is a better general-purpose alternative other than, albeit undesirable, to increase the resolution (e.g., order) of gPC expansions.

6.4 Curse of dimensionality

The dimensionality of the random space of the system (2.1) can be as large as possible, depending on the number of independent random variables involved in parameterizing the random inputs. It is not uncommon in engineering practices to encounter

problems involving $\mathcal{O}(100)$ number of independent random variables. Subsequently the computational cost of stochastic computations can quickly grow out of control – so-called "curse-of-dimensionality". Although with the fast growth of computing power and some newly developed adaptive algorithms, in both stochastic Galerkin and collocation methods [19, 20, 78–80], the difficulty is alleviated to some degree. It still remains one of the most eminent challenges of stochastic computations.

The brute-force Monte Carlo sampling method has a unique property in that its convergence rate, albeit slow, is independent of dimensionality asymptotically. Consequently for a given stochastic problem there should be a critical value such that when the random dimensionality is larger than the critical value, Monte Carlo method becomes advantageous. The precise determination of such a critical value is of course problem dependent.

7 Random domain problem

In the above discussions, we have assumed the computational domain D in (2.1) is fixed and contains no uncertainty. In practice, however, it can be a major source of uncertainty as in many applications the physical domain can not be determined precisely. The problem with uncertain geometry, i.e., rough boundary, has been studied in areas such as wave scattering with many specially designed techniques. (See, for example, a review in [84].) For general purpose PDEs, however, numerical techniques in uncertain domain are less developed. The problem, similar to (2.1), can be formulated as

$$\begin{aligned} &L(x,u)=0, \quad \text{in } D(y), \\ &B(x,u)=0, \quad \text{on } \partial D(y), \end{aligned} \tag{7.1}$$

where for simplicity the only source of uncertainty is assumed to be in the definition of the boundary $\partial D(y)$ which is parameterized by the random vector $y\in\Gamma\subset\mathbb{R}^N$. Note that even though the governing equation is deterministic (it does not need to be), the solution still depends on the random variables y.

A general computational framework is presented in [101], where the key ingredient is the use of a one-to-one mapping to transform the random domain into a deterministic one. Let

$$\xi=\xi(x,y), \qquad x=x(\xi,y), \qquad \forall y\in\Gamma, \tag{7.2}$$

be a one-to-one mapping and its inverse such that the random domain $D(y)$ is transformed to a deterministic one $E\subset\mathbb{R}^d$ whose coordinates are $\xi=(\xi_1,\cdots,\xi_d)$. Then (7.1) is transformed to the following problem: for all $y\in\Gamma$, find $u=u(\xi,y):\bar{E}\times\Gamma\to\mathbb{R}$ such that

$$\begin{aligned} &\mathcal{L}(\xi,u;y)=0, \quad \text{in } E, \\ &\mathcal{B}(\xi,u;y)=0, \quad \text{on } \partial E, \end{aligned} \tag{7.3}$$

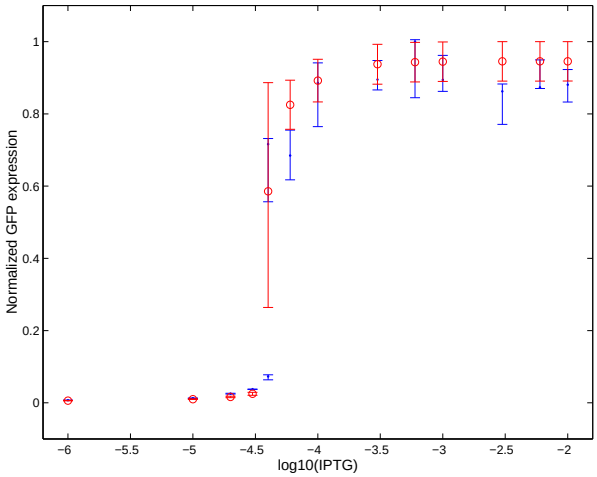

Figure 5: Steady-state gene expression of a genetic toggle switch. Light (and red) error bars centered around circles are numerical results; Dark (and blue) error bars around dots are experimental measurements. The re-production of the experimental results from [22] is courtesy of Dr.Gardner. Numerical simulation details can be found in [86].

where the operators L and B are transformed to $\mathcal{L}$ and $\mathcal{B}$, respectively, because of the random mapping (7.2). The transformed problem (7.3) is a stochastic PDE in a fixed domain and all of the aforementioned gPC techniques apply.

The key is to construct an efficient and robust random mapping (7.2). This can be achieved analytically, as demonstrated in [76]. Often analytical mapping is not available, then a numerical technique can be employed to determine the mapping, as presented in [101]. Other techniques to cast random domain problem into deterministic problem include boundary perturbation method [97], isoparametric mapping [9], and a Lagrangian approach that works well for solid deformation [2]. A different kind approach based on fictitious domain method is presented in [8].

Problems with rough geometry remain an important research direction. Despite these recent algorithm development, computations in random domains are still at an early stage. We note here a recent interesting computational result that reports lift force enhancement in supersonic flow due to surface roughness [45].

8 Summary

This paper presents an extensive review of the current state of numerical methods for stochastic computation and uncertainty quantification. The focus is on fast algorithms based on the generalized polynomial chaos (gPC) expansion. Upon introducing the gPC framework, the two major approaches for implementation, Galerkin and collocation, are discussed. Both approaches, when properly implemented, can achieve fast convergence and high accuracy and be highly efficient in practical computations. This is due to the fact that the gPC framework is a natural extension of spectral methods into multi-dimensional

random space. Important properties of different approaches are discussed without going into too much technical details, and more in-depth discussions can be found in the references which consist of mostly published work. With the field advancing at such a fast pace, new results are expected to appear on a continuously basis to help us further understand and enhance the methods.

We close the discussion by another illustrative example, a stochastic computation of a biological problem in Fig. 5. The figure shows the steady-state of a genetic toggle switch whose mathematical model consists of a system of differential/algebraic equations (DAE) with six random parameters. This is a comparison of numerical error bars (in red) and experimental error bars (in blue). The two sets of bars were generated completely independently and agree each other well. (The larger discrepancy at the switch location is due to a non-standard plotting technique used in the experimental work. More details are in [86].) This kind of comparison is not possible for classical deterministic simulations. By incorporating uncertainty from the beginning of the computations, we are one step closer to the ultimate goal of scientific computing — to predict the true physics.

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