Application of polynomial chaos in modeling one dimensional stochastic heat conduction equation

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I. INTRODUCTION

In most engineering applications, one aims to solve physical problems by converting it into a deterministic mathematical model. This is a rough approximation of reality, as many physical input parameters describing the problem are fixed through this conversion. In reality however, these parameters show some randomness which definitely influence the behavior of the solution. This randomness is not incorporated in the deterministic model. In order to include this uncertainty in the mathematical model, probabilistic methods have been developed.

The traditional statistical approach for uncertainty quantification is the Monte Carlo (MC) method [1, 2]. With the brute force MC implementation, one first generates an ensemble of random realizations with each parameter drawn from its uncertainty distribution. Deterministic solvers are then applied to each member to obtain an ensemble of results. The ensemble of results is post-processed to obtain the relevant statistical properties of the results such as the mean and standard deviation, as well as the probability density function (PDF). Since the estimation of the variance converges with the inverse square root of the number of runs, the MC approach is computationally expensive.

Polynomial Chaos (PC) is one of the modern approaches to quantify uncertainty in system models. The PC method originates from the homogeneous chaos concept define by Wiener [3]. Ghanem and co-worker [4] showed that PC is an effective computational tool for engineering studies. Karniadakis and Xiu [5] generalized and expanded the concept by using orthogonal polynomials from the Askey-scheme class as the expansion basis. K.A.Puvkov et.al. [6] proposed that if the Wiener–Askey polynomial chaos expansion is chosen according to the probability distribution of the random input, then the chaos expansion allows possibility to construct simple algorithms for statistical analysis of dynamic system. Based on the PC expansion, several methods have been proposed that include the Non-Intrusive Polynomial Chaos (NIPC) method [7], the Stochastic Response Surface Method (SRSM) [8], and the Deterministic Equivalent Modeling Method (DEMM) [6, 9].

This work is organized as follows. In the section 2, PC method is briefly introduced. The method is then applied for statistical analysis of one dimensional heat conduction equations with random coefficient and the result is compared with traditional Monte Carlo method.

II. POLYNOMIAL CHAOS THEORY

1. Polynomial chaos theory

Polynomial Chaos (PC) is a spectral representation of random process by completed orthonormal polynomial of random variable.

Consider complete probability space (Ω, F, P). A general second order random process $X(\theta) \in L_2(\Omega, F, P)$ can be presented as

$$X(\theta) = \sum_{i=1}^{\infty} a^i \Phi^i(\xi(\theta)) \tag{1}$$

where θ is random event, and $\Phi^i(\xi(\theta))$ are polynomial functional defined in term of multi-dimensional random variable $\xi(\theta) = (\xi_1(\theta), ..., \xi_n(\theta))$ with joint probability distribution function $w(\xi)$. The family $\{\Phi^i\}$ is complete orthonormal basis

$$\left\langle \Phi^i, \Phi^j \right\rangle = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases} \tag{2}$$

where the inner product on the Hilbert space is the ensemble average $\langle .,. \rangle$

$$\int f(\xi) g(\xi) w(\xi) d\xi \tag{3}$$

If the uncertainties in the model are independent random variables $\xi = (\xi_1, ..., \xi_2)$ with a joint probability distribution

$w(\xi) = w^1(\xi_1)...w^n(\xi_n)$, then a multi-dimensional orthogonal basis is constructed from the tensor products of one-dimensional polynomials $\{P^k{}_m\}$ orthogonal with respect to the density w^k [10]

$$\Phi^i(\xi_1,...,\xi_n) = P_{i_1}^{\,1}(\xi_1)...P_{i_n}^{\,n}(\xi_n) \tag{4}$$

PC expansion involve following steps [6]:

- Choosing appropriate basis based on probability characteristic of random parameters.
- Expanding the uncertainty variables
- Using the Galerkin projection or collocation approaches to find coefficients a^i of PC expansion.

Let consider a simple example to demonstrate idea of PC [11]

$$y'(t) = f(y(t),\xi) \tag{5}$$

The infinite dimension of the polynomial space given in (1) must be replaced for computational use by a finite dimension S

$$y(t) = \sum_{i=1}^{S} a^i(t)\Phi^i(\xi) \tag{6}$$

In general, the number of terms S needed to describe each uncertain variable in a PC expanded model can be obtained by using

$$S = (\frac{(n+k)!}{n!k!} - 1) \tag{7}$$

where n is the number of random variable, k is the order of the polynomial basis to be used.

