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New Developments in Computational Stochastic Mechanics, Part I: Theory

Prasanth B. Nair* and Andy J. Keane†
University of Southampton, Highfield, Southampton SO17 1BJ, U.K

Abstract

The focus of this paper is to develop efficient numerical schemes for analysis of systems governed by stochastic partial differential equations (PDEs). In particular, Stochastic Reduced Basis Approximation (SRBA) methods are proposed for efficient solution of large-scale linear algebraic system of equations with random coefficients. The terms of the Neumann expansion are deployed as stochastic basis vectors in the SRBA methods. The stochastic system response is expressed in terms of these basis vectors and undetermined deterministic scalars (or random functions). Variants of the Bubnov-Galerkin scheme are employed to compute the undetermined terms, which allows explicit expressions for the response quantities to be derived. This enables a *complete probabilistic description* of the response quantities to be obtained in a computationally efficient fashion. The application of SRBA methods in conjunction with stochastic linearization techniques to nonlinear stochastic systems is outlined. In a companion paper (Nair, P. B., and Keane, A. J., "New Developments in Computational Stochastic Mechanics, Part II: Applications," *AIAA-2000-1441*), results are presented for a variety of problems to demonstrate that significant improvements over the Neumann expansion scheme can be achieved.

1. Introduction

The equations governing the physics of many complex systems can be described by ordinary or Partial Differential Equations (PDEs). A wide body of numerical methods based on finite differences, finite elements, and boundary elements are available in the computational mechanics literature to approximately solve the governing equations for the response quantities of interest. Over the last 50 years, significant progress has been made in the theoretical groundwork of these methods for cases when a system is modeled in a deterministic framework, and when a deterministic linear system is subjected to random excitation.

By contrast, the use of probabilistic models for the physical system parameters and the excitation fields lead to a significant increase in the problem complexity. This is primarily due to the difficulties in arriving at tractable descriptions of the system response in terms of the stochastic differential operators and the random excitation field. Exact solutions to this class of problems are possible only under restrictive assumptions for simple problems; see, for example, Pugachev and Sinitsyn[1]. In the context of stochastic analysis of large-scale systems of practical interest, most research work has focused on computationally efficient methods which allow the response statistics to be approximated with reasonable accuracy.

The approaches in the literature can be broadly classified into different categories depending on how the physical system parameters are modeled (random field or random variables), the scheme used for discretizing the random fields, the linearization techniques employed to simplify the nonlinear terms, the spatial discretization scheme, and the algorithm used to solve the resulting random algebraic equations. The interested reader is referred to the monographs of Ghanem and Spanos[2], and Kleiber and Hien[3] for a detailed exposition of computational stochastic mechanics. A recent overview of developments in stochastic mechanics has been presented in Grigoriu[4].

A spectral stochastic finite element method (SSFEM) was proposed by Ghanem and Spanos[2,4,5]. In this approach, the random fields describing the coefficients of the PDEs are discretized using the Karhunen-Loeve (KL) expansion scheme. Subsequently, a finite element procedure was used to derive a system of linear algebraic equations with random coefficients, which is then approximately solved

*Ph.D. Student, Computational Engineering and Design Center, School of Engineering Sciences, Member AIAA. P.B.Nair@soton.ac.uk

†Professor of Computational Engineering, Director Computational Engineering and Design Center.

using the Neumann expansion scheme. An alternative approach was also proposed, wherein the solution vector is represented by the Polynomial chaos decomposition with unknown coefficients. Using the Bubnov-Galerkin scheme, a set of deterministic linear algebraic equations (with increased dimensionality proportional to the number of terms in the polynomial chaos) was obtained for the unknown coefficients. Since, this method increases the dimensionality of the original problem, it is referred to as the *increased basis approximation* method in this paper. This approach was demonstrated to give better results as compared to the Neumann expansion scheme. The reader is directed to Ghanem[6] for a recent review of the mathematical background of the SSFEM.

Monte Carlo Simulation (MCS) techniques[7] and response surface methodology (RSM)[8] have been widely applied to a variety of problems. These approaches are quite general in scope and utilize existing deterministic analysis software. However, due to the requirement of many deterministic simulations, they are practical only for problems where deterministic analysis takes modest computational effort. Methods based on Taylor or Neumann expansion series of the response have been popularly used in the stochastic finite element literature; see, for example, references[3,9,10]. These methods are computationally more efficient as compared to MCS and RSM. However, these approaches give reasonable quality approximations only when the coefficients of variation of the random physical parameters are small.

More recently, Elishakoff and his colleagues (see, for example, references[11,12]) have focused on finite element analysis of structures with large stochastic variations. The key idea has been to develop approaches which do not use perturbation schemes. However, it remains to be seen how readily the methods in references[11,12] can be extended to general finite element analysis. An excellent discussion on the motivation for additional work in the area of stochastic finite element analysis can be found in Elishakoff and Ren[13].

The authors' have developed reduced basis approximation concepts for large-scale random eigenvalue problems[14]. The approach developed in reference[14] is similar in spirit to that presented here, although the choice of basis vectors is different. The fundamentals underpinning the proposed approach are borrowed from the area of reduced basis approximation concepts; see, Noor[15] for an excellent overview of applications to deterministic systems. The choice of basis vectors used in this paper was proposed earlier by Kirsch[16–18] in the context of static structural reanalysis. Subsequently, this method has been applied with a great deal of success to structural reanalysis for topological modifications[19], damage tolerance analysis[20], and evolutionary design optimization[21].

This paper is concerned with the analysis of systems governed by stochastic PDEs. In particular, efficient techniques are proposed for solving large-scale linear algebraic systems of equations with random coefficients, such as those obtained by discretizing linear stochastic PDEs in space and the random dimension. Nonlinear stochastic systems can also be ultimately reduced to this form using stochastic linearization techniques. The fundamental idea used here is to represent the response process as a linear combination of stochastic basis vectors with undetermined coefficients. The undetermined coefficients are either considered as random functions or deterministic scalars. Methods based on this representation, where the number of undetermined terms is less than the dimension of the discretized problem are referred to as *stochastic reduced basis approximation (SRBA) methods* in this paper.

