Elliptic stochastic partial differential equations: An orthonormal vector basis approach

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The stochastic finite element analysis of elliptic type partial differential equations are considered. An alternative approach by projecting the solution of the discretized equation into a finite dimensional orthonormal vector basis is investigated. It is shown that the solution can be obtained using a finite series comprising functions of random variables and orthonormal vectors. These functions, called as the spectral functions, can be expressed in terms of the spectral properties of the deterministic coefficient matrices arising due to the discretization of the governing partial differential equation. Based on the projection in the orthonormal vector basis, a Galerkin error minimization approach is proposed. The constants appearing in the Galerkin method are solved from a system of linear equations which has the same dimension as the original discretized equation. A hybrid analytical and simulation based computational approach is proposed to obtain the moments and pdf of the solution. The method is illustrated using the stochastic nanomechanics of a Zinc Oxide (ZnO) nanowire deflected under the atomic force microscope (AFM) tip. The results are compared with the direct Monte Carlo simulation results for different correlation lengths and strengths of randomness.

Elliptic Stochastic Partial Differential Equation

We consider the stochastic elliptic partial differential equation (PDE)

$$-\nabla\left[a(\mathbf{r},\omega)\nabla u(\mathbf{r},\omega)\right]=p(\mathbf{r});\quad \mathbf{r}\text{ in }\mathcal{D} \tag{1}$$

with suitable boundary conditions. Here $a:\mathbb{R}^d\times\Omega\to\mathbb{R}$ $(d\leq 3)$ is a random field and $\omega\in\Omega$ is a sample point from the sampling space Ω. We assume the random field $a(\mathbf{r},\omega)$ to be stationary and square integrable. The random field $a(\mathbf{r},\omega)$ can be expressed by Karhunen-Loève expansion as

$$a(\mathbf{r},\omega)=a_0(\mathbf{r})+\sum_{i=1}^{\infty}\sqrt{\nu_i}\xi_i(\omega)\varphi_i(\mathbf{r}) \tag{2}$$

Here $a_0(\mathbf{r})$ is the mean function, $\xi_i(\omega)$ are uncorrelated standard Gaussian random variables, ν_i and $\varphi_i(\mathbf{r})$ are eigenvalues and eigenfunctions of the autocorrelation function. Truncating the series (2) upto the M-th term, substituting $a(\mathbf{r},\omega)$ in the governing PDE (1) and applying the boundary conditions, the discretized equation can be written as

$$\left[\mathbf{A}_0+\sum_{i=1}^{M}\xi_i(\omega)\mathbf{A}_i\right]\mathbf{u}(\omega)=\mathbf{f} \tag{3}$$

Our aim is to propose a new solution technique of this equation.

Polynomial Chaos Expansion: After a finite truncation, the polynomial chaos expansion for the solution of Eq. (3) can be written as

$$\hat{\mathbf{u}}(\omega)=\sum_{k=1}^{P}H_k(\boldsymbol{\xi}(\omega))\mathbf{u}_k;\text{ where }P=\sum_{j=0}^{r}\frac{(M+j-1)!}{j!(M-1)!} \tag{4}$$

Here $H_k(\boldsymbol{\xi}(\omega))$ are the polynomial chaoses. Since P increases very rapidly with the order of the chaos r and the number of random variables M, the final number of unknown constants Pn becomes very large.

Spectral decomposition in the vector space

Remark 1. *(The spanning property) Suppose $\{\boldsymbol{\phi}_1,\boldsymbol{\phi}_2,\ldots,\boldsymbol{\phi}_n\}$ is a complete basis in the Hilbert space H. Then for every nonzero $\mathbf{u}\in H$, it is possible to choose $\alpha_1,\alpha_2,\ldots,\alpha_n\neq 0$ uniquely such that $\mathbf{u}=\alpha_1\boldsymbol{\phi}_1+\alpha_2\boldsymbol{\phi}_2+\ldots\alpha_n\boldsymbol{\phi}_n$.*

We can 'split' the Polynomial Chaos type of expansions as $\hat{\mathbf{u}}(\omega)=\sum_{k=1}^{n}H_k(\boldsymbol{\xi}(\omega))\mathbf{u}_k+\sum_{k=n+1}^{P}H_k(\boldsymbol{\xi}(\omega))\mathbf{u}_k$. According to the spanning property of a complete basis in $\mathbb{R}^n$ it is *always* possible to project $\hat{\mathbf{u}}(\omega)$ in a finite dimensional vector basis for any $\omega\in\Omega$. Therefore, in a vector polynomial chaos expansion, all $\mathbf{u}_k$ for $k>n$ must be linearly dependent. This is the motivation behind seeking a finite dimensional expansion.

