Applicability of the spectral stochastic finite element method in time-dependent uncertain problems

By D. Ghosh AND G. Iaccarino

1. Motivation and objectives

While analyzing a physical system, we always observe discrepancies between the response of the system and the predictions obtained using mathematical models. One important source of such discrepancy is the uncertainty, may it be pertaining to insufficient system characteristics, modeling error, natural variability of the system or the physical phenomena, manufacturing variability, etc. Therefore predictive models should take these uncertainties into consideration. One widely accepted framework of developing such models is based on the probability theory, where the uncertain parameters are modeled as random quantities with some known statistical properties, and the statistical description of the response of the model is sought. Perhaps the most straightforward tool in such a framework is the Monte Carlo simulation (MCS), which builds statistics of the response using a large ensemble of realizations obtained by sampling the uncertain input. MCS is however computationally very expensive. Among the alternatives, the spectral stochastic finite element method (SSFEM) has been successful in many applications. The method is briefly described here.

Let the underlying probability space of uncertainty be denoted by $(\Omega, \mathcal{F}, P)$; here Ω denotes the set of elementary events, $\theta \in \Omega$, $\mathcal{F}$ denotes a σ-algebra on that event set, and P denotes the probability measure. Let the physical domain of the system — in general a spatial domain — be denoted by $\mathcal{D}$, and let $\boldsymbol{x} \in \mathcal{D}$. Then a time-dependent problem with uncertainty can expressed as the following equation

$$\begin{aligned} \mathcal{L}(y(\boldsymbol{x}, t, \theta)) &= s(\boldsymbol{x}, t, \theta) \quad \boldsymbol{x} \in \mathcal{D}, \quad t \in [0, T],\ T \in \mathbb{R}, \\ y(\boldsymbol{x}, t, \theta) &= y_b(\boldsymbol{x}, t, \theta) \quad \boldsymbol{x} \in \partial\mathcal{D}, \quad \forall\ t \end{aligned} \tag{1.1}$$

to hold almost everywhere (a.e.) on Ω, where $y(\boldsymbol{x}, t, \theta), s(\boldsymbol{x}, t, \theta) : \mathcal{D} \times [0, T] \times \Omega \to \mathbb{R}$. In effect, the coefficients in this equation, and sometimes in the boundary conditions are random quantities that incorporate the underlying uncertainty in the system. Furthermore, in some cases the external forcing function s also can be random. In a probabilistic framework these parameters are modeled as random variables or as random processes. However, the random processes are infinite dimensional objects, thus introduces a considerable computational challenge. The essence of a stochastic finite element method is to discretize the random processes using a suitable basis set in the space of square-integrable random variables $L_2(\Omega)$. As an example, the Karhunen-Loève (KL) expansion (Ghanem & Spanos 2003) can be used to this end when the covariance of a process is known. The set of all these random variables completely characterizes the uncertainty in the underlying system. These random variables may not be completely independent of each other, and their joint distribution will be non-Gaussian in general. This set can be transformed to

a function of a set of independent standard normal (Gaussian) variables $\{\xi_i(\theta)\}_{i=1}^{i=m}$, also denoted by the m-dimensional vector $\boldsymbol{\xi}$, using various techniques (Ghanem & Doostan 2006; Das *et al.* 2006). In literature, m is often referred to as the stochastic dimension of the problem. Since u, the response of the system, will also be a function of $\boldsymbol{\xi}$, $y(\boldsymbol{x},\theta)$ can now be denoted as $y(\boldsymbol{x},\boldsymbol{\xi})$.

The response of the system is next represented in a tensor product space as $y(\boldsymbol{x},\boldsymbol{\xi}) \in V(\mathcal{D}) \otimes L^2(\Omega)$. Here $V(\mathcal{D})$ may be a space of deterministic finite element bases, for example. Similarly a set of orthogonal bases are chosen in $L^2(\Omega)$. Since the basic random variables $\boldsymbol{\xi}$ are Gaussian, the natural choice of a set of orthogonal polynomials in these variables becomes the set of Hermite polynomials, and the resulting representation is called the polynomial chaos expansion (PCE) (Ghanem & Spanos 2003), described in more details in the following section.

