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Modeling Uncertainty of Elliptic Partial Differential Equations via Generalized Polynomial Chaos

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ABSTRACT

We present a generalized polynomial chaos algorithm to solve the elliptic boundary value problems suject to stochastic uncertain inputs. In particular we focus on the solution of the Poisson equation with random diffusivity and forcing. The stochastic input and solution are represented spectrally by employing the orthogonal polynomial functionals from the Askey scheme, as a generalization of the original polynomial chaos idea of Wiener (1938). A Galerkin projection in random space is applied to satisfy the equations in weak form. The resulting set of deterministic equations is solved iteratively by a block Gauss-Seidel technique. Both discrete and continuous stochastic distributions are considered and convergence is demonstrated for model problems.

Keywords: uncertainty, random diffusion, polynomial chaos

INTRODUCTION

The objective of this paper is to give a broad algorithmic framework to solve stochastic elliptic partial differential equations based on the generalized polynomial chaos expansion. The class of problems we solve has the form

$$\begin{cases} \nabla \cdot [\kappa(x;\omega)\nabla u(x;\omega)] = f(x;\omega), & (x;\omega) \in D \times \Omega \\ u(x;\omega) = g(x;\omega), & (x;\omega) \in \partial D \times \Omega \end{cases} \tag{1}$$

where D is a bounded domain in $\mathbb{R}^d$ $(d = 1, 2, 3)$ and Ω is a probability space. f, g and κ are $\mathbb{R}$-values functions on $D \times \Omega$. This can be considered as a model of steady state diffusion problems subject to internal (diffusivity κ) and/or external (source term f and/or Dirichlet boundary condition g) uncertainties. Similar problems have been considered and their mathematical properties studied (Babuška 1961; Bécus and Cozzarelli 1976; Deb et al. 2000).

In this paper, we solve the steady state diffusion problem (1) by generalized polynomial chaos expansion. The generalized polynomial chaos is a generalization of the classical polynomial chaos, which is based on the theory of Wiener (Wiener 1938), and was applied to various practical problems in mechanics by Ghanem & Spanos (Ghanem and Spanos 1991).

The key ingredient of the chaos expansion is to approximate the random process by a complete and orthogonal polynomial basis in terms of random variables. A second-order random

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process $X(\omega)$ can be represented as

$$X(\omega) = \sum_{j=0}^{\infty} a_j \Phi_j(\boldsymbol{\xi}(\omega)), \tag{2}$$

where $\Phi_n(\boldsymbol{\xi})$ denotes the *generalized polynomial chaos* of order n in terms of the multi-dimensional random variables $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_n, \ldots)$. The expansion bases $\{\Phi_n\}$ are multi-dimensional hypergeometric polynomials defined as tensor-products of the corresponding one-dimensional polynomial bases. The orthogonal polynomials involved in generalized polynomial chaos are listed in table 1, together with their corresponding underlying random variables. These polynomials belong to the class of Askey scheme (Askey and Wilson 1985). The classical polynomial chaos, which employs $Hermite$ polynomials in terms of $Gaussian$ random variables, is a subset of the generalized polynomial chaos. For a detailed account of the generalized polynomial chaos and their applications, see (Xiu and Karniadakis 2001; Xiu and Karniadakis 2002; Xiu et al. 2002).

TABLE 1. Correspondence of the orthogonal polynomials and random variables for different Askey-chaos ($N \geq 0$ is a finite integer).

	Random variables $\boldsymbol{\xi}$	Orthogonal polynomials $\{\Phi_n\}$	Support
Continuous	Gaussian	Hermite	$(-\infty, \infty)$
	Gamma	Laguerre	$[0, \infty)$
	Beta	Jacobi	$[a, b]$
	Uniform	Legendre	$[a, b]$
Discrete	Poisson	Charlier	$\{0, 1, 2, \ldots\}$
	Binomial	Krawtchouk	$\{0, 1, \ldots, N\}$
	Negative Binomial	Meixner	$\{0, 1, 2, \ldots\}$
	Hypergeometric	Hahn	$\{0, 1, \ldots, N\}$

