A Reduced Spectral Projection Method for Stochastic Finite Element Analysis

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Outline of the talk

Stochastic PDEs

We consider the stochastic elliptic partial differential equation (PDE)

$$\mathcal{L}_\theta\{a(\mathbf{r},\theta), u(\mathbf{r},\theta)\} = p(\mathbf{r}) \tag{1}$$

The stochastic operator $\mathcal{L}_\theta$ can be

- $\mathcal{L}_\theta \equiv \frac{\partial}{\partial x} AE(x,\theta)\frac{\partial}{\partial x}$ axial deformation of rods
- $\mathcal{L}_\theta \equiv \frac{\partial^2}{\partial x^2} EI(x,\theta)\frac{\partial}{\partial x}$ axial deformation of rods

Here $a : \mathbb{R}^d \times \Theta \to \mathbb{R}$ is a random field, which can be viewed as a set of random variables indexed by $\mathbf{r} \in \mathbb{R}^d$. We assume the random field $a(\mathbf{r},\theta)$ to be stationary and square integrable. Based on the physical problem the random field $a(\mathbf{r},\theta)$ can be used to model different physical quantities (e.g., $AE(x,\theta)$, $EI(x,\theta)$).

Discretized Stochastic PDE

- The random process $a(\mathbf{r}, \theta)$ can be expressed in a generalized fourier type of series known as the Karhunen-Loève expansion

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

Here $a_0(\mathbf{r})$ is the mean function, $\xi_i(\theta)$ are uncorrelated standard Gaussian random variables, ν_i and $\varphi_i(\mathbf{r})$ are eigenvalues and eigenfunctions satisfying the integral equation

$$\int_{\mathcal{D}} C_a(\mathbf{r}_1, \mathbf{r}_2)\varphi_j(\mathbf{r}_1)\mathrm{d}\mathbf{r}_1 = \nu_j\varphi_j(\mathbf{r}_2), \quad \forall\, j = 1, 2, \cdots \tag{3}$$

Discrete equation for stochastic mechanics

- Truncating the KL expansion upto the M-th term and discretising the displacement field, the equation for static deformation can be expresses as

$$\left[\mathbf{A}_0 + \sum_{i=1}^{M} \xi_i(\theta)\mathbf{A}_i\right] \mathbf{u}(\theta) = \mathbf{f} \tag{4}$$

- The aim is to efficiently solve for $\mathbf{u}(\theta)$.
- Note: Equation (4) can also be obtained with other considerations, such as random variable models.
- For damped structural dynamical systems $\mathbf{A}_i, i = 0, \cdots, M$ matrices in general become frequency dependent and complex.

Polynomial Chaos expansion

- Using the Polynomial Chaos expansion, the solution (a vector valued function) can be expressed as

$$\begin{aligned}\mathbf{u}(\theta) = \mathbf{u}_{i_0} h_0 &+ \sum_{i_1=1}^{\infty} \mathbf{u}_{i_1} h_1(\xi_{i_1}(\theta)) \\ &+ \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} \mathbf{u}_{i_1,i_2} h_2(\xi_{i_1}(\theta), \xi_{i_2}(\theta)) \\ &+ \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} \sum_{i_3=1}^{i_2} \mathbf{u}_{i_1 i_2 i_3} h_3(\xi_{i_1}(\theta), \xi_{i_2}(\theta), \xi_{i_3}(\theta)) \\ &+ \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} \sum_{i_3=1}^{i_2} \sum_{i_4=1}^{i_3} \mathbf{u}_{i_1 i_2 i_3 i_4}\, h_4(\xi_{i_1}(\theta), \xi_{i_2}(\theta), \xi_{i_3}(\theta), \xi_{i_4}(\theta)) + \dots,\end{aligned}$$

Here $\mathbf{u}_{i_1,\dots,i_p} \in \mathbb{R}^n$ are deterministic vectors to be determined.

Polynomial Chaos expansion

- After the finite truncation, concisely, the polynomial chaos expansion can be written as

$$\hat{\mathbf{u}}(\theta) = \sum_{k=1}^{P} H_k(\boldsymbol{\xi}(\theta))\mathbf{u}_k \tag{5}$$

  where $H_k(\boldsymbol{\xi}(\theta))$ are the polynomial chaoses.
- The value of the number of terms P depends on the number of basic random variables M and the order of the PC expansion r as

$$P = \sum_{j=0}^{r} \frac{(M+j-1)!}{j!(M-1)!} \tag{6}$$

Polynomial Chaos expansion

We need to solve a $nP \times nP$ linear equation to obtain all $\mathbf{u}_k \in \mathbb{R}^n$.

$$\begin{bmatrix} \mathbf{A}_{0,0} & \cdots & \mathbf{A}_{0,P-1} \\ \mathbf{A}_{1,0} & \cdots & \mathbf{A}_{1,P-1} \\ \vdots & \vdots & \vdots \\ \mathbf{A}_{P-1,0} & \cdots & \mathbf{A}_{P-1,P-1} \end{bmatrix} \begin{Bmatrix} \mathbf{u}_0 \\ \mathbf{u}_1 \\ \vdots \\ \mathbf{u}_{P-1} \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_0 \\ \mathbf{f}_1 \\ \vdots \\ \mathbf{f}_{P-1} \end{Bmatrix} \tag{7}$$

P increases exponentially with M:

M	2	3	5	10	20	50	100
2nd order PC	5	9	20	65	230	1325	5150
3rd order PC	9	19	55	285	1770	23425	176850

Polynomial Chaos expansion: Some Observations

- The basis is a function of the pdf of the random variables only. For example, Hermite polynomials for Gaussian pdf, Legender's polynomials for uniform pdf.
- The physics of the underlying problem (static, dynamic, heat conduction, transients....) cannot be incorporated in the basis.
- For an n-dimensional output vector, the number of terms in the projection can be more than n (depends on the number of random variables).
- The functional form of the response is a pure polynomial in random variables.

Mathematical nature of the solution

- The elements of the solution vector are not simple polynomials, but ratio of polynomials in $\boldsymbol{\xi}(\theta)$.

Remark

If all $\mathbf{A}_i \in \mathbb{R}^{n\times n}$ are matrices of rank n, then the elements of $\mathbf{u}(\theta)$ are the ratio of polynomials of the form

$$\frac{p^{(n-1)}(\xi_1(\theta), \xi_2(\theta), \ldots, \xi_M(\theta))}{p^{(n)}(\xi_1(\theta), \xi_2(\theta), \ldots, \xi_M(\theta))} \tag{8}$$

where $p^{(n)}(\xi_1(\theta), \xi_2(\theta), \ldots, \xi_M(\theta))$ is an n-th order complete multivariate polynomial of variables $\xi_1(\theta), \xi_2(\theta), \ldots, \xi_M(\theta)$.

Mathematical nature of the solution

Suppose we denote

$$\mathbf{A}(\theta) = \left[\mathbf{A}_0 + \sum_{i=1}^{M} \xi_i(\theta)\mathbf{A}_i\right] \in \mathbb{R}^{n\times n} \tag{9}$$

so that

$$\mathbf{u}(\theta) = \mathbf{A}^{-1}(\theta)\mathbf{f} \tag{10}$$

From the definition of the matrix inverse we have

$$\mathbf{A}^{-1} = \frac{\mathrm{Adj}(\mathbf{A})}{\det(\mathbf{A})} = \frac{\mathbf{C}_a^T}{\det(\mathbf{A})} \tag{11}$$

where $\mathbf{C}_a$ is the matrix of cofactors. The determinant of $\mathbf{A}$ contains a maximum of n number of products of A_{kj} and their linear combinations. Note from Eq. (9) that

$$A_{kj}(\theta) = A_{0_{kj}} + \sum_{i=1}^{M} \xi_i(\theta)\mathbf{A}_{i_{kj}} \tag{12}$$

Mathematical nature of the solution

- Since all the matrices are of full rank, the determinant contains a maximum of n number of products of linear combination of random variables in Eq. (12). On the other hand, each entries of the matrix of cofactors, contains a maximum of $(n-1)$ number of products of linear combination of random variables in Eq. (12). From Eqs. (10) and (11) it follows that

$$\mathbf{u}(\theta) = \frac{\mathbf{C}_a^T \mathbf{f}}{\det(\mathbf{A})} \tag{13}$$

  Therefore, the numerator of each element of the solution vector contains linear combinations of the elements of the cofactor matrix, which are complete polynomials of order $(n-1)$.
- The result derived in this theorem is important because the solution methods proposed for stochastic finite element analysis essentially aim to approximate the ratio of the polynomials given in Eq. (8).

Some basics of linear algebra

Definition

(Linearly independent vectors) A set of vectors $\{\phi_1, \phi_2, \ldots, \phi_n\}$ *is linearly independent if the expression* $\sum_{k=1}^{n} \alpha_k \phi_k = \mathbf{0}$ *if and only if* $\alpha_k = 0$ *for all* $k = 1, 2, \ldots, n$.

Remark

(The spanning property) Suppose $\{\phi_1, \phi_2, \ldots, \phi_n\}$ *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*
$\mathbf{u} = \alpha_1\phi_1 + \alpha_2\phi_2 + \ldots \alpha_n\phi_n$.

Polynomial Chaos expansion

- We can 'split' the Polynomial Chaos type of expansions as

$$\hat{\mathbf{u}}(\theta) = \sum_{k=1}^{n} H_k(\boldsymbol{\xi}(\theta))\mathbf{u}_k + \sum_{k=n+1}^{P} H_k(\boldsymbol{\xi}(\theta))\mathbf{u}_k \tag{14}$$

- According to the spanning property of a complete basis in $\mathbb{R}^n$ it is *always* possible to project $\hat{\mathbf{u}}(\theta)$ in a finite dimensional vector basis for any $\theta \in \Theta$. Therefore, in a vector polynomial chaos expansion (14), all $\mathbf{u}_k$ for $k > n$ must be linearly dependent.
- This is the motivation behind seeking a finite dimensional expansion.