There habe been many developments and adaptations in SFEM such as enrichment (Ghosh & Ghanem 2007), incorporating various orthogonal bases (Xiu & Karniadakis 2003), wavelet bases (LeMaître *et al.* 2007). However, there is no universal choice of bases for every problem. Furthermore, the applicability of SSFEM to time-dependent problems is a current issue and not yet well resolved. Therefore here we explore this issue with a model problem, and upon observing the performance of the SSFEM for this problem, we try to adapt/improve SSFEM to suit our need, and try to suggest a somewhat more general recipe for time-dependent problems.

2. Detailed problem description

2.1. *Background: Polynomial chaos expansion and other related expansions*

The stochastic counterpart of the response $y(\boldsymbol{x},\boldsymbol{\xi})$ can be approximated using various types of square-integrable random bases. In this paper, the polynomial chaos bases (Ghanem & Spanos 2003) are used for this purpose. In the polynomial chaos expansion, any square integrable random variable, vector or process can be represented using a basis set $\{\psi_i(\boldsymbol{\xi})\}_{i=0}^{i=\infty}$, where the bases are chosen to be Hermite polynomials in the set of orthonormal variables $\boldsymbol{\xi}$. Let the function $p(\boldsymbol{\xi})$ denote the joint probability density function of the random vector $\boldsymbol{\xi}$. Introduce the notation

$$\mathbb{E}\{\cdot\} = \int_\Omega \cdot dP(\theta) = \int_{\mathbb{R}^m} \cdot p(\boldsymbol{\xi}) d\boldsymbol{\xi}$$

to denote the mathematical expectation of a random quantity. Then the bases ψ_i have the following properties:

$$\psi_0 \equiv 1 \ , \quad \mathbb{E}\{\psi_i\} = 0 \ \text{ for } \ i > 0 \ , \qquad \text{and } \ \mathbb{E}\{\psi_i \psi_j\} = \delta_{i,j} \mathbb{E}\{\psi_i^2\} \ ,$$

where $\delta_{i,j}$ denotes the Kronecker delta function. For computational purposes, only a finite number of bases — P are used. P depends upon m, the stochastic dimension of the problem and the order of expansion — defined as the highest degree of polynomials retained. Let the physical domain be discretized using an n degrees of freedom (dof) deterministic finite element model, and the response be represented using a P-term PCE. In this case using both the deterministic or physical bases and the stochastic bases $\{\psi_j(\boldsymbol{\xi})\}_{j=0}^{j=P-1}$ the approximation $\hat{y}(\boldsymbol{\xi})$ to the response $y(\boldsymbol{x},\boldsymbol{\xi})$ can be represented as

$$\hat{y}(\boldsymbol{\xi}) = \sum_{i=0}^{P-1} y_i \psi_i(\boldsymbol{\xi}) \ , \quad \hat{y}(\boldsymbol{\xi}), y_i \in \mathbb{R}^n \ . \tag{2.1}$$

The probabilistic description of $\hat{y}(\boldsymbol{\xi})$ can be derived from the chaos coefficients y_i. For example, the mean and variance of the response at the j^{th} node can be computed from Eq. 2.1 as

$$\text{Mean} = \bar{y} = y_0(j), \quad \text{Variance} = Var(\hat{y}) = \sum_{i=1}^{i=P-1} \left(y_i(j)\right)^2 \mathbb{E}\{\psi_i^2\} \ , \tag{2.2}$$

where $y_i(j)$ denotes the j^{th} element of the vector y_i.