Theorem 1. *There exist a finite set of functions $\Gamma_k:(\mathbb{R}^m\times\Omega)\to(\mathbb{R}\times\Omega)$ and an orthonormal basis $\boldsymbol{\phi}_k\in\mathbb{R}^n$ for $k=1,2,\ldots,n$ such that the series*

$$\hat{\mathbf{u}}(\omega)=\sum_{k=1}^{n}\Gamma_k(\boldsymbol{\xi}(\omega))\boldsymbol{\phi}_k \tag{5}$$

converges to the exact solution of the discretized stochastic finite element equation (3) with probability 1.

Outline of the proof: The first step is to generate a complete orthonormal basis. We use the eigenvectors $\boldsymbol{\phi}_k\in\mathbb{R}^n$ of the matrix $\mathbf{A}_0$ such that

$$\mathbf{A}_0\boldsymbol{\phi}_k=\lambda_{0_k}\boldsymbol{\phi}_k;\quad k=1,2,\ldots n \tag{6}$$

We define the matrix of eigenvalues $\boldsymbol{\Lambda}_0=\text{diag}\left[\lambda_{0_1},\lambda_{0_2},\ldots,\lambda_{0_n}\right]$ and eigenvectors $\boldsymbol{\Phi}=[\boldsymbol{\phi}_1,\boldsymbol{\phi}_2,\ldots,\boldsymbol{\phi}_n]$. Suppose the solution of Eq. (3) is given by

$$\hat{\mathbf{u}}(\omega)=\left[\mathbf{A}_0+\sum_{i=1}^{M}\xi_i(\omega)\mathbf{A}_i\right]^{-1}\mathbf{f} \tag{7}$$

Using the orthonormality of $\boldsymbol{\Phi}$ one has $\hat{\mathbf{u}}(\omega)=\boldsymbol{\Phi}\boldsymbol{\Psi}\left(\boldsymbol{\xi}(\omega)\right)\boldsymbol{\Phi}^T\mathbf{f}$ with $\boldsymbol{\Psi}\left(\boldsymbol{\xi}(\omega)\right)=\left[\boldsymbol{\Lambda}_0+\sum_{i=1}^{M}\xi_i(\omega)\widetilde{\mathbf{A}}_i\right]^{-1}$. Separating the diagonal and off-diagonal terms we have

$$\boldsymbol{\Psi}\left(\boldsymbol{\xi}(\omega)\right)=\left[\underbrace{\boldsymbol{\Lambda}_0+\sum_{i=1}^{M}\xi_i(\omega)\boldsymbol{\Lambda}_i}_{\boldsymbol{\Lambda}(\boldsymbol{\xi}(\omega))}+\underbrace{\sum_{i=1}^{M}\xi_i(\omega)\boldsymbol{\Delta}_i}_{\boldsymbol{\Delta}(\boldsymbol{\xi}(\omega))}\right]^{-1} \tag{8}$$

where $\boldsymbol{\Lambda}\left(\boldsymbol{\xi}(\omega)\right)\in\mathbb{R}^{n\times n}$ is a diagonal matrix and $\boldsymbol{\Delta}\left(\boldsymbol{\xi}(\omega)\right)$ is an off-diagonal only matrix.

Expanding this in a Neumann type of matrix series we have

$$\boldsymbol{\Psi}\left(\boldsymbol{\xi}(\omega)\right)=\sum_{s=0}^{\infty}(-1)^s\left[\boldsymbol{\Lambda}^{-1}\left(\boldsymbol{\xi}(\omega)\right)\boldsymbol{\Delta}\left(\boldsymbol{\xi}(\omega)\right)\right]^s\boldsymbol{\Lambda}^{-1}\left(\boldsymbol{\xi}(\omega)\right) \tag{9}$$

