A Vector-Space Approach for Stochastic Finite Element Analysis

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Outline of the talk

1. **Introduction**
   - Uncertainty in computational mechanics
   - 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**
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4. **Numerical illustration**
   - ZnO nanowires
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Sources of uncertainty

(a) parametric uncertainty - e.g., uncertainty in geometric parameters, friction coefficient, strength of the materials involved;
(b) model inadequacy - arising from the lack of scientific knowledge about the model which is a-priori unknown;
(c) experimental error - uncertain and unknown error percolate into the model when they are calibrated against experimental results;
(d) computational uncertainty - e.g, machine precession, error tolerance and the so called ‘h’ and ‘p’ refinements in finite element analysis, and
(e) model uncertainty - genuine randomness in the model such as uncertainty in the position and velocity in quantum mechanics, deterministic chaos.

Stochastic elliptic PDE

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

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

  with the associated boundary condition

$$u(\mathbf{r},\theta) = 0; \quad \mathbf{r} \text{ on } \partial\mathcal{D} \tag{2}$$

- 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.

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

$$a(\mathbf{r}, \theta) = a_0(\mathbf{r}) + \sum_{i=1}^{\infty} \sqrt{\nu_i} \xi_i(\theta) \varphi_i(\mathbf{r}) \tag{3}$$

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

$$\int_{\mathcal{D}} C_a(\mathbf{r}_1, \mathbf{r}_2) \varphi_j(\mathbf{r}_1) \mathrm{d}\mathbf{r}_1 = \nu_j \varphi_j(\mathbf{r}_2), \quad \forall\ j = 1, 2, \cdots \tag{4}$$

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

$$\left[\mathbf{A}_0 + \sum_{i=1}^{M} \xi_i(\theta)\mathbf{A}_i\right] \mathbf{u}(\theta) = \mathbf{f} \tag{5}$$

- The aim is to efficiently solve for $\mathbf{u}(\theta)$.

Polynomial Chaos expansion

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

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

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

Polynomial Chaos expansion

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

$$\hat{\mathbf{u}}(\theta) = \sum_{k=1}^{P} H_k(\xi(\theta))\mathbf{u}_k \tag{6}$$

  where $H_k(\xi(\theta))$ 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

$$P = \sum_{j=0}^{r} \frac{(M+j-1)!}{j!(M-1)!} \tag{7}$$

Polynomial Chaos expansion

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

$$\begin{bmatrix} \mathbf{A}_{0,0} & \cdots & \mathbf{A}_{0,P-1} \\ \mathbf{A}_{1,0} & \cdots & \mathbf{A}_{1,P-1} \\ \vdots & \vdots & \vdots \\ \mathbf{A}_{P-1,0} & \cdots & \mathbf{A}_{P-1,P-1} \end{bmatrix} \begin{Bmatrix} \mathbf{u}_0 \\ \mathbf{u}_1 \\ \vdots \\ \mathbf{u}_{P-1} \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_0 \\ \mathbf{f}_1 \\ \vdots \\ \mathbf{f}_{P-1} \end{Bmatrix} \tag{8}$$

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

Mathematical nature of the solution (1)

- 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

$$\frac{p^{(n-1)}(\xi_1(\theta),\xi_2(\theta),\ldots,\xi_M(\theta))}{p^{(n)}(\xi_1(\theta),\xi_2(\theta),\ldots,\xi_M(\theta))} \tag{9}$$

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 (2)

Suppose we denote

$$\mathbf{A}(\theta) = \left[\mathbf{A}_0 + \sum_{i=1}^{M} \xi_i(\theta)\mathbf{A}_i\right] \in \mathbb{R}^{n\times n} \tag{10}$$

so that

$$\mathbf{u}(\theta) = \mathbf{A}^{-1}(\theta)\mathbf{f} \tag{11}$$

From the definition of the matrix inverse we have

$$\mathbf{A}^{-1} = \frac{\mathrm{Adj}(\mathbf{A})}{\det(\mathbf{A})} = \frac{\mathbf{C}_a^T}{\det(\mathbf{A})} \tag{12}$$

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. (10) that

$$A_{kj}(\theta) = A_{0_{kj}} + \sum_{i=1}^{M} \xi_i(\theta)\mathbf{A}_{i_{kj}} \tag{13}$$

Mathematical nature of the solution (3)

- 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. (13). 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. (13). From Eqs. (11) and (12) it follows that

$$\mathbf{u}(\theta) = \frac{\mathbf{C}_a^T \mathbf{f}}{\det(\mathbf{A})} \tag{14}$$

  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. (9).