The PCE, being by definition a polynomial expansion, often fails to capture the behavior of certain non-smooth functions (here the smoothness is meant with respect to the uncertain parammeter $\boldsymbol{\xi}$), for example, functions with jump. To alleviate this problem, an enrichment scheme to PCE is proposed recently (Ghosh & Ghanem 2007), where the basis set is augmented by a set of special functions (usually non-polynomial) referred to as enrichment functions. Selection of such functions are based upon a-priori knowledge about the behavior of the target function. Including the enrichment terms, $\hat{y}(\boldsymbol{\xi})$ is expressed as

$$\hat{y}(\boldsymbol{\xi}) = \sum_{i=0}^{P-1} y_i \psi_i(\boldsymbol{\xi}) + \sum_{i=P}^{P+E-1} y_i \psi_i(\boldsymbol{\xi}) \ , \quad \hat{y}(\boldsymbol{\xi}), y_i \in \mathbb{R} \ . \tag{2.3}$$

In this expression the first P terms are the Hermite chaos terms, and the remaining E terms are the enrichment terms. The enrichment functions are in general neither zero-mean nor orthogonal to any of the bases. Therefore, the first and second order statistical moments of $\hat{y}(\boldsymbol{\xi})$ at the j^{th} node are expressed as,

$$\text{Mean} = \bar{y} = y_0(j) + \sum_{i=P}^{P+E-1} y_i(j) \mathbb{E}\{\psi_i\}, \tag{2.4}$$

$$\text{Second moment} = \mathbb{E}\{\hat{y}^2\} = \sum_{i=0}^{P+E-1} \mathbb{E}\{\psi_i^2\}(\left(y_i(j)\right)^2 + 2 \sum_{i=0}^{P+E-2} \sum_{k=i+1}^{P+E-1} y_i(j) y_k(j) \mathbb{E}\{\psi_i \psi_k\} \ .$$

In order to obtain the representations (2.1) or (2.3) the coefficients y_i must be estimated. It is observed that for most applications, the computationally fastest method for this estimation is the *stochastic Galerkin finite element method* (Ghanem & Spanos 2003; Babŭska *et al.* 2005), where a variational formulation is constructed using the bases from the tensor product space $V(\mathcal{D}) \otimes L^2(\Omega)$. Procedures for estimating the coefficients are discussed later.

2.2. *The model problem*

The problem considered represents a simple model of CO surface oxidation, for which the mean field evolution equations for the coverages u, v, w of three species on the surface are expressed as (Makeev *et al.* 2002)

$$\frac{du}{dt} = az - cu - 4duv$$
$$\frac{dv}{dt} = 2bz^2 - 4duv$$

$$\frac{dw}{dt} = ez - fw$$
$$z = 1 - u - v - w$$
$$u(0) = v(0) = w(0) = 0 \ , \tag{2.5}$$

where the following parameters are fixed

$$a = 1.6,\ c = 0.04,\ d = 1.0,\ e = 0.36,\ f = 0.016. \tag{2.6}$$

If the parameter b is used as the uncertain parameter, then it is easy to show that the system has two supercritical bifurcation points at $b \approx= 20.3$ and $b \approx 21.2$. In our study the following stochastic model of b is used

$$b = 20.8 + \beta\ \eta \ , \tag{2.7}$$

where η is a zero-mean random variable and β is a constant term that, together with the standard deviation of η determines σ_b — the standard deviation of b. For this model, for a given distribution of η and σ_b, the statistical behavior of u, v and w are estimated using various methods and compared here.

2.3. *Using PCE for this model problem*

First, a Monte Carlo simulation is performed. In this method a random number generator is used to generate realizations of η; each realization corresponds to a realization of the physical system. For each realization, the system of Eqs. 2.5 is solved. Finally, over a large number of realizations the statistical moments of u, v and w are estimated using averaging. Here the Matlab algorithm *ode*45 — which uses the fourth order Runge-Kutta scheme — is used to solve Eq. 2.5. It is further observed that an implicit Runge-Kutta scheme (*ode*23*tb* in Matlab) also yields the same result.