Projection in a finite dimensional vector-space

Theorem

There exist a finite set of functions $\Gamma_k : (\mathbb{R}^m \times \Theta) \rightarrow (\mathbb{R} \times \Theta)$ *and an orthonormal basis* $\phi_k \in \mathbb{R}^n$ *for* $k = 1, 2, \ldots, n$ *such that the series*

$$\hat{\mathbf{u}}(\theta) = \sum_{k=1}^{n} \Gamma_k(\boldsymbol{\xi}(\theta))\phi_k \tag{15}$$

converges to the exact solution of the discretized stochastic finite element equation (4) with probability 1.

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

$$\mathbf{A}_0\phi_k = \lambda_{0_k}\phi_k; \quad k = 1, 2, \ldots n \tag{16}$$

Projection in a finite dimensional vector-space

We define the matrix of eigenvalues and eigenvectors

$$\mathbf{\Lambda}_0 = \mathrm{diag}\left[\lambda_{0_1}, \lambda_{0_2}, \ldots, \lambda_{0_n}\right] \in \mathbb{R}^{n\times n}; \mathbf{\Phi} = [\phi_1, \phi_2, \ldots, \phi_n] \in \mathbb{R}^{n\times n} \quad (17)$$

Eigenvalues are ordered in the ascending order: $\lambda_{0_1} < \lambda_{0_2} < \ldots < \lambda_{0_n}$.
Since $\mathbf{\Phi}$ is an orthogonal matrix we have $\mathbf{\Phi}^{-1} = \mathbf{\Phi}^T$ so that:

$$\mathbf{\Phi}^T \mathbf{A}_0 \mathbf{\Phi} = \mathbf{\Lambda}_0; \quad \mathbf{A}_0 = \mathbf{\Phi}^{-T} \mathbf{\Lambda}_0 \mathbf{\Phi}^{-1} \quad \text{and} \quad \mathbf{A}_0^{-1} = \mathbf{\Phi} \mathbf{\Lambda}_0^{-1} \mathbf{\Phi}^T \quad (18)$$

We also introduce the transformations

$$\widetilde{\mathbf{A}}_i = \mathbf{\Phi}^T \mathbf{A}_i \mathbf{\Phi} \in \mathbb{R}^{n\times n}; i = 0, 1, 2, \ldots, M \quad (19)$$

Note that $\widetilde{\mathbf{A}}_0 = \mathbf{\Lambda}_0$, a diagonal matrix and

$$\mathbf{A}_i = \mathbf{\Phi}^{-T} \widetilde{\mathbf{A}}_i \mathbf{\Phi}^{-1} \in \mathbb{R}^{n\times n}; i = 1, 2, \ldots, M \quad (20)$$

Projection in a finite dimensional vector-space

Suppose the solution of Eq. (4) is given by

$$\hat{\mathbf{u}}(\theta) = \left[\mathbf{A}_0 + \sum_{i=1}^{M} \xi_i(\theta)\mathbf{A}_i\right]^{-1} \mathbf{f} \tag{21}$$

Using Eqs. (17)–(20) and the orthonormality of $\mathbf{\Phi}$ one has

$$\hat{\mathbf{u}}(\theta) = \left[\mathbf{\Phi}^{-T}\mathbf{\Lambda}_0\mathbf{\Phi}^{-1} + \sum_{i=1}^{M} \xi_i(\theta)\mathbf{\Phi}^{-T}\widetilde{\mathbf{A}}_i\mathbf{\Phi}^{-1}\right]^{-1} \mathbf{f} = \mathbf{\Phi}\mathbf{\Psi}\left(\boldsymbol{\xi}(\theta)\right)\mathbf{\Phi}^{T}\mathbf{f} \tag{22}$$

where

$$\mathbf{\Psi}\left(\boldsymbol{\xi}(\theta)\right) = \left[\mathbf{\Lambda}_0 + \sum_{i=1}^{M} \xi_i(\theta)\widetilde{\mathbf{A}}_i\right]^{-1} \tag{23}$$

and the M-dimensional random vector

$$\boldsymbol{\xi}(\theta) = \{\xi_1(\theta), \xi_2(\theta), \ldots, \xi_M(\theta)\}^T \tag{24}$$

Projection in a finite dimensional vector-space

Now we separate the diagonal and off-diagonal terms of the $\widetilde{\mathbf{A}}_i$ matrices as

$$\widetilde{\mathbf{A}}_i = \mathbf{\Lambda}_i + \mathbf{\Delta}_i, \quad i = 1, 2, \ldots, M \tag{25}$$

Here the diagonal matrix

$$\mathbf{\Lambda}_i = \operatorname{diag}\left[\widetilde{\mathbf{A}}\right] = \operatorname{diag}\left[\lambda_{i_1}, \lambda_{i_2}, \ldots, \lambda_{i_n}\right] \in \mathbb{R}^{n \times n} \tag{26}$$

and $\mathbf{\Delta}_i = \widetilde{\mathbf{A}}_i - \mathbf{\Lambda}_i$ is an off-diagonal only matrix.

$$\mathbf{\Psi}\left(\boldsymbol{\xi}(\theta)\right) = \left[\underbrace{\mathbf{\Lambda}_0 + \sum_{i=1}^{M} \xi_i(\theta)\mathbf{\Lambda}_i}_{\mathbf{\Lambda}\left(\boldsymbol{\xi}(\theta)\right)} + \underbrace{\sum_{i=1}^{M} \xi_i(\theta)\mathbf{\Delta}_i}_{\mathbf{\Delta}\left(\boldsymbol{\xi}(\theta)\right)}\right]^{-1} \tag{27}$$

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

Projection in a finite dimensional vector-space

We rewrite Eq. (27) as

$$\boldsymbol{\Psi}\left(\boldsymbol{\xi}(\theta)\right) = \left[\boldsymbol{\Lambda}\left(\boldsymbol{\xi}(\theta)\right)\left[\mathbf{I}_n + \boldsymbol{\Lambda}^{-1}\left(\boldsymbol{\xi}(\theta)\right)\boldsymbol{\Delta}\left(\boldsymbol{\xi}(\theta)\right)\right]\right]^{-1} \tag{28}$$

The above expression can be represented using a Neumann type of matrix series as

$$\boldsymbol{\Psi}\left(\boldsymbol{\xi}(\theta)\right) = \sum_{s=0}^{\infty}(-1)^s\left[\boldsymbol{\Lambda}^{-1}\left(\boldsymbol{\xi}(\theta)\right)\boldsymbol{\Delta}\left(\boldsymbol{\xi}(\theta)\right)\right]^s\boldsymbol{\Lambda}^{-1}\left(\boldsymbol{\xi}(\theta)\right) \tag{29}$$

Polynomial Chaos expansion

Taking an arbitrary r-th element of $\hat{\mathbf{u}}(\theta)$, Eq. (22) can be rearranged to have

$$\hat{u}_r(\theta) = \sum_{k=1}^{n} \Phi_{rk} \left(\sum_{j=1}^{n} \Psi_{kj} \left(\boldsymbol{\xi}(\theta) \right) \left(\phi_j^T \mathbf{f} \right) \right) \tag{30}$$

Defining

$$\Gamma_k \left(\boldsymbol{\xi}(\theta) \right) = \sum_{j=1}^{n} \Psi_{kj} \left(\boldsymbol{\xi}(\theta) \right) \left(\phi_j^T \mathbf{f} \right) \tag{31}$$

and collecting all the elements in Eq. (30) for $r = 1, 2, \ldots, n$ one has

$$\hat{\mathbf{u}}(\theta) = \sum_{k=1}^{n} \Gamma_k \left(\boldsymbol{\xi}(\theta) \right) \phi_k \tag{32}$$

Spectral functions

Definition

The functions $\Gamma_k\left(\boldsymbol{\xi}(\theta)\right), k = 1, 2, \ldots n$ *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 $\Gamma_k\left(\boldsymbol{\xi}(\theta)\right)$ contain infinite number of terms and they are highly nonlinear functions of the random variables $\xi_i(\theta)$.
- 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 $\Gamma_k\left(\boldsymbol{\xi}(\theta)\right)$

First-order spectral functions

Definition

The first-order spectral functions $\Gamma_k^{(1)}(\boldsymbol{\xi}(\theta)), k = 1, 2, \ldots, n$ are obtained by retaining one term in the series (29).

Retaining one term in (29) we have

$$\boldsymbol{\Psi}^{(1)}\left(\boldsymbol{\xi}(\theta)\right) = \boldsymbol{\Lambda}^{-1}\left(\boldsymbol{\xi}(\theta)\right) \quad \text{or} \quad \Psi_{kj}^{(1)}\left(\boldsymbol{\xi}(\theta)\right) = \frac{\delta_{kj}}{\lambda_{0_k} + \sum_{i=1}^{M} \xi_i(\theta)\lambda_{i_k}} \tag{33}$$

Using the definition of the spectral function in Eq. (31), the first-order spectral functions can be explicitly obtained as

$$\Gamma_k^{(1)}\left(\boldsymbol{\xi}(\theta)\right) = \sum_{j=1}^{n} \Psi_{kj}^{(1)}\left(\boldsymbol{\xi}(\theta)\right)\left(\phi_j^T \mathbf{f}\right) = \frac{\phi_k^T \mathbf{f}}{\lambda_{0_k} + \sum_{i=1}^{M} \xi_i(\theta)\lambda_{i_k}} \tag{34}$$

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

Second-order spectral functions

Definition

The second-order spectral functions $\Gamma_k^{(2)}(\boldsymbol{\xi}(\theta)), k = 1, 2, \ldots, n$ *are obtained by retaining two terms in the series (29).*