The terms of the Neumann expansion are chosen as the basis vectors in this research. Two procedures are developed for computing the undetermined coefficients in the SRBA. The first procedure uses an approximate stochastic Bubnov-Galerkin scheme (see Section 2), wherein the coefficients of the SRBA are considered as deterministic scalars. The second procedure uses an exact stochastic Bubnov-Galerkin scheme. This formulation is developed for cases wherein only two/three basis vectors are used. Hence, it becomes possible to treat the SRBA coefficients as random functions, which ensures that all the statistical moments of the weighted residual error are zero. Both these procedures allow explicit expressions for the stochastic response quantities to be derived. This enables a complete probabilistic description of the response quantities to be obtained in a computationally efficient fashion. It is shown that the SRBA methods require of the order of $O(n^2)$ operations in addition to one deterministic analysis; where n is the dimension of the corresponding deterministic problem. The application of SRBA methods to nonlinear stochastic problems in conjunction with stochastic linearization techniques is also outlined. In a companion paper, results are presented for a variety of example problems to demonstrate that high-quality approximations of the response statistics can be achieved for moderate to large coefficient of variation of the random physical parameters.

2. Preliminaries

This section summarizes some of the fundamental concepts used in developing the SRBA methods. The greek characters Θ, θ, ζ, and η are used throughout this paper to reference random quantities. $\langle . \rangle$ is used to refer to the expected value or the ensemble average of a random quantity $\{.\}$.

2.1 Discretization of Random Fields

Random field discretization involves its representation in terms of a finite number of random variables. An excellent overview of discretization procedures for random fields such as the Karhunen Loeve (KL) expansion, Polynomial chaos decomposition, and linear estimation theory can be found in the literature[2,22]. For example, the KL expansion of a random field $w(\mathbf{x}, \Theta)$ defined on the domain Ω with covariance function $\mathbf{R}_{ww}(\mathbf{x}_1, \mathbf{x}_2)$ can be written as

$$w(\mathbf{x}, \Theta) = \langle w(\mathbf{x}, \Theta) \rangle + \sum_{i=0}^{\infty} \eta_i \sqrt{\mu_i} w_i(\mathbf{x}), \quad (1)$$

where μ_i and $w_i(\mathbf{x})$ are the characteristic functions (eigenvalues and eigenvectors, respectively) of the following deterministic integral eigenvalue problem,

$$\mu_i w_i(\mathbf{x}) = \int_{\Omega} \mathbf{R}_{ww}(\mathbf{x}, \mathbf{x}_2) w_i(\mathbf{x}_1) d\mathbf{x}_1. \quad (2)$$

The vector of zero-mean random variables $\{\eta_i\}$ are orthogonal, i.e., $\langle \eta_i \eta_j \rangle = \mu_i \delta_{ij}$; where δ_{ij} denotes the Kronecker delta function. For a detailed overview of the mathematical characteristics of the KL expansion scheme, the reader is referred to the monograph of Ghanem and Spanos[2]. A discussion on numerical solution of equation (2) for complex domains can be found in reference[23]. The application of the Polynomial Chaos decomposition scheme for representing random fields with unknown correlation functions can be found in Ghanem[24].

2.2 Bubnov-Galerkin Scheme for Stochastic Problems

In the computational stochastic mechanics literature, the following definition is used to check the orthogonality of two random vector functions $\mathbf{x}_1(\Theta)$ and $\mathbf{x}_2(\Theta)$

$$\langle \mathbf{x}_1^T(\Theta) \mathbf{x}_2(\Theta) \rangle = 0. \quad (3)$$

Equation (3) is essentially the expected value of the inner product defined in the Hilbert space of random variables, i.e, only the mean value of the inner product is enforced to be zero for values of Θ. The Bubnov-Galerkin scheme used in most of the formulations in the literature uses the above definition to constrain the random residual error to be orthogonal to the approximating space of basis functions. This scheme is henceforth referred to as the *approximate stochastic Bubnov-Galerkin scheme.* An alternative procedure would be to orthogonalize the random residual error to the approximating space such that all the statistical moments of the inner product are zero, i.e.,

$$\langle \left(\mathbf{x}_1^T(\Theta) \mathbf{x}_2(\Theta) \right)^k \rangle = 0, k = 1, 2, \ldots, \infty. \quad (4)$$

The projection scheme which leads to satisfaction of equation (4) is referred to as the *exact stochastic Bubnov-Galerkin scheme* in this paper.

3. Discretization of Linear Stochastic PDEs

This section outlines a general scheme for discretizing linear stochastic PDEs in space and the random dimension on the lines of that presented earlier by Ghanem[6]. A general expression for the discretized equations is derived, which sets the stage for the development of SRBA methods. Consider a linear stochastic PDE of the form

$$\mathcal{T}_\alpha \left[u(\mathbf{x}, t, \Theta) \right] + \mathcal{Q}_\beta \left[u(\mathbf{x}, t, \Theta) \right] = f(\mathbf{x}, t, \Theta), \quad (5)$$

where $\mathbf{x} \in \mathcal{D}$ denotes a point in the space defined by $\mathcal{D}$; $t \in [0, T]$ refers to time; $\Theta \in \Omega$ belongs to the Hilbert space of random variables. $\mathcal{T}_\alpha$ and $\mathcal{Q}_\beta$ denotes linear stochastic differential operators with respect to time and space respectively. These operators have coefficients $\alpha(\mathbf{x}, \Theta)$ and $\beta(\mathbf{x}, \Theta)$ which are considered to be random fields. $f(\mathbf{x}, t, \Theta)$ denotes the random excitation field for which a solution $u(\mathbf{x}, \Theta)$ is sought.

The random fields in equation (5) can be discretized in terms of a finite number of random variables. This can be done using any of the techniques mentioned earlier in section 2. Equation (5) can subsequently be rewritten as

$$\left(\mathcal{T} + \mathcal{T}_\theta \right) \left[u(\mathbf{x}, t, \Theta) \right] + \left(\mathcal{L} + \mathcal{L}_\theta \right) \left[u(\mathbf{x}, t, \Theta) \right] = f^o(\mathbf{x}, t)$$

$$+ f^{'}(\mathbf{x}, t, \eta), \quad (6)$$

where $\mathcal{T}$ and $\mathcal{L}$ are the deterministic components of the stochastic differential operators with respect

to time and space, respectively; $\mathcal{T}_\theta$ and $\mathcal{L}_\theta$ are the random components of the differential operators; $f^o(\mathbf{x},t)$ and $f^{'}(\mathbf{x},t,\eta)$ denote the deterministic and random components of the excitation field.