Then the quantities u, v and w are represented in their PCE as in Eq. (2.1), when the random variable η is standard normal and therefore denoted by ξ. As mentioned earlier, any other bases such as gPCE (when η is non-Gaussian) can be employed using the same techniques presented here. For any such representation, the chaos coefficients are first estimated using the non-intrusive method. In this method, the errors in the solution u, v, and w are orthogonalized with respect to the subspace spanned by the chaos bases $\{\psi_i\}_{i=0}^{P-1}$, therefore yielding expressions

$$u_i(t) = \frac{\mathbb{E}\{u(t)\psi_i\}}{\mathbb{E}\{\psi_i^2\}}\ ,\ v_i(t) = \frac{\mathbb{E}\{v(t)\psi_i\}}{\mathbb{E}\{\psi_i^2\}}\ ,\ w_i(t) = \frac{\mathbb{E}\{w(t)\psi_i\}}{\mathbb{E}\{\psi_i^2\}}\ . \tag{2.8}$$

Here the numerators are estimated using the Monte Carlo method as mentioned above, the denominators are usually precomputed using some computationally inexpensive algorithm and stored in a tabulated form. Therefore the main computational cost in this case is equal to the Monte Carlo sampling. However, here the added advantage is the series representation that offers encapsulation of the process through a set of deterministic coefficients. Clearly, the mean of the response is exactly that obtained by Monte Carlo simulation. However, the standard deviation may vary because of the truncation of PCE after a few number of terms. Note that for estimating the coefficients of an enriched expansion (2.3), a coupled system of equations need to be solved instead of Eq. 2.8.

Next the coefficients are determined using the intrusive method (also referred to as the stochastic Galerkin finite element method, Babŭska *et al.* 2005). Accordingly, the residual in Eq. 1.1 is minimized by using a Galerkin projection on the approximation

subspace in $V(\mathcal{D}) \otimes L^2(\Omega)$. This results in a deterministic system of $3P$ equations of the following form

$$\begin{aligned}
\frac{du_0}{dt} &= g_0 \\
&\cdots \\
\frac{du_{P-1}}{dt} &= g_{P-1} \\
\frac{dv_0}{dt} &= g_P \\
&\cdots \\
\frac{dv_{P-1}}{dt} &= g_{2P-1} \\
\frac{dw_0}{dt} &= g_{2P} \\
&\cdots \\
\frac{dw_{P-1}}{dt} &= g_{3P-1} \\
u_0(0) = \cdots = u_{P-1} = \cdots v_0(0) &= \cdots v_{P-1} = w_0(0) = \cdots = w_{P-1} = 0 \ , \qquad (2.9)
\end{aligned}$$

where g_i are known non-linear functions. For $\sigma_b = 0.3$, that is, about 1.5% standard deviation of b with respect to its mean value, the above system is solved here using *ode*45 in Matlab. Estimates of the mean and standard deviation of u are plotted in Figs. 1 and 2, respectively.

From Fig. 1 we observe that the intrusive method is unable to capture the mean response. Further, from Fig. 2 it is observed that both intrusive and non-intrusive methods are unable to capture the standard deviation.

One possible reason for the discrepancy of the intrusive and Monte Carlo methods can be attributed to the phase error. In the intrusive PCE, at any given time instant, starting from $t = 0$, the PCE is truncated after P terms, thus introducing a truncation error. This error is accumulated in time and, therefore the result deteriorates. On the other hand, the non-intrusive method is not polluted in the same way — at any given time instant the complete system is solved. However, the estimate of standard deviation from the non-intrusive method is not satisfactory. This issue is investigated further.

The evolution of the solution u as a function of the parameter is b (which is a function of η) is plotted in Fig. 3 at different time instants. Here it is seen that as the time grows, the behavior becomes more oscillatory in nature. Therefore, the polynomials may not be the most suitable choice of bases in this case. Similar observation was noted in Pettit & Beran 2006, where the authors tried to approximate a sinusoid function with uncertain frequency using polynomial bases. To circumvent this problem, a number of directions are explored here, as described in the following section.