ALGORITHM

By applying the chaos expansion, we expand the variables as

$$\kappa(x;\omega) = \sum_{i=0}^{M} \kappa_i(x)\Phi_i(\boldsymbol{\xi}), \qquad u(x;\omega) = \sum_{i=0}^{M} u_i(x)\Phi_i(\boldsymbol{\xi}), \qquad f(x;\omega) = \sum_{i=0}^{M} f_i(x)\Phi_i(\boldsymbol{\xi}), \tag{3}$$

where we have replaced the infinite summation of $\boldsymbol{\xi}$ in infinite dimensions in equation (2) by a truncated finite-term summation of $\{\Phi\}$ in the finite dimensions of $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_n)$. The dimensionality n of $\boldsymbol{\xi}$ is determined by the random inputs. By substituting the expansion into governing equation (1) and conducting a Galerkin projection onto each polynomial basis $\{\Phi_i\}$, we obtain

$$\sum_{j=0}^{M} \left[b_{jk}(x)\nabla^2 u_j(x) + h_{jk}(x) \cdot \nabla u_j(x) \right] = f_k(x) < \Phi_k^2 >, \qquad \forall k \in [0, M], \tag{4}$$

where

$$b_{jk}(x) = \sum_{i=0}^{M} \kappa_i(x) e_{ijk}, \qquad h_{jk}(x) = \sum_{i=0}^{M} \nabla\kappa_i(x) e_{ijk} = \nabla b_{jk}(x).$$

The coefficients $e_{ijk} =< \Phi_i \Phi_j \Phi_k >$ and $< \Phi_i^2 >$ can be evaluated analytically from the definition of Φ_i.

Equation (4) is a set of $(M+1)$ coupled *deterministic* elliptic partial differential equations. They can be discretized by any conventional method. In this paper we employ the spectral/hp element method (Karniadakis and Sherwin 1999). The total number of equations $(M+1)$ is determined by the dimensionality of the chaos expansion (n) and the highest order (p) of the polynomials $\{\Phi\}$:

$$(M+1) = (n+p)!/(n!p!). \tag{5}$$

Equation (4) is solved by the block Gauss-Seidel iteration: for all $k = 0, \dots, M$,

$$\begin{aligned} b_{kk}(x)\nabla^2 u_k^{n+1}(x) + h_{kk}(x) \cdot \nabla u_k^{n+1}(x) &= f_k(x) < \Phi_k^2 > \\ &- \sum_{j=0}^{k-1} \left[b_{jk}(x)\nabla^2 u_j^{n+1}(x) + h_{jk}(x) \cdot \nabla u_j^{n+1}(x) \right] \\ &- \sum_{j=k+1}^{M} \left[b_{jk}(x)\nabla^2 u_j^{n}(x) + h_{jk}(x) \cdot \nabla u_j^{n}(x) \right] \end{aligned} \tag{6}$$

where the superscript n denotes the iteration number. The convergence criterion is defined as

$$\frac{\|u_k^{n+1}(x) - u_k^n(x)\|}{\|u_k^1(x) - u_k^0(x)\|} \leq \varepsilon, \qquad \forall k \in [0, M], \tag{7}$$

where ε is a small positive number. In this paper the L_∞ norm for $\| \cdot \|$ is used and ε is $10^{-5} \sim 10^{-7}$. For all the results we present here, the block Gauss-Seidel iteration normally converges within 10 steps.

NUMERICAL RESULTS

In this section we present numerical results. Among the types of chaos expansions listed in table 1, we choose one continuous chaos: Jacobi-chaos; and one discrete chaos: Charlier-chaos for demonstration purposes.