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

$$\hat{\mathbf{u}}(\theta) = \sum_{k=1}^{n} H_k(\xi(\theta))\mathbf{u}_k + \sum_{k=n+1}^{P} H_k(\xi(\theta))\mathbf{u}_k \qquad (15)$$

- 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 (15), 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 $\Gamma_k : (\mathbb{R}^m \times \Theta) \to (\mathbb{R} \times \Theta)$ *and an orthonormal basis* $\phi_k \in \mathbb{R}^n$ *for* $k = 1, 2, \ldots, n$ *such that the series*

$$\hat{\mathbf{u}}(\theta) = \sum_{k=1}^{n} \Gamma_k(\boldsymbol{\xi}(\theta))\phi_k \tag{16}$$

converges to the exact solution of the discretized stochastic finite element equation (5) 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

$$\mathbf{A}_0\phi_k = \lambda_{0_k}\phi_k; \quad k = 1, 2, \ldots n \tag{17}$$

Projection in a finite dimensional vector-space

We define the matrix of eigenvalues and eigenvectors

$$\mathbf{\Lambda}_0 = \mathrm{diag}\left[\lambda_{0_1}, \lambda_{0_2}, \ldots, \lambda_{0_n}\right] \in \mathbb{R}^{n\times n}; \mathbf{\Phi} = \left[\phi_1, \phi_2, \ldots, \phi_n\right] \in \mathbb{R}^{n\times n} \tag{18}$$

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:

$$\mathbf{\Phi}^T \mathbf{A}_0 \mathbf{\Phi} = \mathbf{\Lambda}_0; \quad \mathbf{A}_0 = \mathbf{\Phi}^{-T} \mathbf{\Lambda}_0 \mathbf{\Phi}^{-1} \quad \text{and} \quad \mathbf{A}_0^{-1} = \mathbf{\Phi} \mathbf{\Lambda}_0^{-1} \mathbf{\Phi}^T \tag{19}$$

We also introduce the transformations

$$\widetilde{\mathbf{A}}_i = \mathbf{\Phi}^T \mathbf{A}_i \mathbf{\Phi} \in \mathbb{R}^{n\times n}; i = 0, 1, 2, \ldots, M \tag{20}$$

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

$$\mathbf{A}_i = \mathbf{\Phi}^{-T} \widetilde{\mathbf{A}}_i \mathbf{\Phi}^{-1} \in \mathbb{R}^{n\times n}; i = 1, 2, \ldots, M \tag{21}$$

Projection in a finite dimensional vector-space

Suppose the solution of Eq. (5) is given by

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

Using Eqs. (18)–(21) and the orthonormality of $\boldsymbol{\Phi}$ one has

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

where

$$\boldsymbol{\Psi}\left(\boldsymbol{\xi}(\theta)\right) = \left[\boldsymbol{\Lambda}_0 + \sum_{i=1}^{M} \xi_i(\theta)\widetilde{\mathbf{A}}_i\right]^{-1} \tag{24}$$

and the M-dimensional random vector

$$\boldsymbol{\xi}(\theta) = \left\{\xi_1(\theta), \xi_2(\theta), \ldots, \xi_M(\theta)\right\}^T \tag{25}$$

Projection in a finite dimensional vector-space

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

$$\widetilde{\mathbf{A}}_i = \mathbf{\Lambda}_i + \mathbf{\Delta}_i, \quad i = 1, 2, \ldots, M \tag{26}$$

Here the diagonal matrix

$$\mathbf{\Lambda}_i = \mathrm{diag}\left[\widetilde{\mathbf{A}}\right] = \mathrm{diag}\left[\lambda_{i_1}, \lambda_{i_2}, \ldots, \lambda_{i_n}\right] \in \mathbb{R}^{n\times n} \tag{27}$$

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

$$\mathbf{\Psi}\left(\boldsymbol{\xi}(\theta)\right) = \left[\underbrace{\mathbf{\Lambda}_0 + \sum_{i=1}^{M} \xi_i(\theta)\mathbf{\Lambda}_i}_{\mathbf{\Lambda}(\boldsymbol{\xi}(\theta))} + \underbrace{\sum_{i=1}^{M} \xi_i(\theta)\mathbf{\Delta}_i}_{\mathbf{\Delta}(\boldsymbol{\xi}(\theta))}\right]^{-1} \tag{28}$$

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. (28) as

$$\boldsymbol{\Psi}\left(\xi(\theta)\right) = \left[\boldsymbol{\Lambda}\left(\xi(\theta)\right)\left[\mathbf{I}_n + \boldsymbol{\Lambda}^{-1}\left(\xi(\theta)\right)\boldsymbol{\Delta}\left(\xi(\theta)\right)\right]\right]^{-1} \tag{29}$$