3. Our approach and results

Based on the above observations that the bases of representation might be insufficient to capture the probabilistic nature of the response, it is possible to choose a different sets of bases. As an example, the wavelet bases have been employed by some authors (LeMaître *et al.* 2007; Pettit & Beran 2006), which improves the quality of approximation significantly, however, at a much larger computational cost. Our goal is to use some

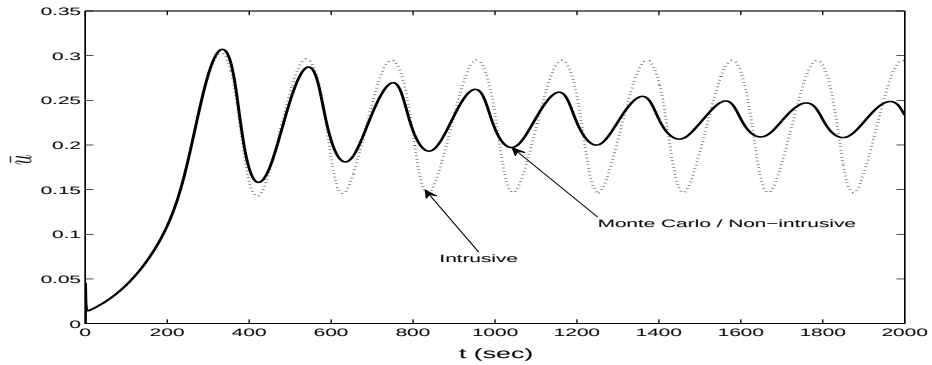

FIGURE 1. Evolution of mean of u with time, estimated using different Monte Carlo simulation (the non-intrusive PCE represents the mean exactly by definition), and intrusive PCE.

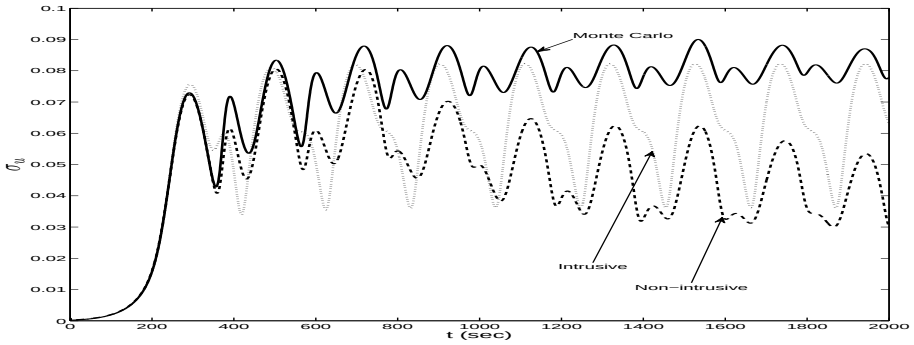

FIGURE 2. Evolution of standard deviation of u with time, estimated using Monte Carlo simulation, non-intrusive PCE, and intrusive PCE.

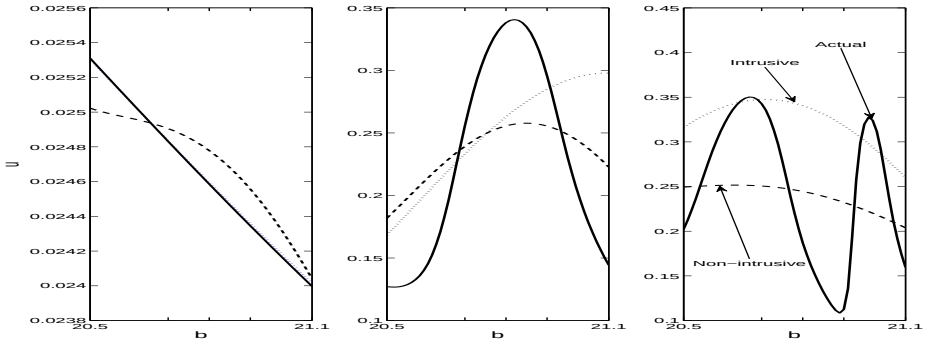

FIGURE 3. Evolution of the parametric response of u with respect to b, measured using actual simulation, non-intrusive PCE, and intrusive PCE. The three subplots from left to right correspond to $t = 50,\ 1000$ and 2000 seconds, respectively.