Consider for the sake of simplicity that the random fields appear as multiplicative terms in the differential operators. Hence, spatial discretization of equation (6) using any conventional finite element formulation and applying the appropriate boundary conditions leads to a matrix system of ordinary differential equations of the form

$$\left(\mathbf{M}^o\mathcal{T} + \sum_{i=1}^{kl1}\theta_i\mathbf{M}^i\mathcal{T}_i\right)\mathbf{u}(t) + \left(\mathbf{K}^o + \sum_{i=1}^{kl2}\zeta_i\mathbf{K}^i\right)\mathbf{u}(t) = \mathbf{f}^o(t) + \sum_{i=1}^{kl3}\eta_i\mathbf{f}^i(t), \quad (7)$$

where $\mathbf{M}^o$, $\mathbf{M}^i$, $\mathbf{K}^o$, and $\mathbf{K}^i \in \Re^{n\times n}$ are deterministic matrices; $\mathcal{T}_i$ denotes a deterministic differential operator with respect to time; n is the total number of degrees of freedom; $\mathbf{f}^o(t)$ and $\mathbf{f}^i(t) \in \Re^{n\times 1}$ are deterministic vectors; $kl1$, $kl2$, and $kl3$ denote the number of terms used in discretization of the random fields $\alpha(\mathbf{x},\boldsymbol{\Theta})$, $\beta(\mathbf{x},\boldsymbol{\Theta})$, and $f(\mathbf{x},t,\boldsymbol{\Theta})$, respectively; θ_i, ζ_i, and η_i are random variables arising from the discretization procedure applied to the appropriate random fields.

For static problems, equation (7) will be a system of linear algebraic equations in terms of the random variables. Similar sets of equations could be arrived at for time dependent problems by transforming the equations to the frequency domain, which leads to a system of complex linear algebraic equations with random coefficients for each excitation frequency of interest. Without any loss of generality, a general form for the resulting system of linear algebraic equations with random coefficients can be written as

$$\left(\mathbf{L} + \sum_{i=1}^{p}\theta_i\mathbf{\Pi}_i\right)\mathbf{u}(\boldsymbol{\Theta}) = \mathbf{f}^o + \sum_{i=1}^{q}\eta_i\mathbf{f}^i \quad (8)$$

where $\mathbf{L} \in \Re^{n\times n}$ and $\mathbf{\Pi}_i \in \Re^{n\times n}$ are deterministic matrices; $\mathbf{f}^o$, $\mathbf{f}^i \in \Re^{n\times 1}$ are deterministic vectors; $\mathbf{u}(\boldsymbol{\Theta}) \in \Re^{n\times 1}$ is the stochastic response vector; $\boldsymbol{\Theta} = \{\theta_i\}$, $i = 1,2,\ldots,p$ is the vector of random variables arising from discretization of all the random fields describing the system properties in equation (5). η_i, $i = 1,2,\ldots,q$ denotes the random variables arising from discretization of the excitation field.

For problems where the system parameters and the external forces are considered as random variables, an equation similar to equation (8) could be derived by expanding the global coefficient matrices using a first-order Taylor series and appropriately representing the random forces.

4. The Neumann Expansion Scheme

The Neumann expansion for $\mathbf{u}(\boldsymbol{\Theta})$ can be written as

$$\mathbf{u}(\boldsymbol{\Theta}) = \sum_{i=0}^{m}(-1)^i\left(\mathbf{L}^{-1}\sum_{j=1}^{p}\theta_j\mathbf{\Pi}_j\right)^i \times\mathbf{L}^{-1}\left(\mathbf{f}^o + \sum_{j=1}^{q}\eta_j\mathbf{f}^j\right), \quad (9)$$

The Neumann expansion series is convergent only when $||\mathbf{L}^{-1}\sum_{j=1}^{p}\theta_j\mathbf{\Pi}_j|| < 1$. More rigorously, equation (9) converges when $\rho(\mathbf{L}^{-1}\sum_{j=1}^{p}\theta_j\mathbf{\Pi}_j) < 1$; where ρ denotes the spectral radius of a matrix. These conditions imply that the Neumann expansion series will convergence only when the magnitude of θ_j is small.

Consider the special case where the governing stochastic PDE is elliptic, i.e., the coefficient matrices of the discretized equations are symmetric positive definite. Then, it can be readily shown (see reference[25]) that equation (9) is unconditionally convergent if the following condition is met for any arbitrary $\mathbf{v}\in \Re^{n\times 1}$.

$$\mathbf{v}^T\left(\mathbf{L} + \sum_{i=1}^{p}\theta_i\mathbf{\Pi}_i\right)\mathbf{v} < \mathbf{v}^T\mathbf{L}\mathbf{v} \quad (10)$$

A detailed discussion on how to choose $\mathbf{L}$ in structural applications so as to satisfy equation (10) was recently presented by Dasgupta[25].

5. Stochastic Reduced Basis Approximation (SRBA) Methods

This section presents SRBA methods to efficiently solve equation (8), particularly for large values of n and for large coefficient of variation of θ_i. The main objective here is to represent $\mathbf{u}(\boldsymbol{\Theta})$ explicitly in terms of the random variable vector $\boldsymbol{\Theta}$.

