# Elliptic stochastic partial differential equations: An orthonormal vector basis approach 

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Uncertainty Quantification Workshop, Edinburgh, 26 May, 2010

## Outline of the talk

(1) Introduction

- Stochastic elliptic PDEs
(2) Spectral decomposition in a vector space
- Projection in a finite dimensional vector-space
- Properties of the spectral functions

3 Error minimization in the Hilbert space

- The Galerkin approach
- Computational method

4 Numerical illustration

- ZnO nanowires
(5) Conclusions


## Stochastic elliptic PDE

- We consider the stochastic elliptic partial differential equation (PDE)

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

with the associated boundary condition

$$
\begin{equation*}
u(\mathbf{r}, \omega)=0 ; \quad \mathbf{r} \text { on } \partial \mathcal{D} \tag{2}
\end{equation*}
$$

- Here $a: \mathbb{R}^{d} \times \Omega \rightarrow \mathbb{R}$ 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 $a(\mathbf{r}, \omega)$ to be stationary and square integrable. Based on the physical problem the random field $a(\mathbf{r}, \omega)$ can be used to model different physical quantities.


## Discretized Stochastic PDE

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

$$
\begin{equation*}
a(\mathbf{r}, \omega)=a_{0}(\mathbf{r})+\sum_{i=1}^{\infty} \sqrt{\nu_{i}} \xi_{i}(\omega) \varphi_{i}(\mathbf{r}) \tag{3}
\end{equation*}
$$

Here $a_{0}(\mathbf{r})$ is the mean function, $\xi_{i}(\omega)$ are uncorrelated standard Gaussian random variables, $\nu_{i}$ and $\varphi_{i}(\mathbf{r})$ are eigenvalues and eigenfunctions satisfying the integral equation

$$
\int_{\mathcal{D}} C_{a}\left(\mathbf{r}_{1}, \mathbf{r}_{2}\right) \varphi_{j}\left(\mathbf{r}_{1}\right) \mathrm{d} \mathbf{r}_{1}=\nu_{j} \varphi_{j}\left(\mathbf{r}_{2}\right), \quad \forall j=1,2, \cdots
$$

- Truncating the series (3) 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

$$
\begin{equation*}
\left[\mathbf{A}_{0}+\sum_{i=1}^{M} \xi_{i}(\omega) \mathbf{A}_{i}\right] \mathbf{u}(\omega)=\mathbf{f} \tag{4}
\end{equation*}
$$

## Polynomial Chaos expansion

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

$$
\begin{equation*}
\hat{\mathbf{u}}(\omega)=\sum_{k=1}^{P} H_{k}(\boldsymbol{\xi}(\omega)) \mathbf{u}_{k} \tag{5}
\end{equation*}
$$

where $H_{k}(\boldsymbol{\xi}(\omega))$ 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

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

## Some basics of linear algebra

## Definition

(Linearly independent vectors) $A$ set of vectors $\left\{\phi_{1}, \phi_{2}, \ldots, \phi_{n}\right\}$ is linearly independent if the expression $\sum_{k=1}^{n} \alpha_{k} \boldsymbol{\phi}_{k}=\mathbf{0}$ if and only if $\alpha_{k}=0$ for all $k=1,2, \ldots, n$.

## Remark

(The spanning property) Suppose $\left\{\phi_{1}, \phi_{2}, \ldots, \phi_{n}\right\}$ 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

$$
\begin{equation*}
\hat{\mathbf{u}}(\omega)=\sum_{k=1}^{n} H_{k}(\boldsymbol{\xi}(\omega)) \mathbf{u}_{k}+\sum_{k=n+1}^{P} H_{k}(\boldsymbol{\xi}(\omega)) \mathbf{u}_{k} \tag{7}
\end{equation*}
$$

- 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 (7), 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 $\Gamma_{k}:\left(\mathbb{R}^{m} \times \Omega\right) \rightarrow(\mathbb{R} \times \Omega)$ and an orthonormal basis $\phi_{k} \in \mathbb{R}^{n}$ for $k=1,2, \ldots, n$ such that the series

$$
\begin{equation*}
\hat{\mathbf{u}}(\omega)=\sum_{k=1}^{n} \Gamma_{k}(\xi(\omega)) \phi_{k} \tag{8}
\end{equation*}
$$