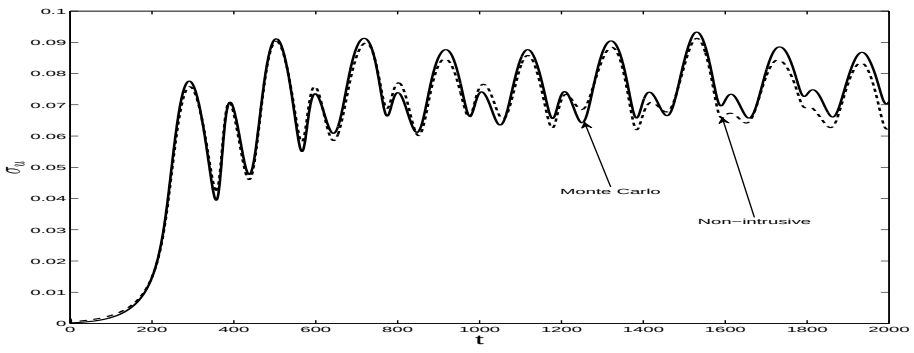

FIGURE 4. Evolution of standard deviation of u with time, estimated using Monte Carlo simulation and expansion using trigonometric bases — the coefficients are estimated using the non-intrusive method.

different kinds of bases, and to enrich the basis set so that only a few terms can give a good approximation of the response. The resulting method should be computationally efficient as well. To begin, we use trigonometric bases. First the random model of b is modified, from a Gaussian distribution to a uniform distribution, that is, in Eq. 2.7, $\eta \sim \mathcal{U}\,[-\pi, \pi]$ and β is chosen such that σ_b still remains as 0.3 — the value used in the previous subsection. The response u, v and w are then represented using trigonometric bases. This way, the representation of u is

$$u = u_0 + \sum_{i=1}^{N} \left(u_{i,s} sin(i\eta) + u_{i,c} cos(i\eta)\right) \ , \tag{3.1}$$

where u_0, $u_{i,s}$ and $u_{i,c}$ are the coefficients to be determined, and N determines the maximum number of terms retained in the expansion. Here the uniform distribution of η is assumed only for convenience, because it is straightforward to construct orthogonal trigonometric bases with respect to uniform measure.

The coefficients of this representation are first estimated using the non-intrusive method, that is, via statistical simulations. Standard deviation of u computed from Monte Carlo simulation and from the above expansion with $N = 4$ — that is, with total 9 terms retained — are plotted in Fig. 4. As shown in this plot, the two estimates of standard deviations are quite close. Therefore it can be concluded from this study that the set of trigonometric bases is a better alternative than the set of polynomial bases. To achieve more confidence in this conclusion, the estimated standard deviation of u obtained from an 8^{th}-order PCE — that is, with total 9 terms retained in the expansion — is plotted in Fig. 5 (the randomness in b is Gaussian and the coefficients are extimated using the non-intrusive method). A comparison between Figs. 4 and 5 re-asserts that the trigonometric bases are indeed the better ones for this problem.

Next the intrusive method will be used in for this expansion. Since the bases are proved to be appropriate, the phase error (or/and the long-term integration error) in intrusive computation can now be decoupled to some extent from the error due to insufficient bases.