The SRBA methods developed in this research attempt to improve the range of validity of the Neumann expansion scheme. The fundamental assumption made here is that a good approximation for the stochastic process $\mathbf{u}(\boldsymbol{\Theta})$ can be obtained in the subspace spanned by the terms of the Neumann expansion series. The stochastic reduced basis representation may be written as

$$\hat{\mathbf{u}}(\boldsymbol{\Theta}) = \sum_{i=0}^{m} \xi_i(\boldsymbol{\Theta}) \left(\sum_{j=1}^{p} \theta_j \mathbf{L}^{-1} \boldsymbol{\Pi}_j \right)^i \left(\mathbf{u}_o + \sum_{j=1}^{q} \eta_j \mathbf{u}_j \right), \tag{11}$$

where $\xi_i(\boldsymbol{\Theta})$ are undetermined quantities in the SRBA; $\mathbf{u}_o = \mathbf{L}^{-1}\mathbf{f}^o$ and $\mathbf{u}_k = \mathbf{L}^{-1}\mathbf{f}^k \in \Re^{n\times 1}$ are deterministic vectors. Equation (11) can be written using matrix notation as

$$\hat{\mathbf{u}}(\boldsymbol{\Theta}) = \boldsymbol{\Psi}(\boldsymbol{\Theta})\boldsymbol{\Xi}(\boldsymbol{\Theta}) \tag{12}$$

where $\boldsymbol{\Psi}(\boldsymbol{\Theta}) = [\Psi_0(\boldsymbol{\Theta}), \Psi_1(\boldsymbol{\Theta}), \ldots, \Psi_m(\boldsymbol{\Theta})] \in \Re^{n\times(m+1)}$ denotes the matrix of stochastic basis vectors, and $\boldsymbol{\Xi}(\boldsymbol{\Theta}) = \{\xi_0(\boldsymbol{\Theta}), \xi_1(\boldsymbol{\Theta}), \ldots, \xi_m(\boldsymbol{\Theta})\}^T \in \Re^{(m+1)\times 1}$ denotes the vector of undetermined coefficients. $\Psi_i(\boldsymbol{\Theta})$ denotes the i^{th} basis vector, which is a polynomial in θ_i. The basis vectors are a sequence of the form

$$\Psi_0(\boldsymbol{\Theta}) = \mathbf{u}_o + \sum_{i=1}^{q} \eta_i \mathbf{u}_i \tag{13}$$

$$\Psi_1(\boldsymbol{\Theta}) = \sum_{i=1}^{p} \theta_i \left(\mathbf{b}_i^{(11)} + \sum_{j=1}^{q} \eta_j \mathbf{b}_{ij}^{(12)} \right), \tag{14}$$

where $\mathbf{b}_i^{(11)} = \mathbf{L}^{-1}\boldsymbol{\Pi}_i\mathbf{u}_o$ and $\mathbf{b}_{ij}^{(12)} = \mathbf{L}^{-1}\boldsymbol{\Pi}_i\mathbf{u}_j \in \Re^{n\times 1}$ are deterministic vectors. A general expression for the m^{th} basis vector can hence be written as

$$\Psi_m = \sum_{i_1,i_2,\ldots,i_m=1}^{p} \theta_{i_1}\theta_{i_2}\ldots\theta_{i_m} \times \left(\mathbf{b}_{i_1 i_2 \ldots i_m}^{(m1)} + \sum_{i_{m+1}=1}^{q} \eta_{i_{m+1}} \mathbf{b}_{i_1 i_2 \ldots i_{m+1}}^{(m2)} \right) \tag{15}$$

where $\mathbf{b}_{i_1 i_2 \ldots i_m}^{(m1)} = \mathbf{L}^{-1}\boldsymbol{\Pi}_{i_1}\mathbf{L}^{-1}\boldsymbol{\Pi}_{i_2}\ldots\mathbf{L}^{-1}\boldsymbol{\Pi}_{i_m}\mathbf{u}^o$ and $\mathbf{b}_{i_1 i_2 \ldots i_{m+1}}^{(m2)} = \mathbf{L}^{-1}\boldsymbol{\Pi}_{i_1}\mathbf{L}^{-1}\boldsymbol{\Pi}_{i_2}\ldots\mathbf{L}^{-1}\boldsymbol{\Pi}_{i_m}\mathbf{u}_{i_{m+1}} \in \Re^{n\times 1}$ are deterministic vectors. From the above equations, it can be seen that the basis vectors can be computed in a recursive form as

$$\Psi_k = \left(\sum_{i=1}^{p} \theta_i \mathbf{L}^{-1}\boldsymbol{\Pi}_i \right) \Psi_{k-1} \tag{16}$$

A recursion equation for the tensors in equation (14) can be similarly written as

$$\mathbf{b}_{i_1 i_2 \ldots i_{k+1}}^{((k+1)1)} = \left(\sum_{k+1=1}^{p} \mathbf{L}^{-1}\boldsymbol{\Pi}_{k+1} \right) \mathbf{b}_{i_1 i_2 \ldots i_k}^{(k1)} \tag{17}$$

$$\mathbf{b}_{i_1 i_2 \ldots i_{k+2}}^{((k+1)2)} = \left(\sum_{k+2=1}^{p} \mathbf{L}^{-1}\boldsymbol{\Pi}_{k+2} \right) \mathbf{b}_{i_1 i_2 \ldots i_{k+1}}^{(k2)} \tag{18}$$

Equations (16-18) enable the computation of the deterministic tensors in the explicit expression for the basis vectors in an efficient fashion. In order to compute $\boldsymbol{\Xi}(\boldsymbol{\Theta})$ via the Bubnov-Galerkin scheme, it is necessary to formulate a stochastic residual error vector $\mathbf{R}(\boldsymbol{\Theta})$. This is achieved by substituting equation (12) in equation (8), which gives

$$\mathbf{R}(\boldsymbol{\Theta}) = \left(\mathbf{L} + \sum_{i=1}^{p} \theta_i \boldsymbol{\Pi}_i \right) \boldsymbol{\Psi}(\boldsymbol{\Theta})\boldsymbol{\Xi}(\boldsymbol{\Theta}) - \mathbf{f}^o - \sum_{i=1}^{q} \eta_i \mathbf{f}^i \tag{19}$$

In the Bubnov-Galerkin scheme, the coefficient vector $\boldsymbol{\Xi}(\boldsymbol{\Theta})$ is computed by enforcing orthogonality of $\mathbf{R}(\boldsymbol{\Theta})$ with respect to the approximating space, i.e., $\boldsymbol{\Psi}(\boldsymbol{\Theta})$. Two procedures are developed in the subsequent sections for computing $\boldsymbol{\Xi}(\boldsymbol{\Theta})$. These procedures are based on the approximate stochastic Bubnov-Galerkin scheme and the exact stochastic Bubnov-Galerkin scheme outlined earlier in Section 2. It is shown that both procedures allow an explicit expression to be derived for the stochastic process $\hat{\mathbf{u}}(\boldsymbol{\Theta})$.