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

Outline of the 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

$$
\begin{equation*}
\mathbf{A}_{0} \phi_{k}=\lambda_{0_{k}} \phi_{k} ; \quad k=1,2, \ldots n \tag{9}
\end{equation*}
$$

## Projection in a finite dimensional vector-space

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

$$
\begin{equation*}
\hat{\mathbf{u}}(\omega)=\left[\mathbf{A}_{0}+\sum_{i=1}^{M} \xi_{i}(\omega) \mathbf{A}_{i}\right]^{-1} \mathbf{f} \tag{10}
\end{equation*}
$$

Using the eigenvector matrix and the orthonormality of $\boldsymbol{\Phi}$ one has

$$
\begin{equation*}
\hat{\mathbf{u}}(\omega)=\left[\boldsymbol{\Phi}^{-T} \boldsymbol{\Lambda}_{0} \boldsymbol{\Phi}^{-1}+\sum_{i=1}^{M} \xi_{i}(\omega) \boldsymbol{\Phi}^{-T} \widetilde{\mathbf{A}}_{i} \boldsymbol{\Phi}^{-1}\right]^{-1} \mathbf{f}=\boldsymbol{\Phi} \boldsymbol{\Psi}(\boldsymbol{\xi}(\omega)) \boldsymbol{\Phi}^{T} \mathbf{f} \tag{11}
\end{equation*}
$$

where

$$
\begin{equation*}
\boldsymbol{\Psi}(\boldsymbol{\xi}(\omega))=\left[\boldsymbol{\Lambda}_{0}+\sum_{i=1}^{M} \xi_{i}(\omega) \widetilde{\mathbf{A}}_{i}\right]^{-1} \tag{12}
\end{equation*}
$$

and the $M$-dimensional random vector

$$
\begin{equation*}
\boldsymbol{\xi}(\omega)=\left\{\xi_{1}(\omega), \xi_{2}(\omega), \ldots, \xi_{M}(\omega)\right\}^{T} \tag{13}
\end{equation*}
$$

## Projection in a finite dimensional vector-space

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

$$
\begin{equation*}
\widetilde{\mathbf{A}}_{i}=\boldsymbol{\Lambda}_{i}+\boldsymbol{\Delta}_{i}, \quad i=1,2, \ldots, M \tag{14}
\end{equation*}
$$

Here the diagonal matrix

$$
\begin{equation*}
\boldsymbol{\Lambda}_{i}=\operatorname{diag}[\widetilde{\mathbf{A}}]=\operatorname{diag}\left[\lambda_{i_{1}}, \lambda_{i_{2}}, \ldots, \lambda_{i_{n}}\right] \in \mathbb{R}^{n \times n} \tag{15}
\end{equation*}
$$

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

$$
\begin{equation*}
\boldsymbol{\Psi}(\boldsymbol{\xi}(\omega))=[\underbrace{\boldsymbol{\Lambda}_{0}+\sum_{i=1}^{M} \xi_{i}(\omega) \boldsymbol{\Lambda}_{i}}_{\boldsymbol{\Lambda}(\boldsymbol{\xi}(\omega))}+\underbrace{\sum_{i=1}^{M} \xi_{i}(\omega) \boldsymbol{\Delta}_{i}}_{\boldsymbol{\Delta}(\boldsymbol{\xi}(\omega))}]^{-1} \tag{16}
\end{equation*}
$$

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

## Projection in a finite dimensional vector-space

We rewrite Eq. (16) as

$$
\begin{equation*}
\boldsymbol{\Psi}(\boldsymbol{\xi}(\omega))=\left[\boldsymbol{\Lambda}(\boldsymbol{\xi}(\omega))\left[\mathbf{I}_{n}+\boldsymbol{\Lambda}^{-1}(\boldsymbol{\xi}(\omega)) \boldsymbol{\Delta}(\boldsymbol{\xi}(\omega))\right]\right]^{-1} \tag{17}
\end{equation*}
$$

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

$$
\begin{equation*}
\boldsymbol{\Psi}(\boldsymbol{\xi}(\omega))=\sum_{s=0}^{\infty}(-1)^{s}\left[\boldsymbol{\Lambda}^{-1}(\boldsymbol{\xi}(\omega)) \boldsymbol{\Delta}(\boldsymbol{\xi}(\omega))\right]^{s} \boldsymbol{\Lambda}^{-1}(\boldsymbol{\xi}(\omega)) \tag{18}
\end{equation*}
$$