Defining

$$\Gamma_k\left(\boldsymbol{\xi}(\omega)\right)=\sum_{j=1}^{n}\Psi_{kj}\left(\boldsymbol{\xi}(\omega)\right)\left(\boldsymbol{\phi}_j^T\mathbf{f}\right) \tag{10}$$

and rearranging one has

$$\hat{\mathbf{u}}(\omega)=\sum_{k=1}^{n}\Gamma_k\left(\boldsymbol{\xi}(\omega)\right)\boldsymbol{\phi}_k \tag{11}$$

Spectral functions

Definition 1. *The functions $\Gamma_k\left(\boldsymbol{\xi}(\omega)\right),k=1,2,\ldots n$ are called the spectral functions as they are expressed in terms of the spectral properties of the coefficient matrices of the governing discretized equation.*

The main difficulty in applying this result is that each of the spectral functions $\Gamma_k\left(\boldsymbol{\xi}(\omega)\right)$ contain infinite number of terms and they are highly nonlinear functions of the random variables $\xi_i(\omega)$. For computational purposes, it is necessary to truncate the series after certain number of terms. Different order of spectral functions can be obtained by using truncation in the expression of $\Gamma_k\left(\boldsymbol{\xi}(\omega)\right)$.

Definition 2. *The first-order spectral functions $\Gamma_k^{(1)}(\boldsymbol{\xi}(\omega)),k=1,2,\ldots,n$ are obtained by retaining one term in the series (9).*

Retaining one term in (9) we have

$$\boldsymbol{\Psi}^{(1)}\left(\boldsymbol{\xi}(\omega)\right)=\boldsymbol{\Lambda}^{-1}\left(\boldsymbol{\xi}(\omega)\right)\quad\text{or}\quad\Psi_{kj}^{(1)}\left(\boldsymbol{\xi}(\omega)\right)=\frac{\delta_{kj}}{\lambda_{0_k}+\sum_{i=1}^{M}\xi_i(\omega)\lambda_{i_k}} \tag{12}$$

Using the definition of the spectral function in Eq. (10), the first-order spectral functions can be explicitly obtained as

$$\Gamma_k^{(1)}\left(\boldsymbol{\xi}(\omega)\right)=\sum_{j=1}^{n}\Psi_{kj}^{(1)}\left(\boldsymbol{\xi}(\omega)\right)\left(\boldsymbol{\phi}_j^T\mathbf{f}\right)=\frac{\boldsymbol{\phi}_k^T\mathbf{f}}{\lambda_{0_k}+\sum_{i=1}^{M}\xi_i(\omega)\lambda_{i_k}} \tag{13}$$

From this expression it is clear that $\Gamma_k^{(1)}\left(\boldsymbol{\xi}(\omega)\right)$ are non-Gaussian random variables even if $\xi_i(\omega)$ are Gaussian random variables.

Definition 3. *The second-order spectral functions $\Gamma_k^{(2)}(\boldsymbol{\xi}(\omega)),k=1,2,\ldots,n$ are obtained by retaining two terms in the series (9).*

Retaining two terms in (9) we have

$$\boldsymbol{\Psi}^{(2)}\left(\boldsymbol{\xi}(\omega)\right)=\boldsymbol{\Lambda}^{-1}\left(\boldsymbol{\xi}(\omega)\right)-\boldsymbol{\Lambda}^{-1}\left(\boldsymbol{\xi}(\omega)\right)\boldsymbol{\Delta}\left(\boldsymbol{\xi}(\omega)\right)\boldsymbol{\Lambda}^{-1}\left(\boldsymbol{\xi}(\omega)\right)$$

Using the definition of the spectral function in Eq. (10), the second-order spectral functions can be obtained in closed-form as

$$\Gamma_k^{(2)}\left(\boldsymbol{\xi}(\omega)\right)=\frac{\boldsymbol{\phi}_k^T\mathbf{f}}{\lambda_{0_k}+\sum_{i=1}^{M}\xi_i(\omega)\lambda_{i_k}}-\sum_{j=1}^{n}\frac{\left(\boldsymbol{\phi}_j^T\mathbf{f}\right)\sum_{i=1}^{M}\xi_i(\omega)\Delta_{i_{kj}}}{\left(\lambda_{0_k}+\sum_{i=1}^{M}\xi_i(\omega)\lambda_{i_k}\right)\left(\lambda_{0_j}+\sum_{i=1}^{M}\xi_i(\omega)\lambda_{i_j}\right)} \tag{14}$$

The spectral basis functions are not simple polynomials, but ratio of polynomials in $\boldsymbol{\xi}(\omega)$.