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

$$\boldsymbol{\Psi}\left(\xi(\theta)\right) = \sum_{s=0}^{\infty}(-1)^s\left[\boldsymbol{\Lambda}^{-1}\left(\xi(\theta)\right)\boldsymbol{\Delta}\left(\xi(\theta)\right)\right]^s\boldsymbol{\Lambda}^{-1}\left(\xi(\theta)\right) \tag{30}$$

Polynomial Chaos expansion

Taking an arbitrary r-th element of $\hat{\mathbf{u}}(\theta)$, Eq. (23) can be rearranged to have

$$\hat{u}_r(\theta) = \sum_{k=1}^{n} \Phi_{rk} \left(\sum_{j=1}^{n} \Psi_{kj} \left(\boldsymbol{\xi}(\theta)\right) \left(\phi_j^T \mathbf{f}\right) \right) \tag{31}$$

Defining

$$\Gamma_k \left(\boldsymbol{\xi}(\theta)\right) = \sum_{j=1}^{n} \Psi_{kj} \left(\boldsymbol{\xi}(\theta)\right) \left(\phi_j^T \mathbf{f}\right) \tag{32}$$

and collecting all the elements in Eq. (31) for $r = 1, 2, \ldots, n$ one has

$$\hat{\mathbf{u}}(\theta) = \sum_{k=1}^{n} \Gamma_k \left(\boldsymbol{\xi}(\theta)\right) \phi_k \tag{33}$$

Spectral functions

Definition

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

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 (30).*

Retaining one term in (30) we have

$$\boldsymbol{\Psi}^{(1)}(\boldsymbol{\xi}(\theta)) = \boldsymbol{\Lambda}^{-1}(\boldsymbol{\xi}(\theta)) \quad \text{or} \quad \Psi_{kj}^{(1)}(\boldsymbol{\xi}(\theta)) = \frac{\delta_{kj}}{\lambda_{0_k} + \sum_{i=1}^{M} \xi_i(\theta)\lambda_{i_k}} \tag{34}$$

Using the definition of the spectral function in Eq. (32), the first-order spectral functions can be explicitly obtained as

$$\Gamma_k^{(1)}(\boldsymbol{\xi}(\theta)) = \sum_{j=1}^{n} \Psi_{kj}^{(1)}(\boldsymbol{\xi}(\theta)) \left(\phi_j^T \mathbf{f}\right) = \frac{\phi_k^T \mathbf{f}}{\lambda_{0_k} + \sum_{i=1}^{M} \xi_i(\theta)\lambda_{i_k}} \tag{35}$$

- From this expression it is clear that $\Gamma_k^{(1)}(\boldsymbol{\xi}(\theta))$ 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 (30).

Retaining two terms in (30) we have

$$\boldsymbol{\Psi}^{(2)}\left(\boldsymbol{\xi}(\theta)\right) = \boldsymbol{\Lambda}^{-1}\left(\boldsymbol{\xi}(\theta)\right) - \boldsymbol{\Lambda}^{-1}\left(\boldsymbol{\xi}(\theta)\right)\boldsymbol{\Delta}\left(\boldsymbol{\xi}(\theta)\right)\boldsymbol{\Lambda}^{-1}\left(\boldsymbol{\xi}(\theta)\right) \tag{36}$$

Using the definition of the spectral function in Eq. (32), the second-order spectral functions can be obtained in closed-form as

$$\Gamma_k^{(2)}\left(\boldsymbol{\xi}(\theta)\right) = \frac{\phi_k^T \mathbf{f}}{\lambda_{0_k} + \sum_{i=1}^M \xi_i(\theta)\lambda_{i_k}} - \sum_{j=1}^{n} \frac{\left(\phi_j^T \mathbf{f}\right)\sum_{i=1}^M \xi_i(\theta)\Delta_{i_{kj}}}{\left(\lambda_{0_k} + \sum_{i=1}^M \xi_i(\theta)\lambda_{i_k}\right)\left(\lambda_{0_j} + \sum_{i=1}^M \xi_i(\theta)\lambda_{i_j}\right)} \tag{37}$$

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,

$$\hat{u}_r(\theta) \equiv \frac{p_r^{(n-1)}(\xi_1(\theta), \xi_2(\theta), \ldots, \xi_M(\theta))}{p_r^{(n)}(\xi_1(\theta), \xi_2(\theta), \ldots, \xi_M(\theta))}, \quad \forall r = 1, 2, \ldots, n \tag{38}$$