## Polynomial Chaos expansion

Taking an arbitrary $r$-th element of $\hat{\mathbf{u}}(\omega)$, Eq. (11) can be rearranged to have

$$
\begin{equation*}
\hat{u}_{r}(\omega)=\sum_{k=1}^{n} \Phi_{r k}\left(\sum_{j=1}^{n} \Psi_{k j}(\boldsymbol{\xi}(\omega))\left(\phi_{j}^{T} \mathbf{f}\right)\right) \tag{19}
\end{equation*}
$$

Defining

$$
\begin{equation*}
\Gamma_{k}(\boldsymbol{\xi}(\omega))=\sum_{j=1}^{n} \Psi_{k j}(\boldsymbol{\xi}(\omega))\left(\phi_{j}^{T} \mathbf{f}\right) \tag{20}
\end{equation*}
$$

and collecting all the elements in Eq. (19) for $r=1,2, \ldots, n$ one has

$$
\begin{equation*}
\hat{\mathbf{u}}(\omega)=\sum_{k=1}^{n} \Gamma_{k}(\boldsymbol{\xi}(\omega)) \phi_{k} \tag{21}
\end{equation*}
$$

## Spectral functions

## Definition

The functions $\Gamma_{k}(\xi(\omega)), k=1,2, \ldots n$ 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 $\Gamma_{k}(\xi(\omega))$ 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 $\Gamma_{k}(\boldsymbol{\xi}(\omega))$


## First-order spectral functions

## Definition

The first-order spectral functions $\Gamma_{k}^{(1)}(\xi(\omega)), k=1,2, \ldots, n$ are obtained by retaining one term in the series (18).

Retaining one term in (18) we have

$$
\begin{equation*}
\boldsymbol{\Psi}^{(1)}(\boldsymbol{\xi}(\omega))=\boldsymbol{\Lambda}^{-1}(\boldsymbol{\xi}(\omega)) \quad \text { or } \quad \Psi_{k j}^{(1)}(\boldsymbol{\xi}(\omega))=\frac{\delta_{k j}}{\lambda_{0_{k}}+\sum_{i=1}^{M} \xi_{i}(\omega) \lambda_{i_{k}}} \tag{22}
\end{equation*}
$$

Using the definition of the spectral function in Eq. (20), the first-order spectral functions can be explicitly obtained as

$$
\begin{equation*}
\Gamma_{k}^{(1)}(\xi(\omega))=\sum_{j=1}^{n} \Psi_{k j}^{(1)}(\xi(\omega))\left(\phi_{j}^{\top} \mathbf{f}\right)=\frac{\phi_{k}^{\top} \mathbf{f}}{\lambda_{0_{k}}+\sum_{i=1}^{M} \xi_{i}(\omega) \lambda_{i_{k}}} \tag{23}
\end{equation*}
$$

- From this expression it is clear that $\Gamma_{k}^{(1)}(\xi(\omega))$ are non-Gaussian random variables even if $\xi_{i}(\omega)$ are Gaussian random variables.


## Second-order spectral functions

## Definition

The second-order spectral functions $\Gamma_{k}^{(2)}(\xi(\omega)), k=1,2, \ldots, n$ are obtained by retaining two terms in the series (18).

Retaining two terms in (18) we have

$$
\begin{equation*}
\boldsymbol{\psi}^{(2)}(\boldsymbol{\xi}(\omega))=\boldsymbol{\Lambda}^{-1}(\boldsymbol{\xi}(\omega))-\boldsymbol{\Lambda}^{-1}(\boldsymbol{\xi}(\omega)) \boldsymbol{\Delta}(\boldsymbol{\xi}(\omega)) \boldsymbol{\Lambda}^{-1}(\boldsymbol{\xi}(\omega)) \tag{24}
\end{equation*}
$$

Using the definition of the spectral function in Eq. (20), the second-order spectral functions can be obtained in closed-form as

$$
\begin{align*}
\Gamma_{k}^{(2)}(\boldsymbol{\xi}(\omega))= & \frac{\phi_{k}^{T} \mathbf{f}}{\lambda_{0_{k}}+\sum_{i=1}^{M} \xi_{i}(\omega) \lambda_{i_{k}}}- \\
& \sum_{j=1}^{n} \frac{\left(\phi_{j}^{T} \mathbf{f}\right) \sum_{i=1}^{M} \xi_{i}(\omega) \Delta_{i_{k j}}}{\left(\lambda_{0_{k}}+\sum_{i=1}^{M} \xi_{i}(\omega) \lambda_{i_{k}}\right)\left(\lambda_{0_{j}}+\sum_{i=1}^{M} \xi_{i}(\omega) \lambda_{i_{j}}\right)} \tag{25}
\end{align*}
$$