One-Dimensional Model Problem

Consider the following problem

$$\frac{d}{dx}\left[\kappa(x;\omega)\frac{du}{dx}(x;\omega)\right] = 0, \qquad x \in [0,1], \tag{8}$$

with boundary conditions $u(0;\omega) = 0$ and $u(1;\omega) = 1$. The random diffusivity has the form $\kappa(x;\omega) = 1 + \epsilon(\omega)x > 0$, where $\epsilon(\omega)$ is a random variable. The exact solution to this problem is

$$u_e(x;\omega) = \begin{cases} \ln\left[1+\epsilon(\omega)x\right] / \ln\left[1+\epsilon(\omega)\right], & \text{for } \epsilon(\omega) \neq 0; \\ x, & \text{for } \epsilon(\omega) = 0. \end{cases} \tag{9}$$

The 'mean-square' error of the p^{th}-order chaos expansion solution $u_p(x,\omega)$ is computed as $e_2(x) = \left(\mathbb{E}\left[u_p(x,\omega) - u_e(x,\omega)\right]^2\right)^{\frac{1}{2}}$, where $\mathbb{E}$ denotes the 'expectation' operator.

We first assume $\epsilon(\omega)$ is a *beta* random variable with probability density function

$$f(\epsilon;\alpha,\beta) = \frac{(1-\epsilon)^\alpha(1+\epsilon)^\beta}{2^{\alpha+\beta+1}B(\alpha+1,\beta+1)}, \qquad \epsilon \in [-1,1],\ \alpha,\beta > -1, \tag{10}$$

where $B(\alpha, \beta) = \Gamma(\alpha)\Gamma(\beta)/\Gamma(\alpha + \beta)$ is the Beta function. The corresponding generalized polynomial chaos is the Jacobi-chaos (table 1). On the left of figure 1 the mean-square convergence of the Jacobi-chaos solution is shown with different standard deviation σ of the input. It can be seen on the semi-log scale that the Jacobi-chaos solution converges exponentially fast as the expansion order p increases. The exponential convergence rate is retained for large input uncertainty such as $\sigma = 0.9$, which is close to the limit of the existence of the solution ($\sigma < 1$).

If $\epsilon(\omega)$ a discrete random variable with Poisson distribution

$$f(\epsilon; \lambda) = e^{-\lambda} \frac{\lambda^{\epsilon}}{\epsilon!}, \qquad \epsilon = 0, 1, 2, \ldots, \ \lambda > 0, \tag{11}$$

we employ the Charlier-chaos (table 1). The exponential convergence of the Charlier-chaos expansion is shown on the right of figure 1 for two different values of the parameter λ.

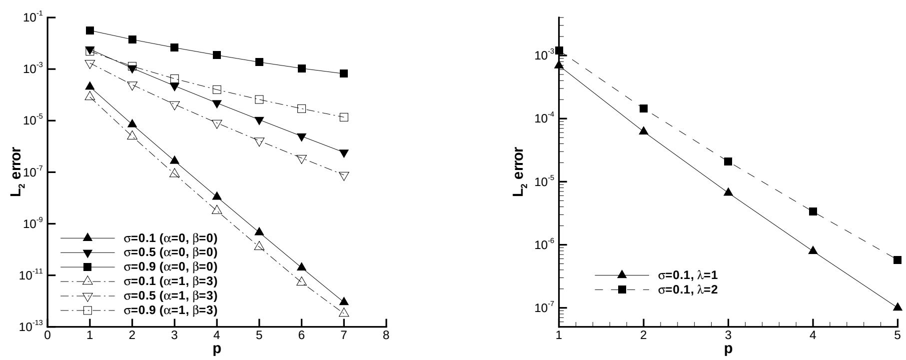

FIG. 1. Convergence of Askey-chaos for the one-dimensional model problem; Left: Jacobi-chaos and beta distribution, Right: Charlier-chaos and Poisson distribution.

Two-Dimensional Model Problem

In this section we consider the two-dimensional problem

$$\nabla \cdot [\kappa(x, y; \omega)\nabla u(x, y; \omega)] = f(x, y; \omega), \qquad (x, y) \in [-1, 1] \times [-1, 1] \tag{12}$$

with boundary conditions

$$u(-1, y; \omega) = 1, \qquad \frac{\partial u}{\partial x}(1, y; \omega) = 0, \qquad u(x, -1; \omega) = 0, \qquad \frac{\partial u}{\partial y}(x, 1; \omega) = 0.$$