Substitute (6) to (5)

$$\sum_{i=1}^{S}(a^i(t))'\Phi^i(\xi) = f(\sum_{i=1}^{S} a^i(t)\Phi^i(\xi)) \tag{8}$$

The coefficient of PC expansion can be calculated by Galerkin or collocation approaches as below

In the Galerkin PC approach, we project system (8) on the spaced spanned by orthonormal polynomial PC, i.e., we take the inner product of (8) with $\Phi^i(\xi)$ to obtain

$$(a_i(t))' = \left\langle \Phi^i(\xi), f(\sum_{i=1}^{S} a^i(t)\Phi^i(\xi)) \right\rangle \quad 1 \le i \le S \tag{9}$$

The original $y(t)$ is substituted by the coefficients of PC expansion $a^1(t),\ a^2(t),\ ...,\ a^S(t)$. With this approach entire stochastic system needs to be evolved in time with the integration executed once. When the number of uncertainties grows significantly, the Galerkin projections usually substituted with collocation method.

In DEMM [6] Gaussian quadrature is used for averaging projection of right-hand side (9).

2. Statistical analysis using polynomial chaos

Consider function $\eta(t,\xi)$ of states of stochastic dynamic system in PC expansion form

$$\eta(t,\xi) = \sum_{i=1}^{S} \hat{q}_i\Phi^i(\xi) \tag{10}$$

Here $\hat{q}_i = q_i(t)$ $i = 1,S$ for convenient of notation.

The expectation of $\eta(t,\xi)$ is

$$M[\eta(t,\xi)] = \int_V \eta(t,\xi)w(\xi)d\xi = \int_V \Phi^1(\xi)\sum_{i=1}^{S}\hat{q}_i\Phi^i(\xi)w(\xi)d\xi = q_1(t) \tag{11}$$

where V is support domain of random variable ξ .

In (11, 12), the properties that polynomial sets starting with $\Phi^0(\xi) = 1$ and the weighting function of the polynomial is the probability density function are used.

The variance of $\eta(t,\xi)$ is

$$\mathrm{var}[\eta(t,\xi)] = \int_V [\sum_{i=1}^{S}\hat{q}_i\Phi^i(\xi) - q_1][\sum_{i=1}^{S}\hat{q}_i\Phi^i(\xi) - q_1]w(\xi)d\xi = \sum_{i=2}^{s} q_i^{\,2} \tag{12}$$

i.e., variance can be calculated as the sum of the squares of all PC coefficients, except the first one.

Thus, if $\eta(t,\xi) = y(t,\xi)$ then the mean and the variance of output of system are approximately given by truncated series (11, 12). Note that performing finite series truncations is a commonly used practice when dealing with orthogonal sets since spectral series generally converges extremely rapidly for well-behaved problems.

3. Legendre polynomial chaos and uniform distribution [6]

For not to build up the orthonormal basis for each uniform random variable, we need to convert the original random variables to of a standard form of the classical laws distribution (uniform in [-1,1]), i.e. to those laws which are already known to the system orthogonal polynomials. If a random variable λ has a uniform law distribution on the interval [a, b], then using the linear transformation

$$\lambda = \frac{b-a}{2}V + \frac{b+a}{2} \tag{13}$$

the interval [a, b] can be transform into the interval [-1, 1], where V is uniform in [-1, 1]. Orthogonal system polynomials on the interval [-1, 1] with weighting $f(V) = \frac{1}{2}$ is a system Legendre polynomials, which can be determined from the following recurrence equation

$$P_0^*(V) = 1,\ P_1(V) = V(n+1); \qquad P_{n+1}^*(V) = (2n+1)VP_n^*(V) - nP_{n-1}^*(V) \tag{14}$$

Thus, orthonormal polynomial Legendre is given by

$$P_n(V) = P_n^*(V)\sqrt{\frac{2n+1}{n}} \tag{15}$$

III. CASE STUDIES

Consider one-dimensional heat conduction equation

Case 1	*Case 2*
$\frac{\partial u}{\partial t} = \kappa \frac{\partial u^2}{\partial^2 x};\quad 0 \le x \le \pi;\quad 0 \le t \le 3$ (16) With initial condition and boundary conditions $u(x,0) = \sin(x)$ (17) $u(0,t) = 0;\ u(\pi,t) = 0$ (18)	$\frac{\partial u}{\partial t} = \kappa \frac{\partial u^2}{\partial^2 x};\quad 0 \le x \le 1;\quad 0 \le t \le 2.5$ (19) With initial condition and boundary condition $u(x,0) = \sin(\frac{\pi x}{2})$ (20) $u(0,t) = 0;\quad u_x(1,t) = 0$ (21)