5.1 Approximate Stochastic Bubnov-Galerkin Approach

The undetermined coefficients in the SRBA are evaluated here such that the stochastic residual error $\mathbf{R}(\boldsymbol{\Theta})$ is orthogonal to $\boldsymbol{\Psi}(\boldsymbol{\Theta})$ in an approximate sense. Here the definition of the inner product of two random vector functions in the Hilbert space of random variables is employed. This can be formally stated as

$$\langle \boldsymbol{\Psi}^T(\boldsymbol{\Theta})\mathbf{R}(\boldsymbol{\Theta}) \rangle = 0 \tag{20}$$

Equation (20) leads to a deterministic matrix system of equations of dimension $(m+1)\times(m+1)$ for the coefficient vector $\boldsymbol{\Xi}$, which is considered here to be deterministic. This formulation is henceforth referred to as the approximate SRBA (ASRBA) method. The order of the approximation is considered to be equal to m; where m+1 is the number of basis vectors used (see equation (11)). The system of equations to be solved for the coefficients $\boldsymbol{\Xi}$ can be written as

$$\left[\langle \boldsymbol{\Psi}^T(\boldsymbol{\Theta})\mathbf{L}\boldsymbol{\Psi}(\boldsymbol{\Theta}) \rangle + \sum_{i=1}^{p} \langle \theta_i \boldsymbol{\Psi}^T(\boldsymbol{\Theta})\boldsymbol{\Pi}_i\boldsymbol{\Psi}(\boldsymbol{\Theta}) \rangle \right] \boldsymbol{\Xi} =$$

$$\left\langle \Psi^T(\Theta)\left(\mathbf{f}^o + \sum_{i=1}^{q} {}_i\mathbf{f}^i\right)\right\rangle \tag{21}$$

The above equation can be rewritten in a compact form as

$$[\mathbf{L}_R + \mathbf{\Pi}_R]\,\Xi = \mathbf{F}_R \tag{22}$$

where $\mathbf{L}_R$, $\mathbf{\Pi}_R \in \Re^{(m+1)\times(m+1)}$ are deterministic matrices; $\mathbf{F}_R \in \Re^{(m+1)\times 1}$ is the deterministic reduced force vector. The elements of these terms can be readily computed using the joint statistics of the random variables θ_i. General expressions for the elements of these terms are presented in Appendix A. These allow the computation of the vector of deterministic constants Ξ, which is then used in conjunction with equation (11) to arrive at an explicit expression for $\hat{\mathbf{u}}(\Theta)$.

The ASRBA formulation can be simplified by rewriting the reduced basis approximation as follows

$$\hat{\mathbf{u}}(\Theta) = \xi_0\Psi_0(\Theta) + \sum_{i=1}^{p}\xi_i\theta_i\left(\mathbf{b}_i^{(11)} + \sum_{j=1}^{q}\eta_j\mathbf{b}_{ij}^{(12)}\right), \tag{23}$$

where $\xi_i, i = 0, 1, 2, \ldots, p$ denote deterministic undetermined scalars.

Equation (23) includes only the first two terms of the Neumann expansion series, and the number of undetermined scalars is $p+1$. Substituting equation (23) in (8) and using the approximate stochastic Bubnov-Galerkin scheme leads to a system of deterministic equations of dimension $p+1$ similar to equation (21). General expressions for this matrix system of equations are considerably simpler as compared to the ASRBA formulation presented earlier. This simplified formulation is henceforth referred to as the simplified ASRBA method.

5.2 An Exact Stochastic Bubnov-Galerkin Procedure

In contrast to the earlier formulation, here it is aimed to *exactly orthogonalize* the stochastic residual error vector $\mathbf{R}(\Theta)$ with respect to the approximating space $\Psi(\Theta)$. This implies that all the statistical moments of the inner product of $\Psi(\Theta)$ and $\mathbf{R}(\Theta)$ should be zero. This condition can be written as

$$\langle\left(\Psi^T(\Theta)\mathbf{R}(\Theta)\right)^k\rangle = 0; k = 1, 2, \ldots, \infty \tag{24}$$

It can be seen that equation (24) will be satisfied only when, for each realization of the random variable vector Θ , the term in the brackets is zero. Hence, $\Xi(\Theta)$ should be computed as

$$\Xi(\Theta) = \left[\Psi^T(\Theta)\left(\mathbf{L} + \sum_{i=1}^{p}\theta_i\mathbf{\Pi}_i\right)\Psi(\Theta)\right]^{-1} \times\Psi^T(\Theta)\left(\mathbf{f}^o + \sum_{i=1}^{q}\eta_i\mathbf{f}^i\right) \tag{25}$$

It can be observed from equation (25) that, achieving an explicit expression for $\Xi(\Theta)$, would involve symbolically inverting a random matrix of dimension $(m+1)\times(m+1)$. This could be readily achieved for small values of m. From the authors' previous experience, it has been observed that generally two or three basis vectors are sufficient to ensure good approximations for large variations in θ_i. Experimental evidence for this observation is presented in the companion paper. Consider, for example, the first-order SRBA method where $\mathbf{u}(\Theta)$ is approximated using two basis vectors as given below

$$\hat{\mathbf{u}}(\Theta) = \xi_0(\Theta)\left(\mathbf{u}_o + \sum_{i=1}^{p}\theta_i\mathbf{u}_i\right) + \xi_1(\Theta)\left(\sum_{i=1}^{p}\theta_i\mathbf{b}_i^{(11)} + \sum_{i=1}^{p}\sum_{j=1}^{q}\theta_i\eta_j\mathbf{b}_{ij}^{(12)}\right) \tag{26}$$

The corresponding 2×2 matrix system of equations to be explicitly solved for $\Xi(\Theta)$ can be written as

$$[\mathbf{L}_R(\Theta) + \mathbf{\Pi}_R(\Theta)]\,\Xi(\Theta) = \mathbf{F}_R(\Theta) \tag{27}$$

Explicit expressions for $\mathbf{L}_R$, $\mathbf{\Pi}_R$, and $\mathbf{F}_R$ can be readily derived in terms of the random variables using tensor notation (see Appendix B). These explicit expressions can be used to represent the random functions $\xi_0(\Theta)$ and $\xi_1(\Theta)$. Similar equations can also be derived for the case when three basis vectors are used in the SRBA. The use of symbolic computation software is expected to greatly alleviate the tediousness of the derivation. It is expected that the explicit expressions for the reduced matrices can be simplified by replacing terms of order greater than four by their ensemble averages, without significant loss of accuracy.