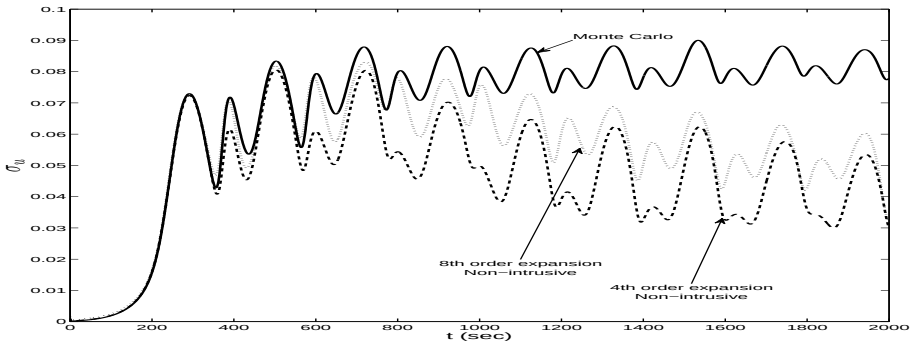

FIGURE 5. Evolution of standard deviation of u with time, estimated using Monte Carlo simulation and non-intrusive PCE, 4^{th} and 8^{th} order. When compared with Fig. 4, clearly the estimate from the expansion with 9-term trigonometric bases is better than the expansion with 9-term Hermite polynomial bases.

4. Conclusions and future direction

For some time-dependent problems, application of the spectral stochastic finite element methods (SSFEM) is by no means a straightforward task. This study adresses two such problems — selection of suitable bases, and the phase error in long time integration in intrusive computation. For the given problem, the trigonometric bases are found to be good candidates. The next goals are (i) to decouple the integration error from the truncation error, and (ii) to develop a scheme to build enrichment functions that will reduce the number of terms in the representation, and to develop an efficient numerical algorithm to compute the coefficients of such enriched expansion.

Acknowledgment

Financial support from the Advanced Simulation and Computing Program of the Department of Energy is gratefully acknowledged.

REFERENCES

BABŮSKA I. , TEMPONE R. & ZOURARIS G. E. 2005 Solving elliptic boundary value problems with uncertain coefficients by the finite element method: the stochastic formulation *Computer Methods in Applied Mechanics and Engineering* **194**, 1251–1294.

DAS S. , GHANEM R. & SPALL J. 2006, Asymptotic sampling distribution for polynomial chaos representation of data: A maximum entropy and Fisher information approach. *45th IEEE Conference on Decision and Control, San Diego, CA.* December 13-15.

GHANEM R. & DOOSTAN A. 2006 On the construction and analysis of stochastic predictive models: Characterization and propagation of the errors associated with limited data. *Journal of Computational Physics* **217(1)**, 63–81.

GHANEM R. & SPANOS P. D. 2003 Stochastic Finite Elements: A Spectral Approach. *Revised Edition, Dover Publications*

GHOSH D. & GHANEM R. Stochastic convergence acceleration through basis enrichment

of polynomial chaos expansions *International Journal for Numerical Methods in Engineering. Forthcoming.*

Le Maître O. P. , Najm H. N. , Pébay P. P. , Ghanem R. & Knio O. M. 2007 Multi-resolution-analysis for uncertainty quantification in chemical systems. *SIAM Journal on Scientic Computing* **29(2)**, 864–889.

Makeev A. G. , Maroudas D. & Kevrikedis I. G. 2002 "Coarse" stability and bifurcation analysis using stochastic simulators: Kinetic Monte Carlo examples. *Journal of Chemical Physics* **116(23)**, 10083–10091.

Pellissetti M. & Ghanem R. 2000 Iterative solution of systems of linear equations arising in the context of stochastic finite elements *Advances in Engng. Software* **31**, 607–616.

Pettit C. L. & Beran P. S. 2006 Spectral and multiresolution Wiener expansions of oscillatory stochastic processes. *Journal of Sound and Vibration* **294**, 752–779.

Xiu D. & Karniadakis G. 2003 Modeling uncertainty in flow simulations via generalized polynomial chaos. *Journal of Computational Physics* **187(1)**, 137–167.

http://www.mathworks.com/products/matlab/.