## Relationship with PC

## Theorem

There exist a finite set of functions $\widetilde{\Gamma}_{k}:\left(\mathbb{R}^{m} \times \Omega\right) \rightarrow(\mathbb{R} \times \Omega)$ and an orthonormal basis $\phi_{k} \in \mathbb{R}^{n}$ for $k=1,2, \ldots, n$ such that a vector polynomial chaos expansion can be expressed by

$$
\begin{equation*}
\hat{\mathbf{u}}(\omega)=\sum_{k=1}^{n} \widetilde{\Gamma}_{k}(\boldsymbol{\xi}(\omega)) \phi_{k} \tag{26}
\end{equation*}
$$

## Relationship with PC

Outline of the proof:

$$
\begin{align*}
\mathbf{u}(\omega) & =\mathbf{u}_{i_{0}} h_{0}+\sum_{i_{1}=1}^{\infty} \mathbf{u}_{i_{1}} h_{1}\left(\xi_{i_{1}}(\omega)\right) \\
& +\sum_{i_{1}=1}^{\infty} \sum_{i_{2}=1}^{i_{1}} \mathbf{u}_{i_{1}, i_{2}} h_{2}\left(\xi_{i_{1}}(\omega), \xi_{i_{2}}(\omega)\right)+\sum_{i_{1}=1}^{\infty} \sum_{i_{2}=1}^{i_{1}} \sum_{i_{3}=1}^{i_{2}} \mathbf{u}_{i_{1} i_{2} i_{3}} h_{3}\left(\xi_{i_{1}}(\omega), \xi_{i_{2}}(\omega), \xi_{i}\right. \\
& +\sum_{i_{1}=1}^{\infty} \sum_{i_{2}=1}^{i_{1}} \sum_{i_{3}=1}^{i_{2}} \sum_{i_{4}=1}^{i_{3}} \mathbf{u}_{i_{1} i_{2} i_{3} i_{4}} h_{4}\left(\xi_{i_{1}}(\omega), \xi_{i_{2}}(\omega), \xi_{i_{3}}(\omega), \xi_{i_{4}}(\omega)\right)+\ldots, \tag{27}
\end{align*}
$$

where $\mathbf{u}_{i_{1}, \ldots, i_{p}} \in \mathbb{R}^{n}$ are deterministic vectors to be determined. Using the spanning property of the orthonormal basis $\phi_{k} \in \mathbb{R}^{n}$ in Remark 1, each of the $\mathbf{u}_{i_{1}, \ldots, i_{p}}$ can be uniquely expressed as

$$
\begin{equation*}
\mathbf{u}_{i_{1}, \ldots, i_{p}}=\alpha_{i_{1}, \ldots, i_{p}}^{(1)} \phi_{1}+\alpha_{i_{1}, \ldots, i_{p}}^{(2)} \phi_{2}+\ldots+\alpha_{i_{1}, \ldots, i_{p}}^{(n)} \phi_{n} \tag{28}
\end{equation*}
$$

## Relationship with PC

Substituting this in Eq. (27) and collecting all the coefficients associated with each orthonormal vector $\phi_{k}$ the theorem is proved where

$$
\begin{align*}
\tilde{\Gamma}_{k}(\boldsymbol{\xi}(\omega)) & =\alpha_{i_{0}}^{(k)} h_{0}+\sum_{i_{1}=1}^{\infty} \alpha_{i_{1}}^{(k)} h_{1}\left(\xi_{i_{1}}(\omega)\right) \\
& +\sum_{i_{1}=1}^{\infty} \sum_{i_{2}=1}^{i_{1}} \alpha_{i_{1}, i_{2}}^{(k)} h_{2}\left(\xi_{i_{1}}(\omega), \xi_{i_{2}}(\omega)\right)+\sum_{i_{1}=1}^{\infty} \sum_{i_{2}=1}^{i_{1}} \sum_{i_{3}=1}^{i_{2}} \alpha_{i_{1} i_{2}}^{(k)} h_{3}\left(\xi_{i_{1}}(\omega), \xi_{i_{2}}(u\right. \\
& +\sum_{i_{1}=1}^{\infty} \sum_{i_{2}=1}^{i_{1}} \sum_{i_{3}=1}^{i_{2}} \sum_{i_{4}=1}^{i_{3}} \alpha_{i_{1} i_{2} i_{3} i_{4}}^{(k)} h_{4}\left(\xi_{i_{1}}(\omega), \xi_{i_{2}}(\omega), \xi_{i_{3}}(\omega), \xi_{i_{4}}(\omega)\right)+\ldots, \tag{29}
\end{align*}
$$