Retaining two terms in (29) we have

$$\boldsymbol{\Psi}^{(2)}\left(\boldsymbol{\xi}(\theta)\right) = \boldsymbol{\Lambda}^{-1}\left(\boldsymbol{\xi}(\theta)\right) - \boldsymbol{\Lambda}^{-1}\left(\boldsymbol{\xi}(\theta)\right)\boldsymbol{\Delta}\left(\boldsymbol{\xi}(\theta)\right)\boldsymbol{\Lambda}^{-1}\left(\boldsymbol{\xi}(\theta)\right) \tag{35}$$

Using the definition of the spectral function in Eq. (31), the second-order spectral functions can be obtained in closed-form as

$$\Gamma_k^{(2)}\left(\boldsymbol{\xi}(\theta)\right) = \frac{\phi_k^T \mathbf{f}}{\lambda_{0_k} + \sum_{i=1}^{M} \xi_i(\theta)\lambda_{i_k}} - \sum_{j=1}^{n} \frac{\left(\phi_j^T \mathbf{f}\right) \sum_{i=1}^{M} \xi_i(\theta)\Delta_{i_{kj}}}{\left(\lambda_{0_k} + \sum_{i=1}^{M} \xi_i(\theta)\lambda_{i_k}\right)\left(\lambda_{0_j} + \sum_{i=1}^{M} \xi_i(\theta)\lambda_{i_j}\right)} \tag{36}$$

Analysis of spectral functions

Remark

The linear combination of the spectral functions has the same functional form in $(\xi_1(\theta), \xi_2(\theta), \ldots, \xi_M(\theta))$ *as the elements of the solution vector, that is,*

$$\hat{u}_r(\theta) \equiv \frac{p_r^{(n-1)}(\xi_1(\theta), \xi_2(\theta), \ldots, \xi_M(\theta))}{p_r^{(n)}(\xi_1(\theta), \xi_2(\theta), \ldots, \xi_M(\theta))}, \quad \forall r = 1, 2, \ldots, n \tag{37}$$

When first-order spectral functions (34) are considered, we have

$$\hat{u}_r^{(1)}(\theta) = \sum_{k=1}^{n} \Gamma_k^{(1)}(\boldsymbol{\xi}(\theta))\, \phi_{rk} = \sum_{k=1}^{n} \frac{\phi_k^T \mathbf{f}}{\lambda_{0_k} + \sum_{i=1}^{M} \xi_i(\theta) \lambda_{i_k}} \phi_{rk} \tag{38}$$

All $(\lambda_{0_k} + \sum_{i=1}^{M} \xi_i(\theta)\lambda_{i_k})$ are different for different k because it is assumed that all eigenvalues λ_{0_k} are distinct.

Analysis of spectral functions

Carrying out the above summation one has n number of products of $(\lambda_{0_k} + \sum_{i=1}^{M} \xi_i(\theta)\lambda_{i_k})$ in the denominator and n sums of $(n-1)$ number of products of $(\lambda_{0_k} + \sum_{i=1}^{M} \xi_i(\theta)\lambda_{i_k})$ in the numerator, that is,

$$\hat{u}_r^{(1)}(\theta) = \frac{\sum_{k=1}^{n} (\phi_k^T \mathbf{f}) \phi_{rk} \prod_{j=1 \neq k}^{n-1} \left(\lambda_{0_j} + \sum_{i=1}^{M} \xi_i(\theta)\lambda_{i_j}\right)}{\prod_{k=1}^{n-1} \left(\lambda_{0_j} + \sum_{i=1}^{M} \xi_i(\theta)\lambda_{i_j}\right)} \tag{39}$$

Summary of the basis functions (spectral functions)

The basis functions are:

1. not polynomials in $\xi_j(\theta)$ but ratio of polynomials.
2. independent of the nature of the random variables (i.e. applicable to Gaussian, non-Gaussian or even mixed random variables).
3. not general but specific to a problem as it utilizes the eigenvalues and eigenvectors of the systems matrices.
4. such that truncation error depends on the off-diagonal terms of the matrix $\mathbf{\Delta}(\boldsymbol{\xi}(\theta))$.

Next we use these spectral functions as trial functions within a Galerkin error minimization scheme.

The Galerkin approach

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

$$\hat{\mathbf{u}}(\theta) = \sum_{k=1}^{n} c_k \widehat{\Gamma}_k(\boldsymbol{\xi}(\theta))\phi_k \tag{40}$$

converges to the exact solution of the discretized stochastic finite element equation (4) 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*

$$S_{jk} = \sum_{i=0}^{M} \widetilde{A}_{i_{jk}} D_{ijk}; \quad \forall\, j, k = 1, 2, \ldots, n; \widetilde{A}_{i_{jk}} = \phi_j^T \mathbf{A}_i \phi_k, \tag{41}$$

$$D_{ijk} = \mathrm{E}\left[\xi_i(\theta)\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\widehat{\Gamma}_k(\boldsymbol{\xi}(\theta))\right] \quad \text{and} \quad b_j = \mathrm{E}\left[\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\right]\left(\phi_j^T \mathbf{f}\right). \tag{42}$$

The Galerkin approach

- The error vector can be obtained as

$$\varepsilon(\theta) = \left(\sum_{i=0}^{M} \mathbf{A}_i \xi_i(\theta)\right)\left(\sum_{k=1}^{n} c_k \widehat{\Gamma}_k(\boldsymbol{\xi}(\theta))\boldsymbol{\phi}_k\right) - \mathbf{f} \in \mathbb{R}^n \tag{43}$$

  The solution is viewed as a projection where $\left\{\widehat{\Gamma}_k(\boldsymbol{\xi}(\theta))\boldsymbol{\phi}_k\right\} \in \mathbb{R}^n$ are the basis functions and c_k are the unknown constants to be determined.

- The coefficients c_k are evaluated using the Galerkin approach so that the error is made orthogonal to the basis functions, that is, mathematically

$$\varepsilon(\theta) \perp \left(\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\boldsymbol{\phi}_j\right) \quad \text{or} \quad \left\langle \widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\boldsymbol{\phi}_j, \varepsilon(\theta)\right\rangle = 0 \,\forall j = 1, 2, \ldots, n \tag{44}$$

The Galerkin approach

- Imposing the orthogonality condition and using the expression of the error one has

$$\mathrm{E}\left[\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\phi_j^T\left(\sum_{i=0}^{M}\mathbf{A}_i\xi_i(\theta)\right)\left(\sum_{k=1}^{n}c_k\widehat{\Gamma}_k(\boldsymbol{\xi}(\theta))\phi_k\right)-\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\phi_j^T\mathbf{f}\right]=0 \tag{45}$$

- Interchanging the $\mathrm{E}[\bullet]$ and summation operations, this can be simplified to

$$\sum_{k=1}^{n}\left(\sum_{i=0}^{M}\left(\phi_j^T\mathbf{A}_i\phi_k\right)\mathrm{E}\left[\xi_i(\theta)\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\widehat{\Gamma}_k(\boldsymbol{\xi}(\theta))\right]\right)c_k=$$

$$\mathrm{E}\left[\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\right]\left(\phi_j^T\mathbf{f}\right) \tag{46}$$

$$\text{or}\quad\sum_{k=1}^{n}\left(\sum_{i=0}^{M}\widetilde{A}_{i_{jk}}D_{ijk}\right)c_k=b_j \tag{47}$$

Model Reduction by reduced number of basis

- Suppose the eigenvalues of $\mathbf{A}_0$ are arranged in an increasing order such that

$$\lambda_{0_1} < \lambda_{0_2} < \ldots < \lambda_{0_n} \tag{48}$$

- From the expression of the spectral functions observe that the eigenvalues appear in the denominator:

$$\Gamma_k^{(1)}\left(\boldsymbol{\xi}(\omega)\right) = \frac{\phi_k^T \mathbf{f}}{\lambda_{0_k} + \sum_{i=1}^{M} \xi_i(\omega)\lambda_{i_k}} \tag{49}$$

- The series can be truncated based on the magnitude of the eigenvalues as the higher terms becomes smaller. Therefore one could only retain the dominant terms in the series (POD like reduction).

Model Reduction by reduced number of basis

- One can select a small value ϵ such that $\lambda_{0_1}/\lambda_{0_p} < \epsilon$ for some value of p. Based on this discussion we have the following proposition.

Proposition

(reduced orthonormal basis) Suppose there exist an ϵ and $p < n$ such that $\lambda_{0_1}/\lambda_{0_p} < \epsilon$. Then the solution of the discretized stochastic finite element equation (4) can be expressed by the series representation

$$\hat{\mathbf{u}}(\omega) = \sum_{k=1}^{p} c_k \widehat{\Gamma}_k(\boldsymbol{\xi}(\omega))\phi_k \tag{50}$$

such that the error is minimized in a least-square sense. c_k, $\widehat{\Gamma}_k(\boldsymbol{\xi}(\omega))$ and ϕ_k can be obtained following the procedure described in the previous section by letting the indices j, k upto p in Eqs. (41) and (42).