5.3 Remarks

It can be readily shown that the computational cost involved in both the SRBA methods for constructing the reduced-order problem are of the order of $O(n^2)$, since only matrix vector multiplications are

involved. It is assumed here that for most problems of practical interest, the number of random variables $p \ll n$. Further, as is shown later in the companion paper, two or three basis vectors are sufficient to obtain nearly exact results for cases when the coefficient of variation of θ_i is of the order of 20%.

Consider the case when $rank(\sum_{i=1}^{p} \theta_i \mathbf{\Pi}_i) = 1$ Then it can be readily shown that the first-order SRBA method will give the exact results with probability one. For example, for a truss structure with one member having random Young's modulus, exact results can be obtained using the first-order SRBA method. This can be formally proved using the observations made earlier in reference[26].

Currently, it is not clear how to compute *a priori* error estimates for the SRBA methods. However, *a posteriori* error estimates of the response statistics can be estimated using the statistics of $\mathbf{R}(\mathbf{\Theta})$.

6. Determination of Response Statistics from SRBA

Consider the case wherein the ASRBA method of order m is used to approximate the stochastic response quantities. The ASRBA method leads to a random polynomial for the response process of the form

$$\hat{\mathbf{u}}(\mathbf{\Theta}) = \sum_{i=0}^{m} \xi_i \Psi_i(\mathbf{\Theta}) \tag{28}$$

Since the coefficients ξ_i are considered here to be deterministic scalars, the mean and variance of the response quantities can be expressed in terms of the statistics of Ψ_i. Note that these statistics can be analytically computed using using equation (15) and the joint statistics of θ_i; see, for example, McCullagh[27] and chapter 4 of reference[2] for details on statistical analysis of random polynomials. The moments of the response can also be analytically computed for the simplified ASRBA formulation.

In contrast, the SRBA method leads to the coefficients being highly nonlinear functions of the random variable vector $\mathbf{\Theta}$. Hence analytical solutions for the statistics of $\hat{\mathbf{u}}(\mathbf{\Theta})$ are not readily possible. Fortunately, sampling the SRBA representation for each realization of $\mathbf{\Theta}$ involves only a few operations when $p \ll n$. In particular, the first and second-order SRBA method requires of the order of p^3 and p^5 operations, respectively. This operation count can be further reduced by replacing all terms of order greater than 2 by their ensemble averages. Hence, Monte Carlo integration techniques can be readily applied to compute the response statistics in a computationally efficient fashion. In fact, the complete probability density function of the response is within reach by using a simulation scheme in conjunction with non-parametric kernel density estimation techniques. However, it may be possible to simplify the SRBA representation by assuming the random functions to be random variables. The effects of such approximations on the accuracy of the SRBA methods remain to be seen.

In the context of reliability analysis (see, for example, reference[28−29]), SRBA methods allow the derivation of an explicit expression for the multi-dimensional limit state curve. This potentially enables the efficient computation of failure probabilities without resorting to first or second order reliability approximations. Furthermore, the explicit expressions for $\hat{\mathbf{u}}(\mathbf{\Theta})$ can also be used to efficiently compute response sensitivities for robust design optimization studies.

6. Application to Nonlinear Stochastic Systems

This section discusses how SRBA methods can be applied in conjunction with stochastic linearization techniques to analysis of nonlinear stochastic systems subjected to random excitation. Consider for example, random vibration analysis of a geometrically nonlinear stochastic structural system. Discretization of the governing nonlinear PDEs in space and the random dimension typically leads to a system of nonlinear ordinary differential equations of the form

$$\mathbf{M}(\mathbf{\Theta})\ddot{\mathbf{u}}(\mathbf{\Theta}) + \mathbf{C}(\mathbf{\Theta})\dot{\mathbf{u}}(\mathbf{\Theta}) + \mathbf{K}(\mathbf{\Theta})\mathbf{u}(\mathbf{\Theta}) + \mathbf{\Gamma}(\mathbf{\Theta}, \mathbf{u}(\mathbf{\Theta})) = \mathbf{F}(\mathbf{\Theta}) \tag{28}$$

where $\mathbf{M}(\mathbf{\Theta})$, $\mathbf{C}(\mathbf{\Theta})$, and $\mathbf{K}(\mathbf{\Theta}) \in \Re^{n \times n}$ are the linear stochastic mass, damping, and stiffness matrices; $\mathbf{\Gamma}(\mathbf{\Theta}, \mathbf{u}(\mathbf{\Theta})) \in \Re^{n \times 1}$ denotes the stochastic nonlinear restoring force vector; $\mathbf{\Theta}$ denotes the random variables arising from discretization of the underlying random fields of the physical parameters.

Consider the case when the random system parameters appear as multiplicative terms in all the differential operators. The nonlinear stochastic vector can hence be written as

$$\mathbf{\Gamma}(\mathbf{\Theta}, \mathbf{u}(\mathbf{\Theta})) = \mathbf{\Gamma}^o(\mathbf{u}(\mathbf{\Theta})) + \sum_{i=1}^{p} \theta_i \mathbf{\Gamma}^i(\mathbf{u}(\mathbf{\Theta})) \tag{29}$$

where $\mathbf{\Gamma}^o$ and $\mathbf{\Gamma}^i \in \Re^{n \times 1}$ are functions of the displacement vector alone. These terms can be replaced by an equivalent linear matrix using any

stochastic linearization formulation; see, for example, references[30-31]. Expressions similar to equation (28) can also be arrived at for the linear stochastic terms. Transformation of the linearized equations to the frequency domain leads to a system of linear algebraic equations with random coefficients of the form :

$$\left[\mathbf{D}^o(\omega) + \sum_{i=1}^{p} \theta_i \mathbf{D}^i(\omega)\right] \mathbf{u}(\boldsymbol{\Theta}) = \mathbf{F}^o(\omega) + \sum_{i=1}^{q} \eta_i \mathbf{F}^i(\omega) \tag{30}$$