Error minimization: The Galerkin approach

Theorem 2. *There exist a set of finite functions $\Gamma_k:(\mathbb{R}^m\times\Omega)\to(\mathbb{R}\times\Omega)$, constants $c_k\in\mathbb{R}$ and orthonormal vectors $\boldsymbol{\phi}_k\in\mathbb{R}^n$ for $k=1,2,\ldots,n$ such that the series*

$$\hat{\mathbf{u}}(\omega)=\sum_{k=1}^{n}c_k\widehat{\Gamma}_k(\boldsymbol{\xi}(\omega))\boldsymbol{\phi}_k \tag{15}$$

converges to the exact solution of the discretized stochastic finite element equation (3) in the mean-square sense provided the vector $\mathbf{c}=\{c_1,c_2,\ldots,c_n\}^T$ satisfies the $n\times n$ algebraic equations $\mathbf{S}\,\mathbf{c}=\mathbf{b}$ with

$$S_{jk}=\sum_{i=0}^{M}\widetilde{A}_{i_{jk}}D_{ijk};\quad\forall\,j,k=1,2,\ldots,n;\widetilde{A}_{i_{jk}}=\boldsymbol{\phi}_j^T\mathbf{A}_i\boldsymbol{\phi}_k, \tag{16}$$

$$D_{ijk}=\text{E}\left[\xi_i(\omega)\widehat{\Gamma}_j(\boldsymbol{\xi}(\omega))\widehat{\Gamma}_k(\boldsymbol{\xi}(\omega))\right],b_j=\text{E}\left[\widehat{\Gamma}_j(\boldsymbol{\xi}(\omega))\right]\left(\boldsymbol{\phi}_j^T\mathbf{f}\right).$$

This can be proved by defining the error vector $\boldsymbol{\varepsilon}(\omega)=\left(\sum_{i=0}^{M}\mathbf{A}_i\xi_i(\omega)\right)\left(\sum_{k=1}^{n}c_k\widehat{\Gamma}_k(\boldsymbol{\xi}(\omega))\boldsymbol{\phi}_k\right)-\mathbf{f}$ and making it orthogonal to the basis functions $\left\{\widehat{\Gamma}_k(\boldsymbol{\xi}(\omega))\boldsymbol{\phi}_k\right\}\in\mathbb{R}^n$, that is, mathematically $\boldsymbol{\varepsilon}(\omega)\perp\left(\widehat{\Gamma}_j(\boldsymbol{\xi}(\omega))\boldsymbol{\phi}_j\right)$ or $\left\langle\widehat{\Gamma}_j(\boldsymbol{\xi}(\omega))\boldsymbol{\phi}_j,\boldsymbol{\varepsilon}(\omega)\right\rangle=0$.

Post processing and computational approach

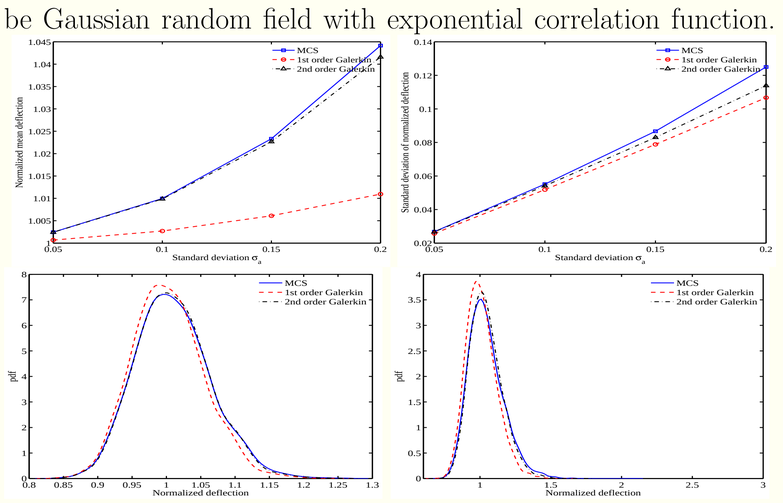
The spectral functions $\widehat{\Gamma}_k(\boldsymbol{\xi}(\omega))$ are highly non-Gaussian in nature and do not in general enjoy any orthogonality properties like the Hermite polynomials or any other orthogonal polynomials with respect to the underlying probability measure. The coefficient matrix $\mathbf{S}$ and the vector $\mathbf{b}$ should be obtained numerically using the Monte Carlo simulation or other numerical integration technique. The simulated spectral functions can also be 'recycled' to obtain the statistics and probability density function (pdf) of the solution.