The diffusivity $\kappa(x, y; \omega)$ and source term $f(x, y; \omega)$ are stochastic processes with mean fields $\bar{\kappa}(x, y; \omega) = 1$ and $\bar{f}(x, y; \omega) = 0$, and correlation functions in the form of $C(r) = \frac{r}{b} K_1\left(\frac{r}{b}\right)$, where K_1 is the modified Bessel function of the second kind with order 1, b scales as the correlation length and r is the distance between two points. It has been shown that this is the 'elementary' correlation function in *two dimensions* (Whittle 1954). The Karhunen-Loeve decomposition (Loève 1977) is applied to the correlation function to reduce the dimensionality in the random space. The first four eigenmodes are employed from the Karhunen-Loeve decomposition, which results in a four-dimensional ($n = 4$) chaos expansion. For computational simplicity, we further arrsum k and f fully cross-correlated. For spatial spectral/hp element discretization, an array of 5×5 elements are used and sixth-order (Jacobi) polynomials are employed in each element. In random space, third-order ($p = 3$) chaos expansion is used. The total number of expansion terms is then 35 (see equation (5)). Numerical results show that this is sufficient to resolve the problem in both physical space and random space. The Monte Carlo simulations are conducted to validate the chaos solution.

We first assume $\kappa(x, y; \omega)$ and $f(x, y; \omega)$ are random fields with uniform distribution, with $\sigma_\kappa = \sigma_f = 0.4$. The solution profiles along the horizontal centerline through the domain are shown in figure 2 and figure 3, for mean and variance profiles, respectively. A noticeable difference between the stochastic mean profile and the deterministic profile is observed. It can be seen that the Monte Carlo solution converges to the chaos solution as the number of realizations increases. Good agreement is obtained with $50,000$ realizations.

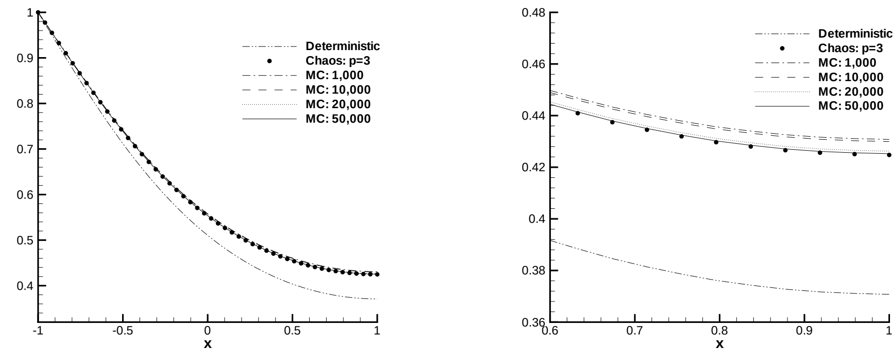

FIG. 2. Two-dimensional model problem: uniform random distribution and Legendre-chaos; Left: Mean solution along the horizontal centerline, Right: Close-up view.

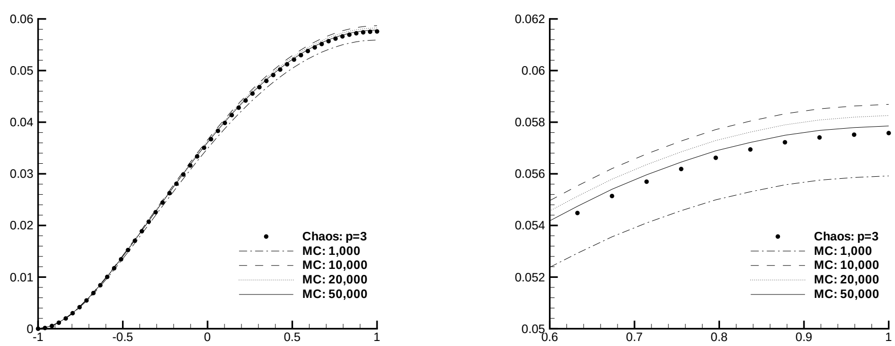

FIG. 3. Two-dimensional model problem: uniform random distribution and Legendre-chaos; Left: Variance along the horizontal centerline, Right: Close-up view.