Computational method

- The mean vector can be obtained as

$$\overline{\mathbf{u}} = \mathrm{E}\left[\hat{\mathbf{u}}(\theta)\right] = \sum_{k=1}^{p} c_k \mathrm{E}\left[\widehat{\Gamma}_k(\boldsymbol{\xi}(\theta))\right] \boldsymbol{\phi}_k \tag{51}$$

- The covariance of the solution vector can be expressed as

$$\boldsymbol{\Sigma}_u = \mathrm{E}\left[\left(\hat{\mathbf{u}}(\theta) - \overline{\mathbf{u}}\right)\left(\hat{\mathbf{u}}(\theta) - \overline{\mathbf{u}}\right)^T\right] = \sum_{k=1}^{p}\sum_{j=1}^{p} c_k c_j \Sigma_{\Gamma_{kj}} \boldsymbol{\phi}_k \boldsymbol{\phi}_j^T \tag{52}$$

where the elements of the covariance matrix of the spectral functions are given by

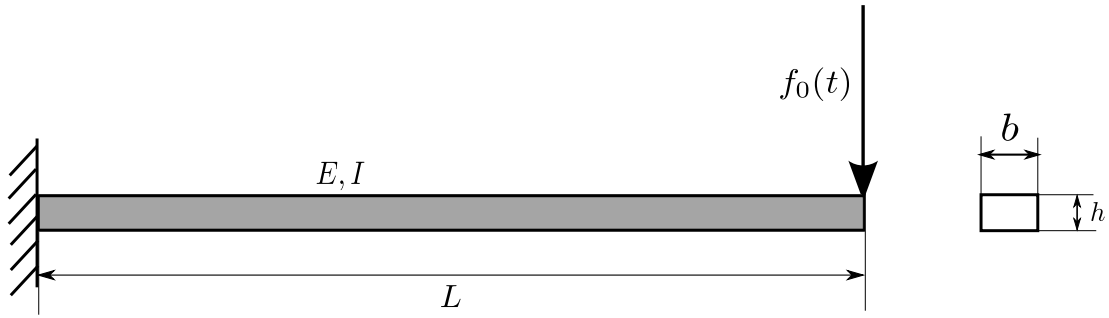
$$\Sigma_{\Gamma_{kj}} = \mathrm{E}\left[\left(\widehat{\Gamma}_k(\boldsymbol{\xi}(\theta)) - \mathrm{E}\left[\widehat{\Gamma}_k(\boldsymbol{\xi}(\theta))\right]\right)\left(\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta)) - \mathrm{E}\left[\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\right]\right)\right] \tag{53}$$

Summary of the computational method

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

The Euler-Bernoulli beam example

- An Euler-Bernoulli cantilever beam with stochastic bending modulus



- Length : 1.0 m, Cross-section : $39 \times 5.93\ mm^2$, Young's Modulus: $2 \times 10^{11}\ Pa$.
- We study the deflection of the beam under the action of a point load on the free end.

Problem details

- We assume that the bending modulus of the cantilever beam is a homogeneous stationary Gaussian random field of the form

$$EI(x,\theta) = EI_0(1 + a(x,\theta)) \tag{54}$$

where x is the coordinate along the length of ZnO NW, EI_0 is the estimate of the mean bending modulus, $a(x,\theta)$ is a zero mean stationary random field.

- The autocorrelation function of this random field is assumed to be

$$C_a(x_1,x_2) = \sigma_a^2 e^{-(|x_1-x_2|)/\mu_a} \tag{55}$$

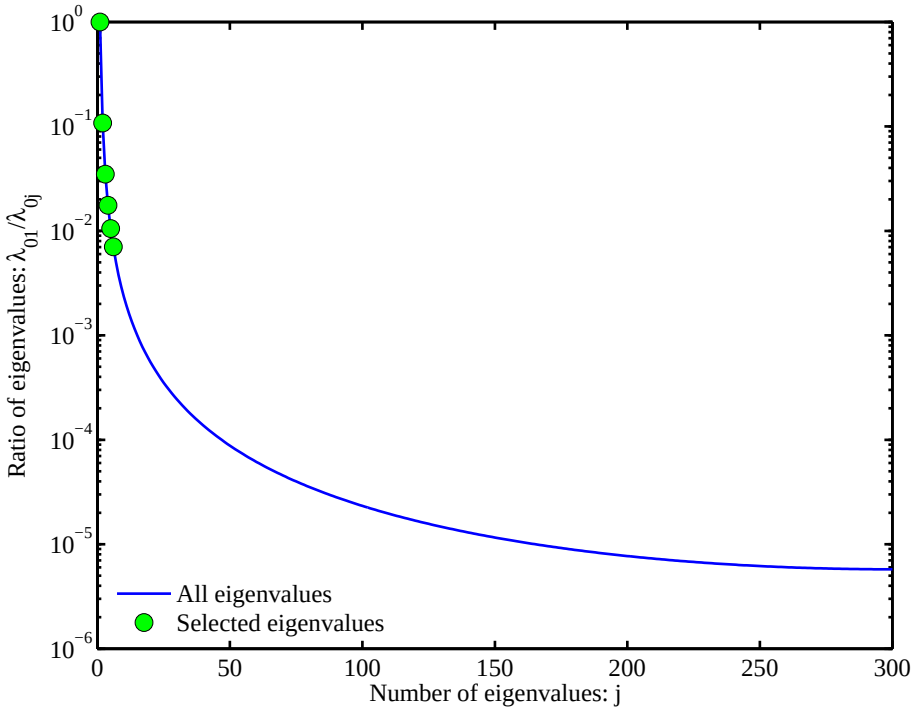
where μ_a is the correlation length and σ_a is the standard deviation.

- Two correlation lengths are considered in the numerical studies: $\mu_a = L/2$ and $\mu_a = L/10$.

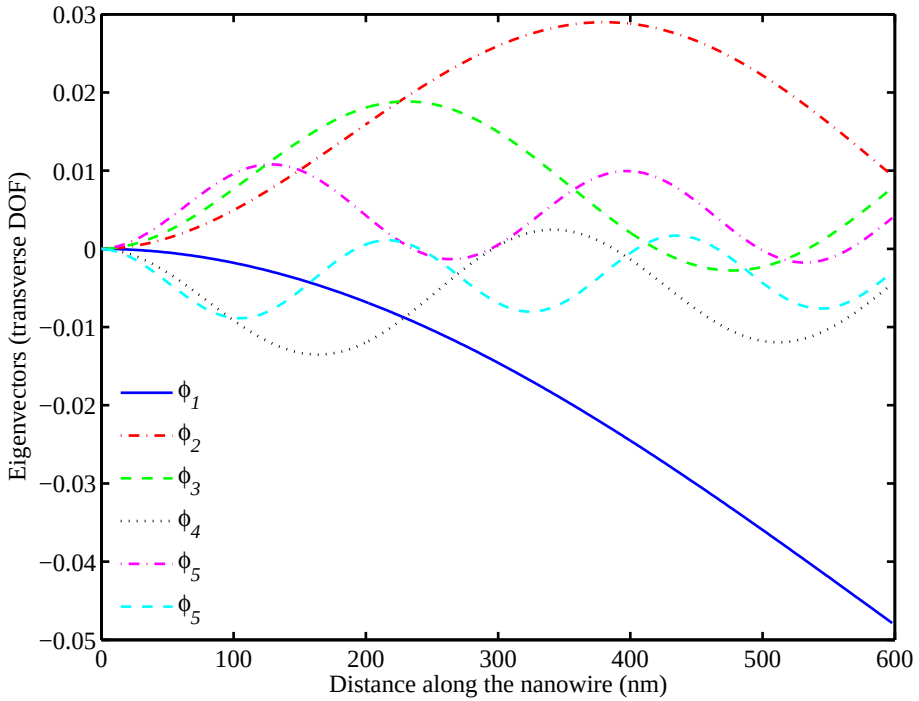
Problem details

- *Case 1:* The random field is Gaussian with $\mu_a = L/2$ with $n = 600$ and $M = 4$. The results are compared with the polynomial chaos expansion.
- *Case 2:* The random field is Uniform with $\mu_a = L/2$ with $n = 2400$ and $M = 29$.
- *Case 3:* The random field is Uniform with $\mu_a = L/2$ with $n = 2400$ and $M = 111$.

Eigensolutions of the beam



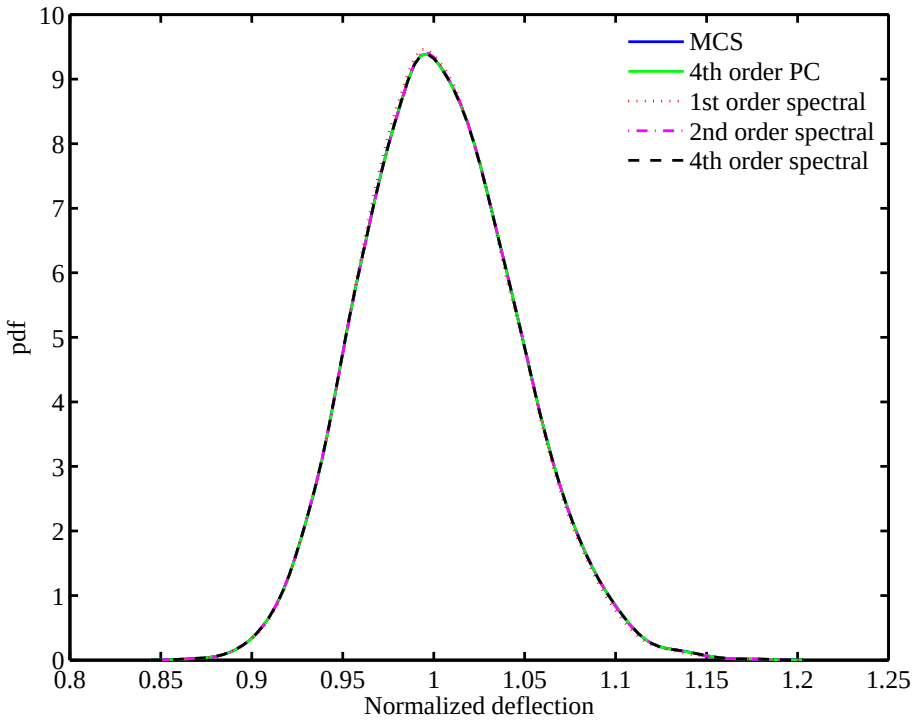
(a) Ratio of eigenvalues of the stiffness matrix $\mathbf{A}_0$.