where $\mathbf{D}^o(\omega) = (\mathbf{K}^o + \mathbf{K}_e^o - \omega^2\mathbf{M}^o + \mathrm{j}\omega\mathbf{C}^o)$ and $\mathbf{D}^i(\omega) = (\mathbf{K}^i + \mathbf{K}_e^i - \omega^2\mathbf{M}^i + \mathrm{j}\omega\mathbf{C}^i)$; $\mathbf{K}_e^o$ and $\mathbf{K}_e^i$ are deterministic linear matrices obtained by stochastic linearization of the nonlinear vectors $\boldsymbol{\Gamma}^o(\mathbf{u}(\boldsymbol{\Theta}))$ and $\boldsymbol{\Gamma}^i(\mathbf{u}(\boldsymbol{\Theta}))$, respectively; $\mathrm{j} = \sqrt{-1}$; $\mathbf{K}^o$, $\mathbf{K}^i$, $\mathbf{M}^o$, $\mathbf{M}^i$, $\mathbf{C}^o$, and $\mathbf{C}^i$ are deterministic matrices obtained by representing the linear stochastic matrices in a form similar to equation (29).

Equation (30) can be readily solved using either the ASRBA or SRBA method to arrive at an explicit expression for the stochastic response vector $\mathbf{u}(\boldsymbol{\Theta})$. An iterative procedure is employed to compute the response statistics, wherein the linear stochastic equations are solved first to arrive at an initial guess for the statistics of $\mathbf{u}(\boldsymbol{\Theta})$. In subsequent iterations, the response statistics at the previous step are used to compute the equivalent linear matrices $\mathbf{K}_e^o$ and $\mathbf{K}_e^i$. The iterations are terminated when the response statistics do not change appreciably across subsequent iterations. Further, it is also possible to reduce the dimensionality of the problem at each iteration by using the eigenvectors of the deterministic eigenvalue problem $(\mathbf{K}^o + \mathbf{K}_e^o)\phi = \lambda\mathbf{M}^o\phi$ to transform equation (30) to modal coordinates.

8. Concluding Remarks

Efficient numerical schemes based on stochastic reduced basis approximations are presented for analysis of systems governed by stochastic PDEs. The methods presented here are quite general in scope and can be applied to a wide spectrum of problem domains. A major advantage of the present approach is that an explicit representation of the response quantities in terms of the random system parameters can be achieved. This enables a complete probabilistic description of the response quantities to obtained in a computationally efficient fashion.

More importantly, in contrast to the increased basis approximation procedure wherein a polynomial chaos decomposition is used for $\mathbf{u}(\boldsymbol{\Theta})$, the stochastic reduced basis methods developed here lead to a substantial reduction in the problem size. SRBA methods are hence expected to be computationally more efficient, particularly for large-scale systems. Further, in contrast to the increased basis method, the random variables which appear in the expression for the response vector have physical meaning. In a companion paper, numerical results are presented for a class of problems in computational mechanics. It is shown that SRBA methods do not compromise on accuracy while achieving this substantial reduction in the computational cost. Some comparison studies with the Neumann expansion scheme are also presented to demonstrate that SRBA methods give significantly better results.

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Appendix A

The expressions for the deterministic reduced matrices which arise in the ASRBA method (see equation (22)) are summarized below. $\mathbf{L}_R \in \Re^{(m+1)\times(m+1)}$ is a deterministic matrix, a typical element of which can be computed as

$$\begin{aligned}
\mathbf{L}_R(k,l) &= \langle \Psi_k^T \mathbf{L} \Psi_l \rangle \\
&= C^1_{i_1 i_2 \ldots i_k j_1 j_2 \ldots j_l} (\mathbf{b}^{(k1)}_{i_1 i_2 \ldots i_k})^T \mathbf{L} (\mathbf{b}^{(l1)}_{j_1 j_2 \ldots j_l}) \\
&+ C^2_{i_1 i_2 \ldots i_k j_1 j_2 \ldots j_{l+1}} (\mathbf{b}^{(k1)}_{i_1 i_2 \ldots i_k})^T \mathbf{L} (\mathbf{b}^{(l2)}_{j_1 j_2 \ldots j_{l+1}}) \\
&+ C^3_{i_1 i_2 \ldots i_{k+1} j_1 j_2 \ldots j_l} (\mathbf{b}^{(k2)}_{i_1 i_2 \ldots i_{k+1}})^T \mathbf{L} (\mathbf{b}^{(l1)}_{j_1 j_2 \ldots j_l}) \\
&+ C^4_{i_1 i_2 \ldots i_{k+1} j_1 j_2 \ldots j_{l+1}} (\mathbf{b}^{(k2)}_{i_1 i_2 \ldots i_{k+1}})^T \mathbf{L} (\mathbf{b}^{(l2)}_{j_1 j_2 \ldots j_{l+1}}),
\end{aligned}$$

$\mathbf{\Pi}_R \in \Re^{(m+1)\times(m+1)}$ is a deterministic matrix, a typical element of which can be written as

$$\begin{aligned}
\mathbf{\Pi}_R(k,l) &= \langle \sum_{i=1}^{p} \theta_i \Psi_k^T \mathbf{\Pi}_i \Psi_l \rangle \\
&= B^1_{i_1 i_2 \ldots i_{k+1} j_1 j_2 \ldots j_l} (\mathbf{b}^{(k1)}_{i_1 i_2 \ldots i_k})^T \mathbf{\Pi}_{k+1} (\mathbf{b}^{(l1)}_{j_1 j_2 \ldots j_l}) \\
&+ B^2_{i_1 i_2 \ldots i_{k+1} j_1 j_2 \ldots j_{l+1}} (\mathbf{b}^{(k1)}_{i_1 i_2 \ldots i_k})^T \mathbf{\Pi}_{k+1} (\mathbf{b}^{(l2)}_{j_1 j_2 \ldots j_{l+1}}) \\
&+ B^3_{i_1 i_2 \ldots i_{k+2} j_1 j_2 \ldots j_l} (\mathbf{b}^{(k2)}_{i_1 i_2 \ldots i_{k+1}})^T \mathbf{\Pi}_{k+1} (\mathbf{b}^{(l1)}_{j_1 j_2 \ldots j_l}) \\
&+ B^4_{i_1 i_2 \ldots i_{k+2} j_1 j_2 \ldots j_{l+1}} (\mathbf{b}^{(k2)}_{i_1 i_2 \ldots i_{k+1}})^T \mathbf{\Pi}_{k+1} (\mathbf{b}^{(l2)}_{j_1 j_2 \ldots j_{l+1}}),
\end{aligned}$$