Summary of the proposed computational approach:

1. Solve the eigenvalue problem associated with the mean matrix $\mathbf{A}_0$ to generate the orthonormal basis vectors: $\mathbf{A}_0\boldsymbol{\Phi}=\boldsymbol{\Lambda}_0\boldsymbol{\Phi}$
2. Select a number of samples, say N_{samp}. Generate the samples of basic random variables $\xi_i(\omega),i=1,2,\ldots,M$.
3. Calculate the spectral basis functions (for example, first-order): $\Gamma_k\left(\boldsymbol{\xi}(\omega)\right)=\frac{\boldsymbol{\phi}_k^T\mathbf{f}}{\lambda_{0_k}+\sum_{i=1}^{M}\xi_i(\omega)\lambda_{i_k}}$
4. Obtain the coefficient vector: $\mathbf{c}=\mathbf{S}^{-1}\mathbf{b}\in\mathbb{R}^n$, where $\mathbf{b}=\widetilde{\mathbf{f}}\odot\overline{\boldsymbol{\Gamma}}$, $\mathbf{S}=\boldsymbol{\Lambda}_0\odot\mathbf{D}_0+\sum_{i=1}^{M}\widetilde{\mathbf{A}}_i\odot\mathbf{D}_i$ and $\mathbf{D}_i=\text{E}\left[\boldsymbol{\Gamma}(\omega)\xi_i(\omega)\boldsymbol{\Gamma}^T(\omega)\right],\forall\,i=0,1,2,\ldots,M$
5. Obtain the samples of the response from the spectral series: $\hat{\mathbf{u}}(\omega)=\sum_{k=1}^{n}c_k\Gamma_k(\boldsymbol{\xi}(\omega))\boldsymbol{\phi}_k$

Numerical Example

We consider the tip deflection of ZnO nanowire of length $L=600$nm, diameter $d=50$nm and the lateral point force at the tip $f_T=80$nN. The bending stiffness of the NW is assumed to be Gaussian random field with exponential correlation function.



(a) Pdf for $\sigma_a=0.1$ (b) Pdf for $\sigma_a=0.2$

The mean, standard deviation and probability density function of the normalized deflection δ/δ_0 of the ZnO NW under the AFM tip (δ_0=145nm). The correlation length of the random field describing the bending rigidity is assumed to be $\mu_a=L/10$. The number of random variable used: $M=67$. The number of degrees of freedom: $n=100$. The results are obtained with 10,000-sample MCS and four values of σ_a (standard deviation of the random field) have been used. If the second-order PC was used, one would need to solve a linear system of equation of size 234,500. The results shown here are obtained by solving a linear system of equation of size 100 using the proposed Galerkin approach.

Statistics	Methods	$\sigma_a=0.05$	$\sigma_a=0.10$	$\sigma_a=0.15$	$\sigma_a=0.20$
Mean	1st order	0.1761	0.7206	1.6829	3.1794
	2nd order	0.0007	0.0113	0.0642	0.6738
Standard deviation	1st order	3.9543	5.9581	9.0305	14.6568
	2nd order	0.3222	1.8425	4.6781	8.9037

Percentage error in the mean and standard deviation of δ/δ_0.

Conclusions

We consider discretised stochastic elliptic partial differential equations. The solution is projected into a finite dimensional complete orthonormal vector basis and the associated coefficient functions are obtained. The coefficient functions, called as the spectral functions, are expressed in terms of the spectral properties of the system matrices. If n is the size of the discretized matrices and M is the number of random variables, then the computational complexity grows in $O(Mn^2)+O(n^3)$ for large M and n in the worse case.

Acknowledgements: The author gratefully acknowledges the support of The Leverhulme Trust for the award of the Philip Leverhulme Prize and The Royal Society of London through the Wolfson Research Merit award.