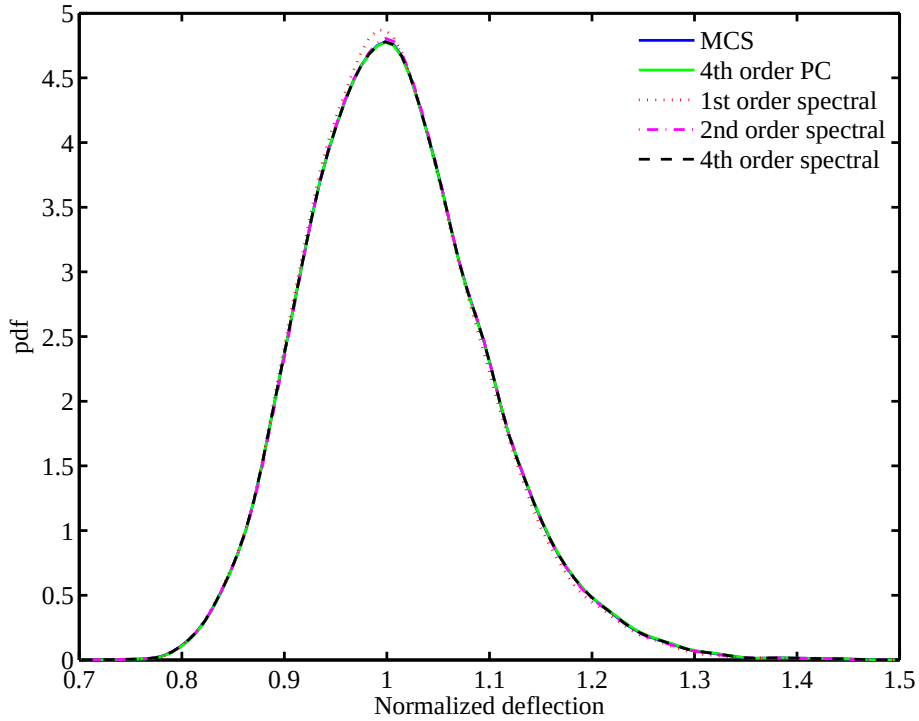
(b) First six eigenvectors of $\mathbf{A}_0$ (transverse DOF).

Figure: The eigenvalues and eigenvectors of the stiffness matrix $\mathbf{A}_0$. For $\epsilon = 0.01$, the number of reduced eigenvectors $p = 6$ such that $\lambda_{0_1}/\lambda_{0_p} < \epsilon$.

Pdf: larger correlation length



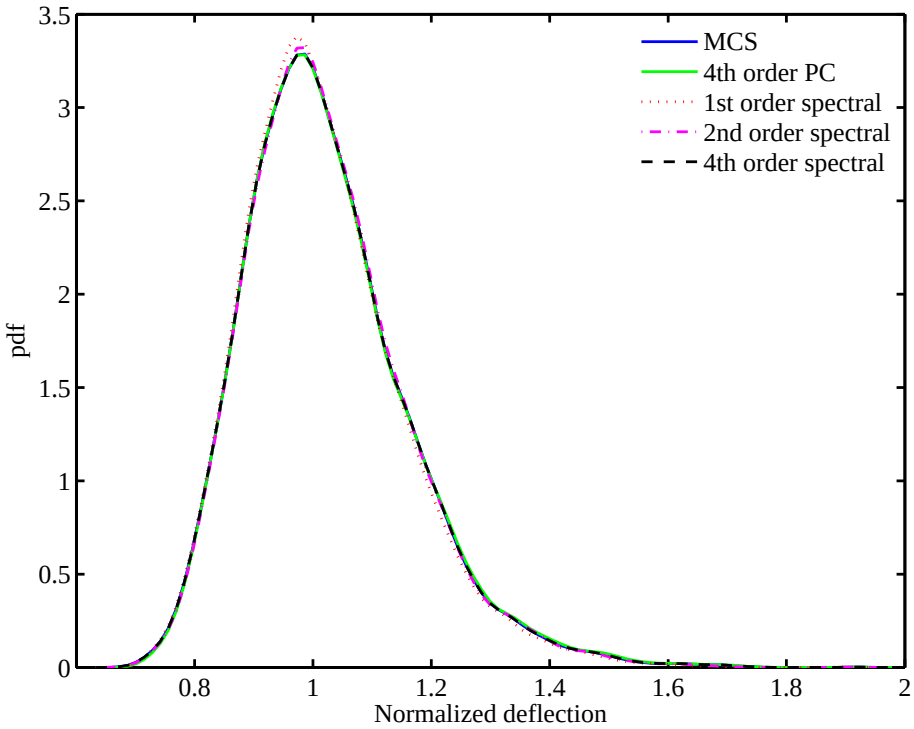
(a) Probability density function for $\sigma_a = 0.05$.



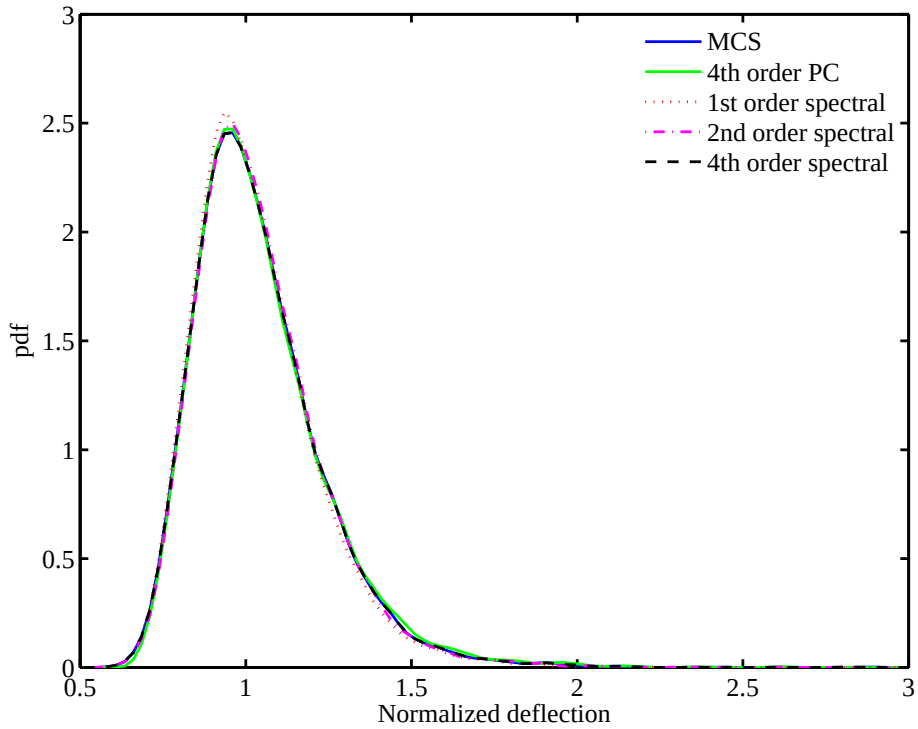
(b) Probability density function for $\sigma_a = 0.1$.

The probability density function of the normalized tip deflection of the cantilever beam under the action of point load on the free end (10,000 sample MCS).

Pdf: larger correlation length



(c) Probability density function for $\sigma_a = 0.15$.



(d) Probability density function for $\sigma_a = 0.2$.

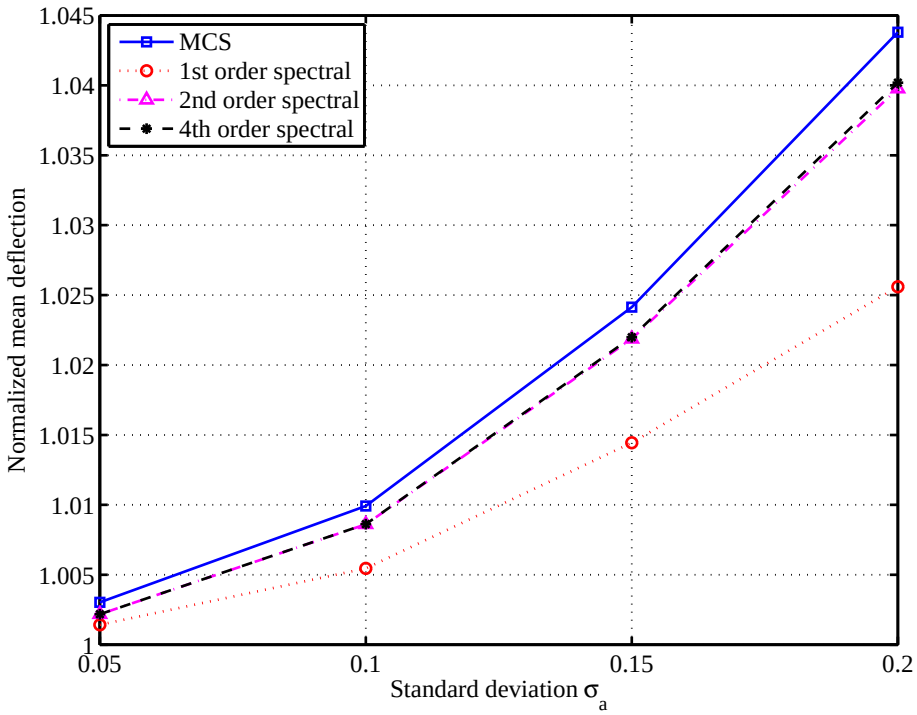
For $n = 600$ and $M = 4$, the fourth-order PC needs solution of a linear system of equation of size 42,000, compared to only 6 with the proposed Galerkin approach. Direct MCS: 43.2131m; PC: 16.8559m; 1st order spectral: 2.8860m; 2nd order spectral: 3.2448m; and 4th order spectral: 3.2604s.