When first-order spectral functions (35) are considered, we have

$$\hat{u}_r^{(1)}(\theta) = \sum_{k=1}^{n} \Gamma_k^{(1)}\left(\boldsymbol{\xi}(\theta)\right)\phi_{rk} = \sum_{k=1}^{n} \frac{\phi_k^T \mathbf{f}}{\lambda_{0_k} + \sum_{i=1}^{M} \xi_i(\theta)\lambda_{i_k}} \phi_{rk} \tag{39}$$

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,

$$\hat{u}_r^{(1)}(\theta) = \frac{\sum_{k=1}^{n} (\phi_k^T \mathbf{f}) \phi_{rk} \prod_{j=1 \neq k}^{n-1} \left(\lambda_{0_j} + \sum_{i=1}^{M} \xi_i(\theta)\lambda_{i_j} \right)}{\prod_{k=1}^{n-1} \left(\lambda_{0_j} + \sum_{i=1}^{M} \xi_i(\theta)\lambda_{i_j} \right)} \tag{40}$$

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*

$$\hat{\mathbf{u}}(\theta) = \sum_{k=1}^{n} c_k \widehat{\Gamma}_k(\boldsymbol{\xi}(\theta))\phi_k \tag{41}$$

converges to the exact solution of the discretized stochastic finite element equation (5) 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*

$$S_{jk} = \sum_{i=0}^{M} \widetilde{A}_{i_{jk}} D_{ijk}; \quad \forall\, j, k = 1, 2, \ldots, n; \widetilde{A}_{i_{jk}} = \phi_j^T \mathbf{A}_i \phi_k, \tag{42}$$

$$D_{ijk} = \mathrm{E}\left[\xi_i(\theta)\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\widehat{\Gamma}_k(\boldsymbol{\xi}(\theta))\right] \quad \text{and} \quad b_j = \mathrm{E}\left[\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\right]\left(\phi_j^T \mathbf{f}\right). \tag{43}$$

The Galerkin approach

- The error vector can be obtained as

$$\varepsilon(\theta) = \left(\sum_{i=0}^{M} \mathbf{A}_i \xi_i(\theta)\right) \left(\sum_{k=1}^{n} c_k \widehat{\Gamma}_k(\boldsymbol{\xi}(\theta))\phi_k\right) - \mathbf{f} \in \mathbb{R}^n \qquad (44)$$

  The solution is viewed as a projection where $\left\{\widehat{\Gamma}_k(\boldsymbol{\xi}(\theta))\phi_k\right\} \in \mathbb{R}^n$ 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 $\chi^2 = \langle \varepsilon(\theta), \varepsilon(\theta) \rangle$ is minimum. This can be achieved using the Galerkin approach so that the error is made orthogonal to the basis functions, that is, mathematically

$$\varepsilon(\theta) \perp \left(\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\phi_j\right) \quad \text{or} \quad \left\langle \widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\phi_j, \varepsilon(\theta) \right\rangle = 0 \; \forall \, j = 1, 2, \ldots, n \qquad (45)$$

The Galerkin approach

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

$$\mathrm{E}\left[\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\phi_j^T\left(\sum_{i=0}^{M}\mathbf{A}_i\xi_i(\theta)\right)\left(\sum_{k=1}^{n}c_k\widehat{\Gamma}_k(\boldsymbol{\xi}(\theta))\phi_k\right)-\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\phi_j^T\mathbf{f}\right]=0 \tag{46}$$

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

$$\sum_{k=1}^{n}\left(\sum_{i=0}^{M}\left(\phi_j^T\mathbf{A}_i\phi_k\right)\mathrm{E}\left[\xi_i(\theta)\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\widehat{\Gamma}_k(\boldsymbol{\xi}(\theta))\right]\right)c_k = \mathrm{E}\left[\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\right]\left(\phi_j^T\mathbf{f}\right) \tag{47}$$

$$\text{or}\quad \sum_{k=1}^{n}\left(\sum_{i=0}^{M}\widetilde{A}_{i_{jk}}D_{ijk}\right)c_k = b_j \tag{48}$$

Model Reduction by reduced number of basis

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

$$\lambda_{0_1} < \lambda_{0_2} < \ldots < \lambda_{0_n} \tag{49}$$

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

$$\Gamma_k^{(1)}(\boldsymbol{\xi}(\omega)) = \frac{\phi_k^T \mathbf{f}}{\lambda_{0_k} + \sum_{i=1}^{M} \xi_i(\omega)\lambda_{i_k}} \tag{50}$$

- 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.