## The Galerkin approach

There exist a set of finite functions $\hat{\Gamma}_{k}:\left(\mathbb{R}^{m} \times \Omega\right) \rightarrow(\mathbb{R} \times \Omega)$, 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

$$
\begin{equation*}
\hat{\mathbf{u}}(\omega)=\sum_{k=1}^{n} c_{k} \widehat{\Gamma}_{k}(\boldsymbol{\xi}(\omega)) \phi_{k} \tag{30}
\end{equation*}
$$

converges to the exact solution of the discretized stochastic finite element equation (4) in the mean-square sense provided the vector $\mathbf{c}=\left\{c_{1}, c_{2}, \ldots, c_{n}\right\}^{\top}$ satisfies the $n \times n$ algebraic equations $\mathbf{S} \mathbf{c}=\mathbf{b}$ with

$$
\begin{gather*}
S_{j k}=\sum_{i=0}^{M} \widetilde{A}_{i j k} D_{i j k} ; \quad \forall j, k=1,2, \ldots, n ; \tilde{A}_{i j k}=\phi_{j}^{T} \mathbf{A}_{i} \phi_{k},  \tag{31}\\
D_{i j k}=\mathrm{E}\left[\xi_{i}(\omega) \widehat{\Gamma}_{j}(\xi(\omega)) \widehat{\Gamma}_{k}(\xi(\omega))\right] \quad \text { and } \quad b_{j}=\mathrm{E}\left[\widehat{\Gamma}_{j}(\xi(\omega))\right]\left(\phi_{j}^{T} \mathbf{f}\right) . \tag{32}
\end{gather*}
$$

## The Galerkin approach

- The error vector can be obtained as

$$
\begin{equation*}
\varepsilon(\omega)=\left(\sum_{i=0}^{M} \mathbf{A}_{i} \xi_{i}(\omega)\right)\left(\sum_{k=1}^{n} c_{k} \hat{\Gamma}_{k}(\boldsymbol{\xi}(\omega)) \phi_{k}\right)-\mathbf{f} \in \mathbb{R}^{n} \tag{33}
\end{equation*}
$$

The solution is viewed as a projection where $\left\{\hat{\Gamma}_{k}(\xi(\omega)) \phi_{k}\right\} \in \mathbb{R}^{n}$ are the basis functions and $c_{k}$ are the unknown constants to be determined.

- We wish to obtain the coefficients $c_{k}$ such that the error norm $\chi^{2}=\langle\varepsilon(\omega), \varepsilon(\omega)\rangle$ is minimum. This can be achieved using the Galerkin approach so that the error is made orthogonal to the basis functions, that is, mathematically
$\varepsilon(\omega) \perp\left(\widehat{\Gamma}_{j}(\xi(\omega)) \phi_{j}\right) \quad$ or $\quad\left\langle\hat{\Gamma}_{j}(\xi(\omega)) \phi_{j}, \varepsilon(\omega)\right\rangle=0 \forall j=1,2, \ldots, n$


## Summary of the computational method

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

## Computational complexity

- The spectral functions $\hat{\Gamma}_{k}(\xi(\omega))$ 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.
- The main computational cost of the proposed method depends on (a) the solution of the matrix eigenvalue problem, (b) the generation of the coefficient matrices $\mathbf{D}_{i}$, and (c) the calculation of the coefficient vector by solving linear matrix equation.
- For large $M$ and $n$, asymptotically the computational cost becomes $C_{s}=O\left(M n^{2}\right)+O\left(n^{3}\right)$.


## Collection of ZnO



Uncertainties in ZnO NWs in the close up view. The uncertain parameter include geometric parameters such as the length and the cross sectional area along the length, boundary condition and material properties.