Error in moments: larger correlation length

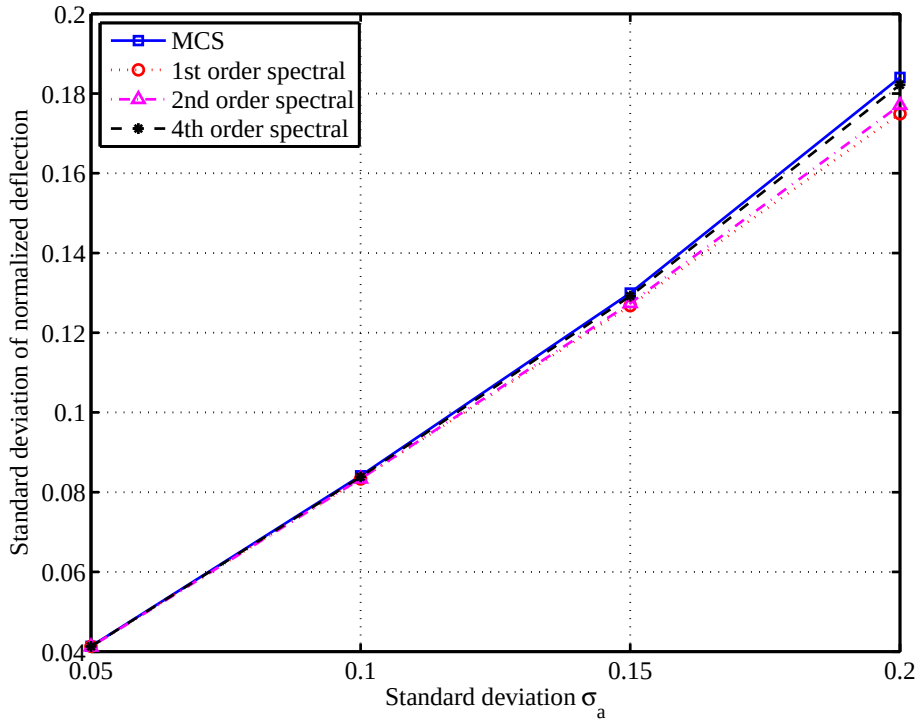
Methods	$\sigma_a = 0.05$	$\sigma_a = 0.10$	$\sigma_a = 0.15$	$\sigma_a = 0.20$
4th order PC	0.0864	0.0267	0.1041	0.1462
1st order spectral	0.0603	0.2289	0.5384	1.0589
2nd order spectral	0.0048	0.0062	0.0140	0.0454
4th order spectral	0.0047	0.0048	0.0053	0.0069
4th order PC	0.7143	0.9065	1.4948	0.1800
1st order spectral	1.1871	1.6784	3.0980	5.1614
2nd order spectral	0.1011	0.5166	1.4668	3.2479
4th order spectral	0.0179	0.0153	0.0004	0.0886

Percentage errors in the mean and standard deviation of the normalized tip deflection with Gaussian random field model. The direct MCS results are used as the reference solution. The fourth-order spectral method turns out to be the most accurate, followed by the fourth-order PC.

Moments: larger correlation length



(e) Mean of the normalized deflection.



(f) Standard deviation of the normalized deflection.

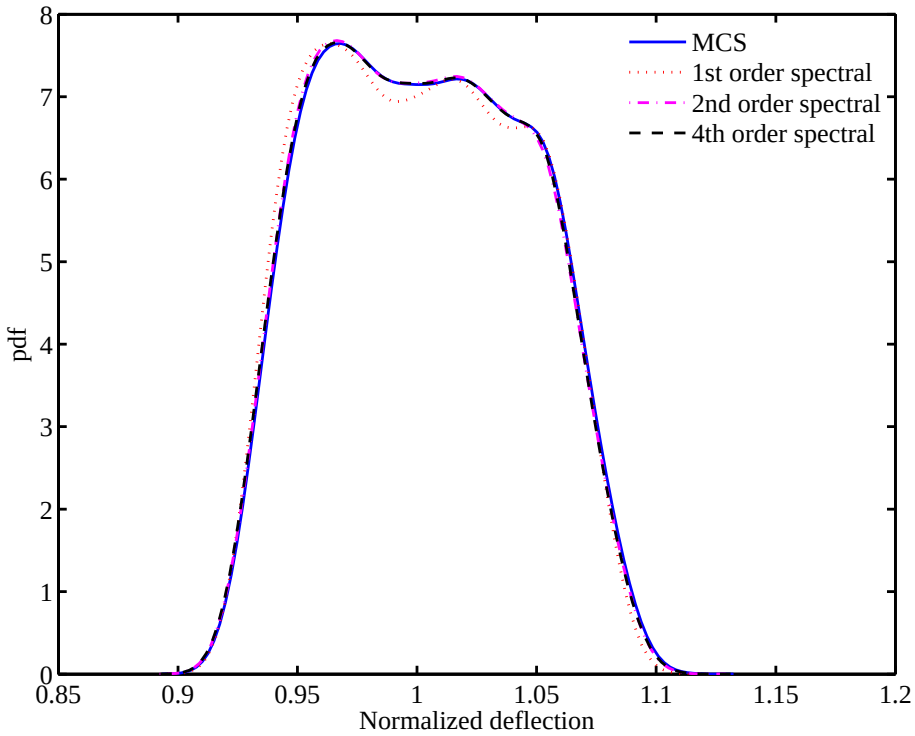
Figure: The number of random variable used: $M = 29$. The number of degrees of freedom: $n = 2400$.

Error in moments: larger correlation length

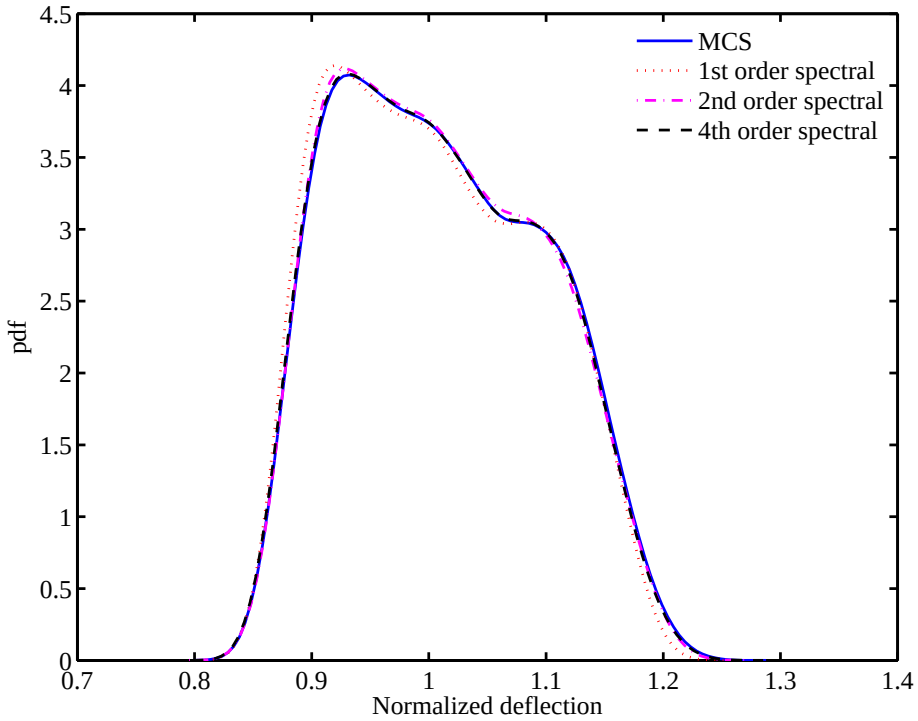
Statistics	Methods	$\sigma_a = 0.05$	$\sigma_a = 0.10$	$\sigma_a = 0.15$	$\sigma_a = 0.20$
Mean	1st order spectral	0.1602	0.4415	0.9475	1.7444
	2nd order spectral	0.0845	0.1303	0.2211	0.3867
	4th order spectral	0.0845	0.1285	0.2105	0.3458
Standard deviation	1st order spectral	0.0350	0.9037	2.4522	4.9665
	2nd order spectral	0.2958	0.8689	1.9842	3.7927
	4th order spectral	0.1642	0.3030	0.5618	1.0063

Percentage errors in the mean and standard deviation of the tip deflection with uniform random field and correlation length $\mu_a = L/2$ ($n = 2400$ and $M = 29$).

Pdf: larger correlation length



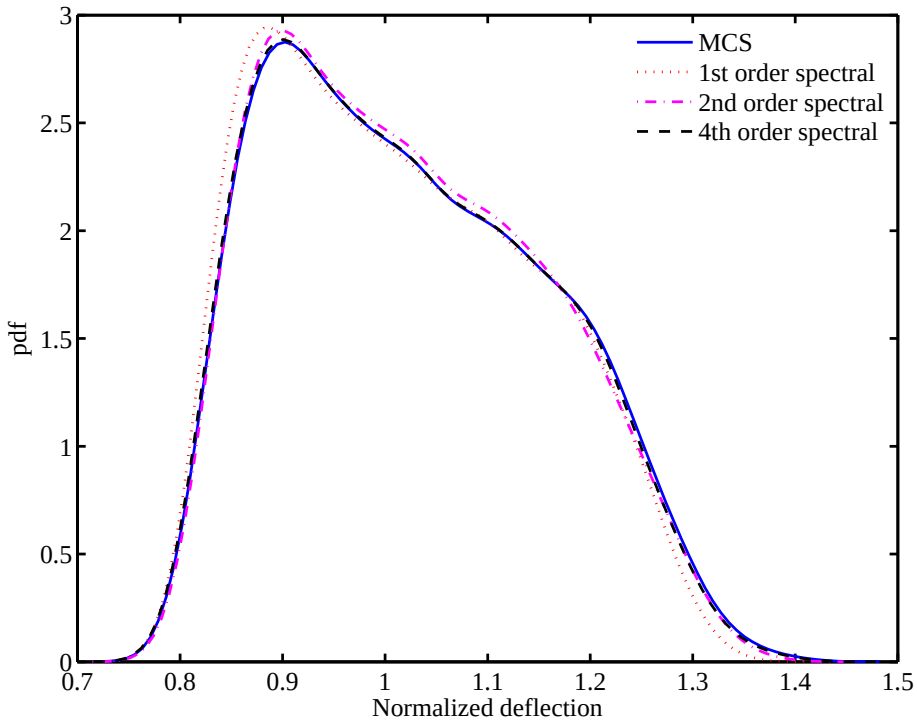
(a) Probability density function for $\sigma_a = 0.05$.