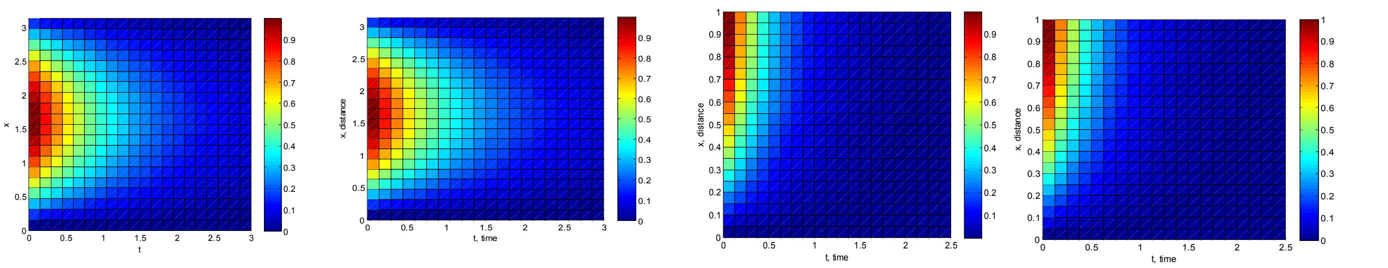
Prediction of mean and variance of the solution by PC method and Monte Carlo method is shown in figure 1, 2, 3. Simulation parameter and computational time for both cases are listed in table 1, 2 respectively. The computer with AMD Phenom II X3 2.81 GHz 2GB RAM was used for the test. Calculations were made using the library DEMM [6] .

Case	Monte-Carlo	Polynomial Chaos
1	Number of samples for κ 6000	Order of Legendre chaos: 5
2	Number of samples for κ 6000	Order of Legendre chaos :5

Table 1 Simulation parameters for case studies

Case	Monte-Carlo	Polynomial Chaos
1	45 sec.	1 sec
2	60 sec	1 sec

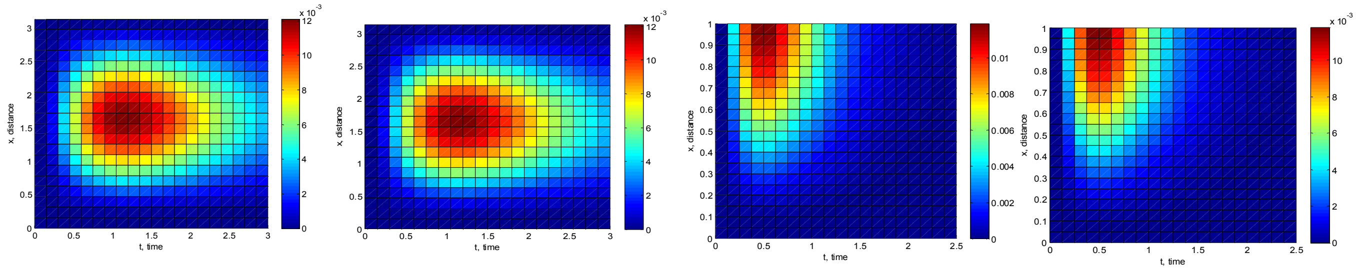
Table 2 Computation time for case studies



PC Monte Carlo PC Monte Carlo

Case1 Case 2

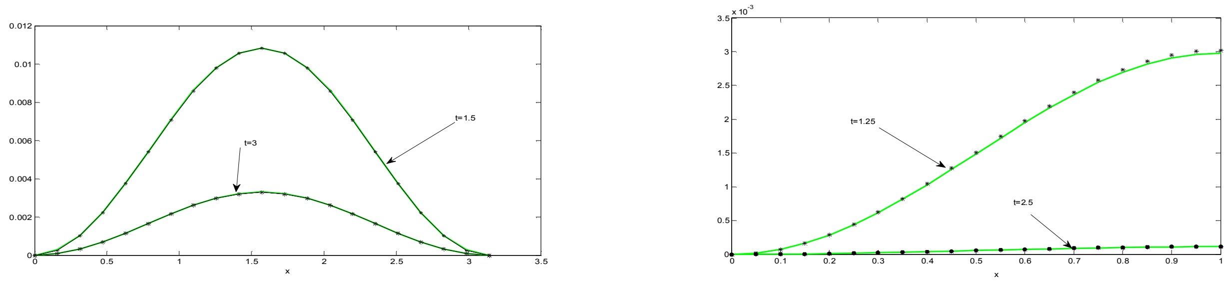
Fig. 1. Mean of solution $M[u(x,t)]$



PC Monte PC Monte

Case 1 Case 2

Fig. 2. Variance of solution $D[u(x,t)]$



Case 1 Case 2

Fig. 3. Slices of variance surface at different time moment. Monte-Carlo: green line, PC: black line

IV. Conclusions

In this work, a statistical analysis for one dimensional stochastic heat conduction equation was studied. It is shown that the use of Polynomial Chaos method drastically reduces a computation time with a desired accuracy over that by the traditional Monte-Carlo method. Simulation examples have shown that the method gives accurate results for prediction statistical characteristic of one dimensional stochastic heat conduction equation.

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