## ZnO nanowires


(a) The SEM image of a collection of ZnO NW showing hexagonal cross sectional area.
(b) The continuum idealization of a cantilevered ZnO NW under an AFM tip

## Problem details

- We study the deflection of ZnO NW under the AFM tip considering stochastically varying bending modulus. The variability of the deflection is particularly important as the harvested energy from the bending depends on it.
- We assume that the bending modulus of the ZnO NW is a homogeneous stationary Gaussian random field of the form

$$
\begin{equation*}
E l(x, \omega)=E l_{0}(1+a(x, \omega)) \tag{35}
\end{equation*}
$$

where $x$ is the coordinate along the length of $\mathrm{ZnO} \mathrm{NW}, E I_{0}$ is the estimate of the mean bending modulus, $a(x, \omega)$ is a zero mean stationary Gaussian random field.

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

$$
\begin{equation*}
C_{a}\left(x_{1}, x_{2}\right)=\sigma_{a}^{2} e^{-\left(\left|x_{1}-x_{2}\right|\right) / \mu_{a}} \tag{36}
\end{equation*}
$$

where $\mu_{a}$ is the correlation length and $\sigma_{a}$ is the standard deviation.

## Problem details

- We consider a long nanowire where the continuum model has been validated.
- We use the baseline parameters for the ZnO NW from Gao and Wang (Nano Letters 7 (8) (2007), 2499-2505) as the length $L=600 \mathrm{~nm}$, diameter $d=50 \mathrm{~nm}$ and the lateral point force at the tip $f_{T}=80 \mathrm{nN}$.
- Using these data, the baseline deflection can be obtained as $\delta_{0}=145 \mathrm{~nm}$. We normalize our results with this baseline value for convenience.
- The correlation length considered in the numerical studies: $\mu_{a}=L / 10$.
- The number of terms $M$ in the KL expansion becomes 67 (95\% capture).
- The nanowire is divided into 50 beam elements of equal length. The number of degrees of freedom of the model $n=100$ (standard beam element).


## Moments



Figure: The number of random variable used: $M=67$. The number of degrees of freedom: $n=100$.

## Error in moments

| Statistics | Methods | $\sigma_{a}=0.05$ | $\sigma_{a}=0.10$ | $\sigma_{a}=0.15$ | $\sigma_{a}=0.20$ |
| :---: | :--- | :---: | :---: | :---: | :---: |
| Mean | 1st order <br> Galerkin <br> 2nd order <br> Galerkin | 0.1761 | 0.0007 | 0.0113 | 0.0642 |
| Standard | 1st order <br> Galerkin | 3.9543 | 5.9581 | 0.6738 |  |
|  | 0.3222 | 1.8425 | 4.6781 | 8.903 | 14.6568 |
| deviation | 2nd order <br> Galerkin |  |  |  |  |

Percentage error in the mean and standard deviation of the deflection of the ZnO NW under the AFM tip when correlation length is $\mu_{a}=L / 3$. For $n=100$ and $M=67$, 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.

## Pdf


(a) Probability density function for $\sigma_{a}=(\mathrm{b})$ Probability density function for $\sigma_{a}=$ 0.1.

The probability density function of the normalized deflection $\delta / \delta_{0}$ of the ZnO NW under the AFM tip ( $\delta_{0}=145 \mathrm{~nm}$ ).

## Conclusions

- The only informaion used in the classical PC is the pdf of the random variables.
- Here, additionally, the following information, coming from the discreised PDE, are used:
- $\mathbf{A}_{0}$ is symmetric and positive definite (used to generate the orthonormal basis)
- $\left\|\mathbf{A}_{i}\right\| \geq\left\|\mathbf{A}_{i+1}\right\|, i=0,1,2,3 \ldots$ (used to generate the coefficient functions)
- This is a 'bespoke' approach


## Conclusions


(c) Basic building blocks.

(d) Possible 'solution'.

An analogy of PC based solution.

## Conclusions



Basic building blocks for the proposed method

## Conclusions

(1) We consider discretised stochastic elliptic 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 $n$ is the size of the discretized matrices and $M$ is the number of random variables, then the computational complexity grows in $O\left(M n^{2}\right)+O\left(n^{3}\right)$ for large $M$ and $n$ in the worse case.
(5) We consider a problem with 67 random variables and $n=100$ degrees of freedom. A second-order PC would require the solution of equations of dimension 234,500. In comparison, the proposed Galerkin approach requires the solution of algebraic equations of dimension $n$ only.