Next we assume the $\kappa(x, y; \omega)$ and $f(x, y; \omega)$ are Poisson processes, with $\sigma_\kappa = \sigma_f = 0.2$ and $\lambda = 1$ in (11). The solution profiles of the mean and variance along the horizontal centerline are shown in figure 4 and 5, respectively. The Monte Carlo solution converges to the solution of Charlier-chaos; with $100,000$ realizations we obtain good agreement.

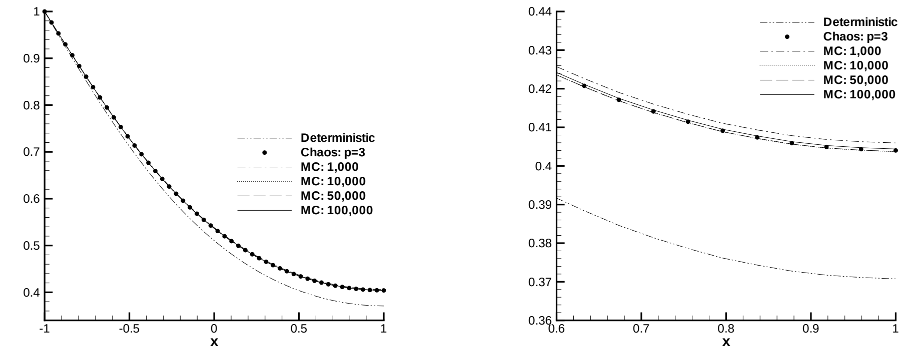

FIG. 4. Two-dimensional model problem: Poisson random distribution and Charlier-chaos; Left: Mean solution along the horizontal centerline, Right: Close-up view.

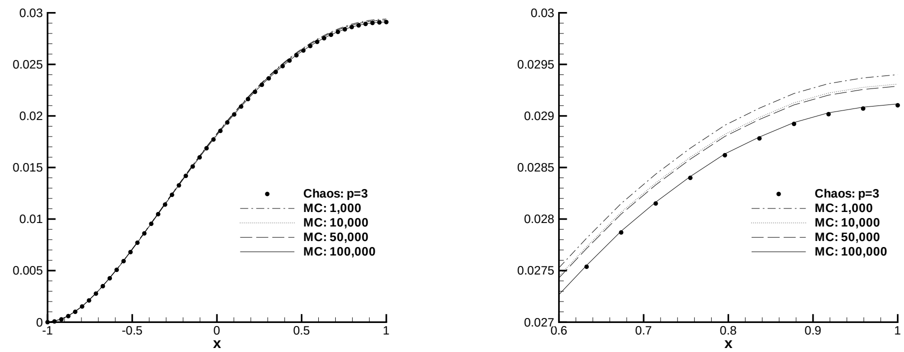

FIG. 5. Two-dimensional model problem: Poisson random distribution and Charlier-chaos; Left: Variance along the horizontal centerline, Right: Close-up view.

Random Heat Conduction in a Grooved Channel

In this section we consider the steady state heat conduction in a grooved channel subject to uncertainties in boundary conditions and diffusivity.

$$\nabla \cdot [\kappa(x, y; \omega) \nabla u(x, y; \omega)] = 0, \qquad (x, y) \in D, \tag{13}$$

where the computational domain D is shown in figure 6. The boundary conditions are

$$u|_{\Gamma_T} = 0, \qquad u|_{\Gamma_B} = 1, \qquad \left.\frac{\partial u}{\partial x}\right|_{\Gamma_S} = 0, \qquad u|_{\Gamma_C} = 1 + \xi, \tag{14}$$

where ξ is a random variable with uniform distribution. The diffusivity $\kappa(x, y; \omega)$ is a uniformly distributed random field, with mean field $\bar{\kappa}(x, y; \omega) = 1$ and the Bessel correlation function.