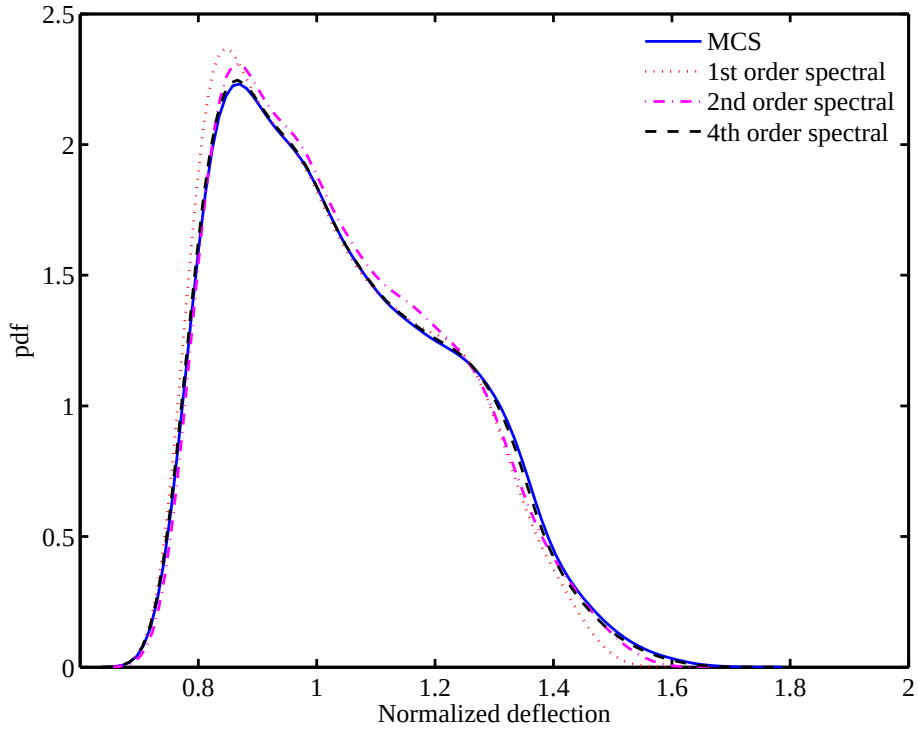
(b) Probability density function for $\sigma_a = 0.1$.

The probability density function of the normalized deflection.

Pdf: larger correlation length



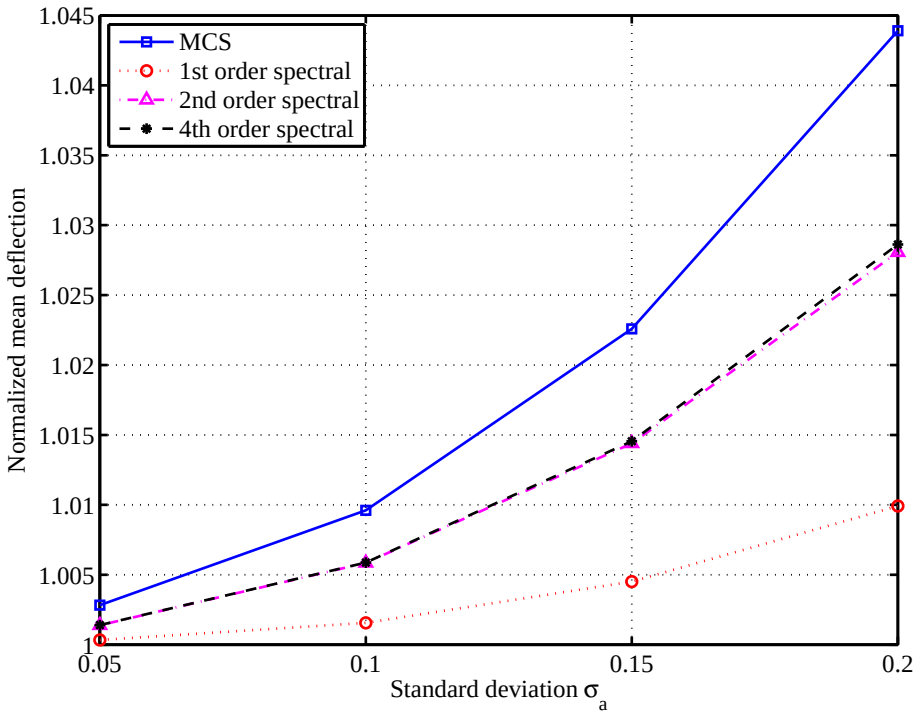
(c) Probability density function for $\sigma_a = 0.15$.



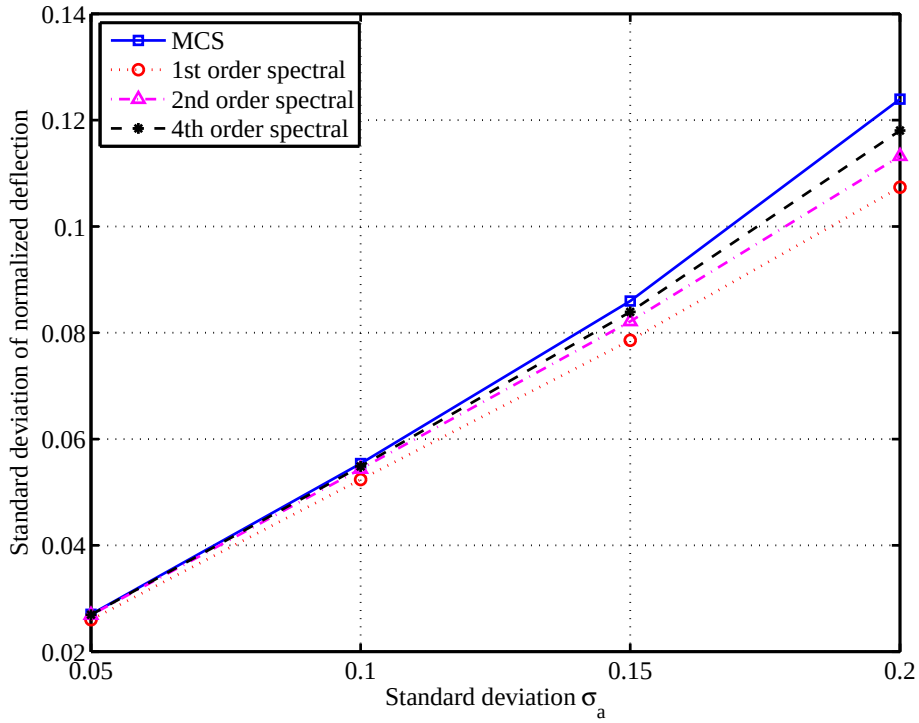
(d) Probability density function for $\sigma_a = 0.2$.

For $n = 2400$ and $M = 29$, the second-order PC needs solution of a linear system of equation of size 72,000. Direct MCS: 19.2590 hours; 1st order spectral: 109.6687 seconds; 2nd order spectral: 112.7731 seconds; and 4th order spectral: 116.6419 seconds

Moments: smaller correlation length



(e) Mean of the normalized deflection.



(f) Standard deviation of the normalized deflection.

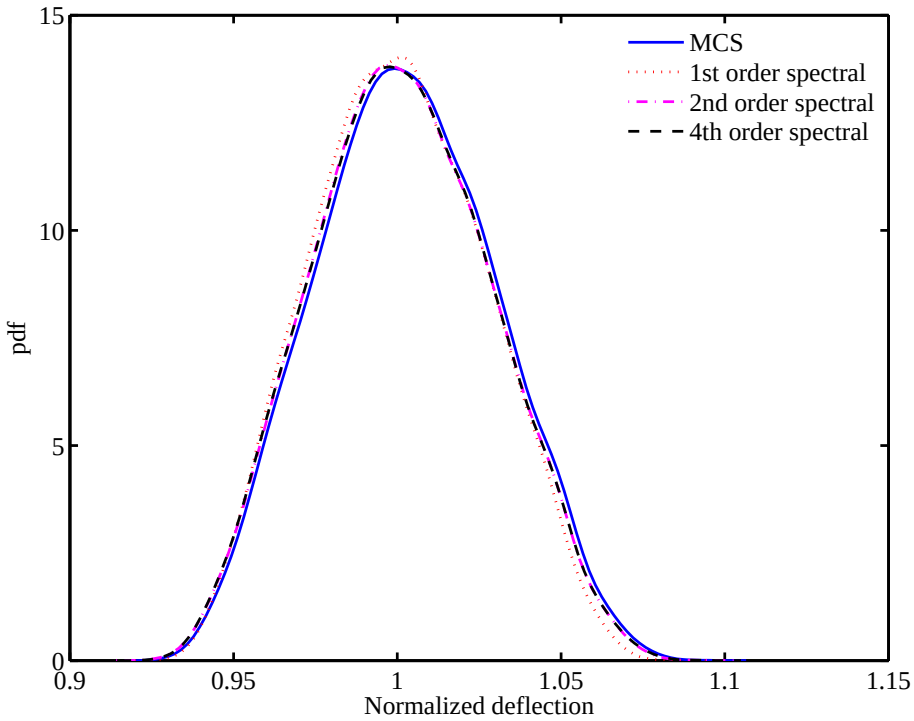
Figure: The number of random variable used: $M = 111$. The number of degrees of freedom: $n = 2400$.