The tensors B and C are tabulated below :

$$C^1_{i_1 \ldots i_k j_1 \ldots j_k} = \langle \theta_{i_1} \theta_{i_2} \ldots \theta_{i_k} \theta_{j_1} \theta_{j_2} \ldots \theta_{j_l} \rangle \qquad C^2_{i_1 \ldots i_k j_1 \ldots j_{l+1}} = \langle \theta_{i_1} \theta_{i_2} \ldots \theta_{i_k} \theta_{j_1} \theta_{j_2} \ldots \theta_{j_l} \eta_{j_{l+1}} \rangle$$

$$C^3_{i_1 \ldots i_{k+1} j_1 \ldots j_l} = \langle \theta_{i_1} \theta_{i_2} \ldots \theta_{i_k} \eta_{i_{k+1}} \theta_{j_1} \theta_{j_2} \ldots \theta_{j_l} \rangle \qquad C^4_{i_1 \ldots i_{k+1} j_1 \ldots j_{l+1}} = \langle \theta_{i_1} \theta_{i_2} \ldots \theta_{i_k} \eta_{i_{k+1}} \theta_{j_1} \theta_{j_2} \ldots \theta_{j_l} \eta_{j_{l+1}} \rangle$$

$$B^1_{i_1 \ldots i_{k+1} j_1 \ldots j_l} = \langle \theta_{i_1} \theta_{i_2} \ldots \theta_{i_{k+1}} \theta_{j_1} \theta_{j_2} \ldots \theta_{j_l} \rangle \qquad B^2_{i_1 \ldots i_{k+1} j_1 \ldots j_{l+1}} = \langle \theta_{i_1} \theta_{i_2} \ldots \theta_{i_{k+1}} \theta_{j_1} \theta_{j_2} \ldots \theta_{j_l} \eta_{j_{l+1}} \rangle$$

$$B^3_{i_1 \ldots i_{k+2} j_1 \ldots j_l} = \langle \theta_{i_1} \theta_{i_2} \ldots \theta_{i_{k+1}} \eta_{i_{k+2}} \theta_{j_1} \theta_{j_2} \ldots \theta_{j_l} \rangle \qquad B^4_{i_1 \ldots i_{k+2} j_1 \ldots j_{l+1}} = \langle \theta_{i_1} \theta_{i_2} \ldots \theta_{i_{k+1}} \eta_{i_{k+2}} \theta_{j_1} \theta_{j_2} \ldots \theta_{j_l} \eta_{j_{l+1}} \rangle.$$

Similarly, a typical element of $\mathbf{F}_R \in \Re^{(m+1)\times 1}$ can be evaluated as

$$\begin{aligned}
\mathbf{F}_R(k) &= \langle \mathbf{\Psi}_k^T \rangle \mathbf{f}^o + \sum_{i=1}^{q} \langle \mathbf{\Psi}_k^T \eta_i \rangle \mathbf{f}^i \\
&= \langle \theta_{i_1} \theta_{i_2} \ldots \theta_{i_k} \rangle (\mathbf{b}^{(k1)}_{i_1 i_2 \ldots i_k})^T \mathbf{f}^o \\
&+ \langle \theta_{i_1} \theta_{i_2} \ldots \theta_{i_k} \eta_{i_{k+1}} \rangle (\mathbf{b}^{(k2)}_{i_1 i_2 \ldots i_{k+1}})^T \mathbf{f}^o \\
&+ \langle \theta_{i_1} \theta_{i_2} \ldots \theta_{i_k} \eta_{k+1} \rangle (\mathbf{b}^{(k1)}_{i_1 i_2 \ldots i_k})^T \mathbf{f}^{k+1} \\
&+ \langle \theta_{i_1} \theta_{i_2} \ldots \theta_{i_k} \eta_{i_{k+1}} \eta_{i_{k+2}} \rangle (\mathbf{b}^{(k2)}_{i_1 i_2 \ldots i_{k+1}})^T \mathbf{f}^{k+2}
\end{aligned}$$

When the random variables θ_i and η_i are uncorrelated, the expectation operations for the tensors B and C can be readily calculated. In the notation used here, repeated indices indicate summation with respect to that index over its range. Using this, the values of the deterministic coefficients $\mathbf{\Xi}$ can be computed.

Appendix B

For the sake of notational simplicity consider the case when the force vector is deterministic. Then the reduced-order matrices for the first-order SRBA method (see equation (27)) can be written using tensor notation as

$$\mathbf{L}_R + \mathbf{\Pi}_R = \begin{bmatrix} \mathbf{u}^{oT}\mathbf{L}\mathbf{u}^o + \theta_i \mathbf{u}^{oT}\mathbf{\Pi}_i\mathbf{u}^o & \theta_i \mathbf{u}^{oT}\mathbf{L}\mathbf{b}_i^{11} + \theta_i\theta_j \mathbf{u}^{oT}\mathbf{\Pi}_i\mathbf{b}_j^{11} \\ \text{sym} & \theta_i\theta_j(\mathbf{b}_i^{11})^T\mathbf{L}\mathbf{b}_j^{11} + \theta_i\theta_j\theta_k(\mathbf{b}_i^{11})^T\mathbf{\Pi}_j\mathbf{b}_k^{11} \end{bmatrix} \tag{17}$$

$$\mathbf{F}_R = \begin{bmatrix} \mathbf{u}^{oT}\mathbf{f}^o \\ \theta_i(\mathbf{b}_i^{11})^T\mathbf{f}^o \end{bmatrix} \tag{18}$$

In the notation used here, repeated index implies summation with respect to it over its range. Using equations (17) and (18), an explicit expression can be derived for the random functions in the reduced basis representation.