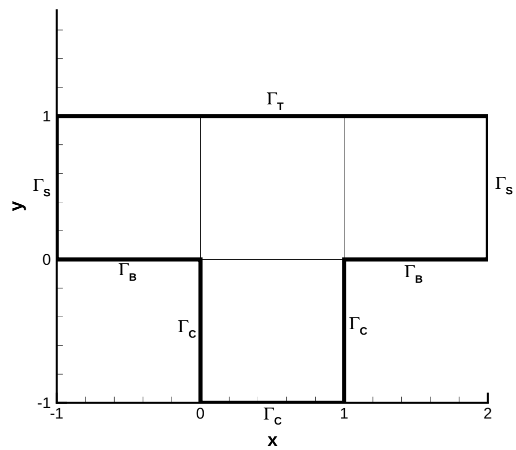

FIG. 6. Schematic of the domain of the grooved channel

In physical space, 10^{th}-order polynomials are employed within each of the four elements as shown in figure 6; in random space, the third-order Legendre-chaos is used.

We consider two cases: the first case is when only the diffusivity κ is random, while the boundary condition along Γ_C is deterministic, i.e. $u|_{\Gamma_C} = 1$. Again, four-dimensional ($n = 4$), third-order chaos ($p = 3$) with 35 expansion terms is used. In the second case, we further assume the boundary condition along Γ_C is random as in (14), and is independent of the random field κ. This introduces one more dimension in the random space and a total of 56 expansion terms are needed for third-order chaos; $n = 5$, $p = 3$ from (5).

In figure 7, the contours of the standard deviations of the solution are plotted. The solution of the first case is shown on the left, while solution of the second case on the right. In both cases, the standard deviations of the random inputs are $\sigma = 0.2$. No noticeable difference is observed between the mean solutions of the two cases, and that of the corresponding deterministic case. However, the standard deviations of the solutions are very different: the effect of uncertainty in the diffusivity is subdominant (maximum deviation about only 0.15%). By introducing the uncertainty in boundary condition, the output uncertainty is greatly enhanced in the entire domain (maximum deviation about 12%), and its maximum moves from the center of the channel to the lower wall of the cavity.

SUMMARY

We have developed a stochastic spectral method to model uncertainty in steady state diffusion problems. The generalized polynomial chaos we introduced is an extension of the original chaos idea of Wiener (1938) and of the work of Ghanem & Spanos (1991). It incorporates different types of chaos expansion corresponding to several important distribution functions, including some $discrete$ distributions. We have applied the generalized polynomial chaos to the solution of steady state random diffusion problems. It is shown for model problem that, when the appropriate chaos expansion is chosen, the generalized polynomial chaos expansion converges exponentially fast, in accordance with the result of (Xiu and Karniadakis 2001). For more complicated problems, we observe good agreement between the well-resolved chaos expansion solution and the converged Monte Carlo simulation results. For the problems considered here, the generalized polynomial chaos expansion is at least two to three orders faster

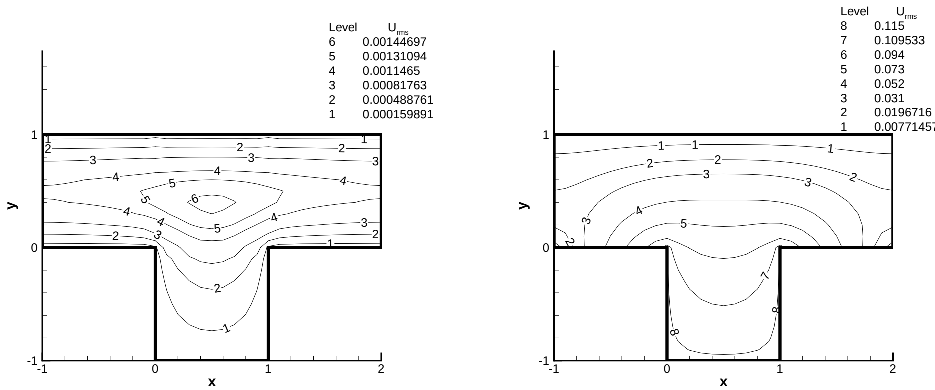

FIG. 7. Standard deviations of heat conduction in the grooved channel; Left: solution subject to random diffusivity only; Right: solution subject to random diffusivity and random boundary conditions.

than the Monte Carlo simulation.

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