Error in moments: smaller correlation length

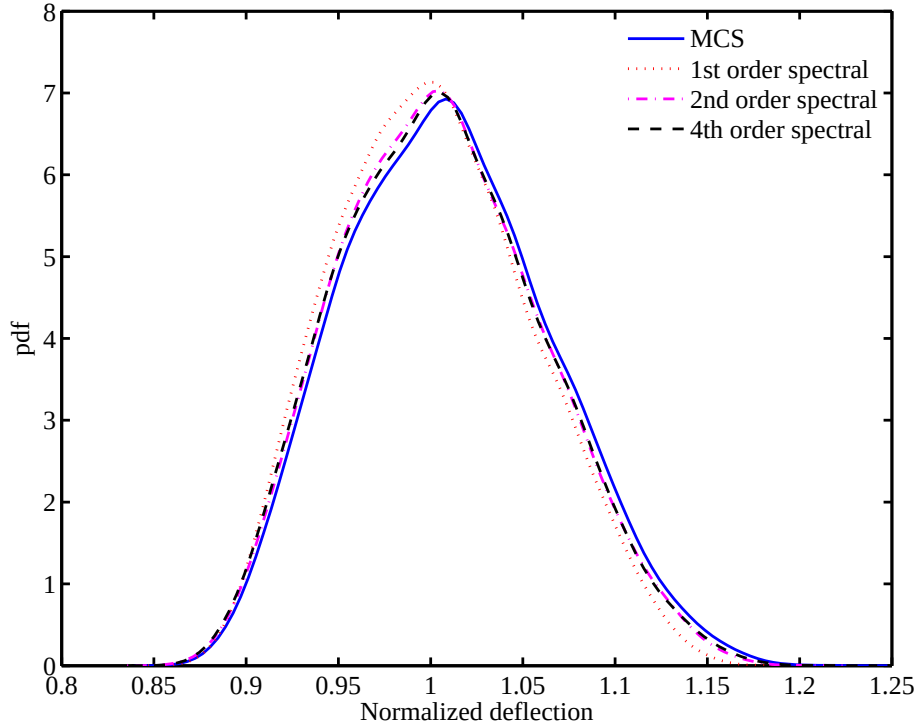
Statistics	Methods	$\sigma_a = 0.05$	$\sigma_a = 0.10$	$\sigma_a = 0.15$	$\sigma_a = 0.20$
Mean	1st order spectral	0.2488	0.7974	1.7671	3.2555
	2nd order spectral	0.1434	0.3725	0.8007	1.5174
	4th order spectral	0.1432	0.3697	0.7854	1.4641
Standard deviation	1st order spectral	3.7039	5.4718	8.5930	13.3714
	2nd order spectral	0.4704	1.8630	4.4737	8.6448
	4th order spectral	0.2561	0.9733	2.3849	4.7576

Percentage errors in the mean and standard deviation of the tip deflection with uniform random field and correlation length $\mu_a = L/10$ ($n = 2400$ and $M = 111$).

Pdf: smaller correlation length



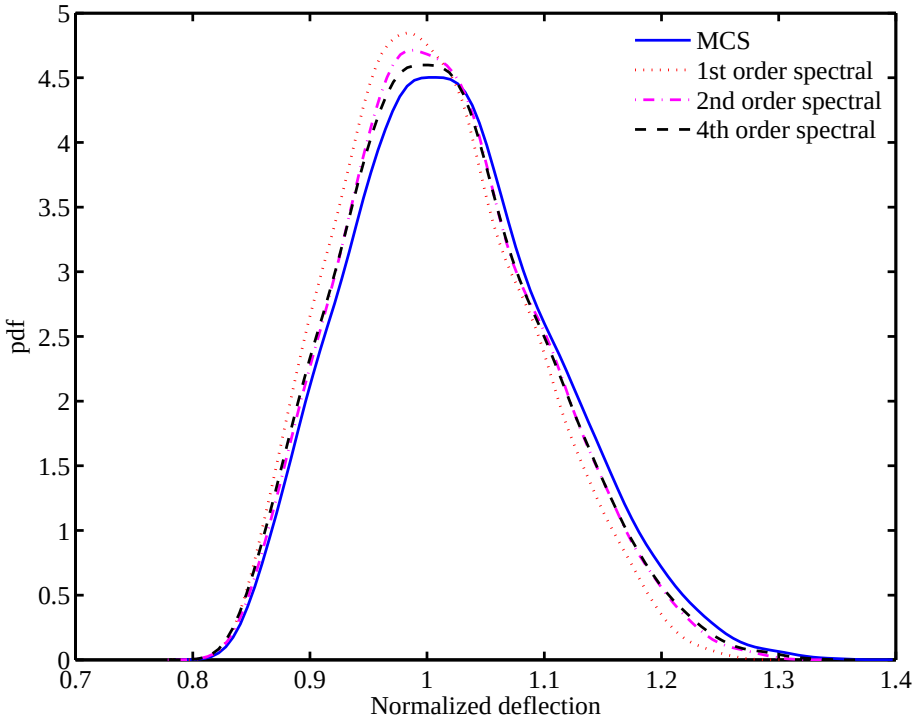
(a) Probability density function for $\sigma_a = 0.05$.



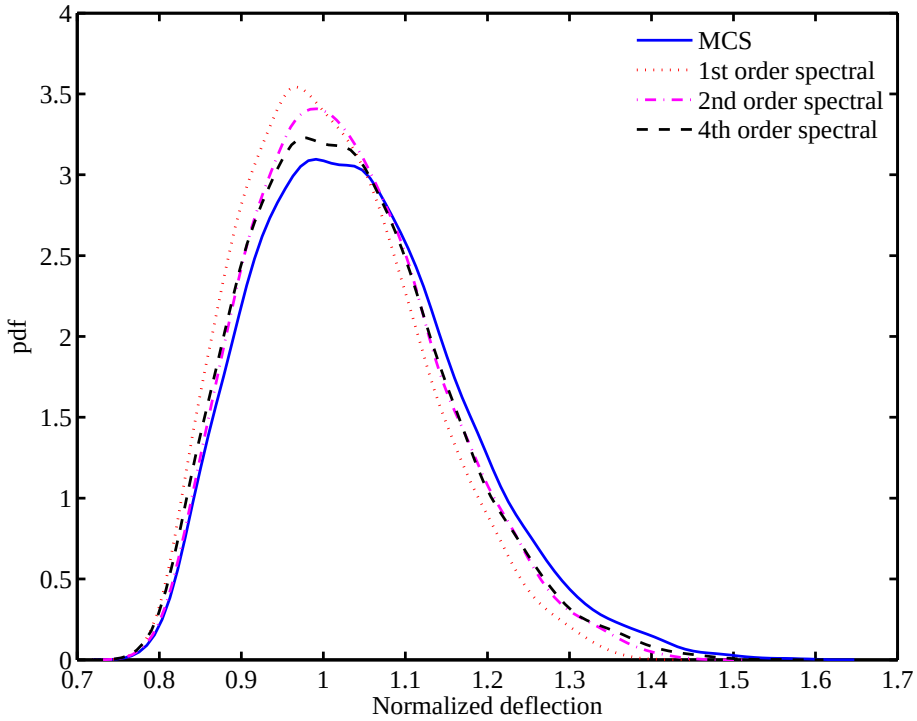
(b) Probability density function for $\sigma_a = 0.1$.

The probability density function of the normalized deflection.

Pdf: smaller correlation length



(c) Probability density function for $\sigma_a = 0.15$.



(d) Probability density function for $\sigma_a = 0.2$.

For $n = 2400$ and $M = 111$, the second-order PC needs solution of a linear system of equation of size 268,800. Direct MCS: 37.1910 hours; 1st order spectral: 137.6085 seconds; 2nd order spectral: 140.9937 seconds; and 4th order spectral: 142.7097 seconds.

Conclusions

1. We consider discretized stochastic partial differential equations.
2. The solution is projected into a finite dimensional complete orthonormal vector basis and the associated coefficient functions are obtained.
3. The coefficient functions, called as the spectral functions, are expressed in terms of the spectral properties of the system matrices.
4. If $p < n$ number of orthonormal vectors are used and M is the number of random variables, then the computational complexity grows in $O(Mp^2) + O(p^3)$ for large M and p in the worse case.
5. We consider a problem with 29 and 111 random variables and $n = 2400$ degrees of freedom. A second-order PC would require the solution of equations of dimension 72,000 and 268,800 respectively. In comparison, the proposed Galerkin approach requires the solution of algebraic equations of dimension $p = 6$ only.

Discussions

- The *only* information used in constructing the polynomial chaos basis is the probability density function of the random variables involved.
- However, more information is available - these include (a) there are matrices $\mathbf{A}_i, i = 0, 1, 2 \ldots M$, (b) they are symmetric and of dimension n, (c) $\mathbf{A}_0$ is positive definite, and (d) there exist a ordering $\|\mathbf{A}_i\| \geq \|\mathbf{A}_{i+1}\|$. The proposed method constructs a customized basis for elliptic problems using these 'additional' information.
- In the PC method these information are used in the Galerkin error minimization step, which is much further down the line. Whereas in the proposed method, the basis functions themselves are created using these information. As a result, the error to be minimized in the Galerkin is much smaller to start with compared to the PC and consequently a very small number of constants are necessary.

Discussions

- The true nature of the solution is *not* polynomials in the random variables but a ratio of two polynomials where the denominator has higher degree than the numerator. The proposed spectral basis functions have this correct mathematical form.
- A vector of dimension n can be uniquely represented as a linear combination of n orthogonal vectors. In the PC approach, whenever $P > n$, the additional $P - n$ coefficient vectors are linearly independent. Therefore they can be simply represented as a constant times the other vectors. But the PC method explicitly determines these *linearly dependent* vectors by solving large number of equations. This huge additional cost has been avoided in the proposed approach by a-priori selecting a orthonormal basis from the system matrices.

Discussions

- The proposed method takes advantage of the difference in the magnitude of the eigenvalues of the $\mathbf{A}_0$. This POD-like model reduction leads to a significantly smaller basis. This type of reduction is difficult to incorporate within the scope of PC as no information regarding the system matrices are used in constructing the orthogonal polynomial basis.