Proposiion

(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 (5) can be expressed by the series representation

$$\hat{\mathbf{u}}(\omega) = \sum_{k=1}^{p} c_k \widehat{\Gamma}_k(\boldsymbol{\xi}(\omega))\phi_k \tag{51}$$

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. (42) and (43).

Computational method

- The mean vector can be obtained as

$$\bar{\mathbf{u}} = \mathrm{E}\left[\hat{\mathbf{u}}(\theta)\right] = \sum_{k=1}^{p} c_k \mathrm{E}\left[\widehat{\Gamma}_k(\boldsymbol{\xi}(\theta))\right] \phi_k \tag{52}$$

- The covariance of the solution vector can be expressed as

$$\boldsymbol{\Sigma}_u = \mathrm{E}\left[\left(\hat{\mathbf{u}}(\theta) - \bar{\mathbf{u}}\right)\left(\hat{\mathbf{u}}(\theta) - \bar{\mathbf{u}}\right)^T\right] = \sum_{k=1}^{p}\sum_{j=1}^{p} c_k c_j \Sigma_{\Gamma_{kj}} \phi_k \phi_j^T \tag{53}$$

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

$$\Sigma_{\Gamma_{kj}} = \mathrm{E}\left[\left(\widehat{\Gamma}_k(\boldsymbol{\xi}(\theta)) - \mathrm{E}\left[\widehat{\Gamma}_k(\boldsymbol{\xi}(\theta))\right]\right)\left(\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta)) - \mathrm{E}\left[\widehat{\Gamma}_j(\boldsymbol{\xi}(\theta))\right]\right)\right] \tag{54}$$

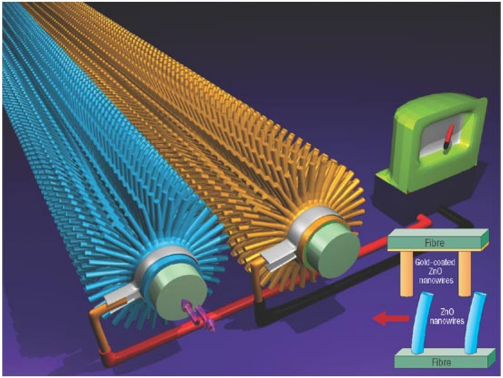
Summary of the computational method

1. Solve the eigenvalue problem associated with the mean matrix $\mathbf{A}_0$ to generate the orthonormal basis vectors: $\mathbf{A}_0 \mathbf{\Phi} = \mathbf{\Lambda}_0 \mathbf{\Phi}$
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): $\Gamma_k(\boldsymbol{\xi}(\theta)) = \frac{\phi_k^T \mathbf{f}}{\lambda_{0_k} + \sum_{i=1}^{M} \xi_i(\theta) \lambda_{i_k}}$, 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: $\hat{\mathbf{u}}(\theta) = \sum_{k=1}^{p} c_k \Gamma_k(\boldsymbol{\xi}(\theta)) \phi_k$

Nanoscale Energy Harvesting: ZnO nanowires

- ZnO materials have attracted extensive attention due to their excellent performance in electronic, ferroelectric and piezoelectric applications.
- Nano-scale ZnO is an important material for the nanoscale energy harvesting and scavenging.
- Investigation and understanding of the bending of ZnO nanowires are valuable for their potential application. For example, ZnO nanowires are bend by rubbing against each other for energy scavenging.

Rubbing the right way



When ambient vibrations move a microfibre covered with zinc oxide nanowires (blue) back and forth with respect to a similar fibre that has been coated with gold (orange), electrical energy is produced because ZnO is a piezoelectric material; *Nature Nanotechnology, Vol 3, March 2008, pp 123*.

Power shirt

Science News

Share Blog Cite

Power Shirt: Nanotechnology In Clothing Could Harvest Energy From Body Movement

ScienceDaily (Feb. 14, 2008) — Nanotechnology researchers are developing the perfect complement to the power tie: a "power shirt" able to generate electricity to power small electronic devices for soldiers in the field, hikers and others whose physical motion could be harnessed and converted to electrical energy.

The February 14 issue of the journal Nature details how pairs of textile fibers covered with zinc oxide nanowires can generate electrical current using the piezoelectric effect. Combining current flow from many fiber pairs woven into a shirt or jacket could allow the wearer's body movement to power a range of portable electronic devices. The fibers could also be woven into curtains, tents or other structures to capture energy from wind motion, sound vibration or other mechanical energy.

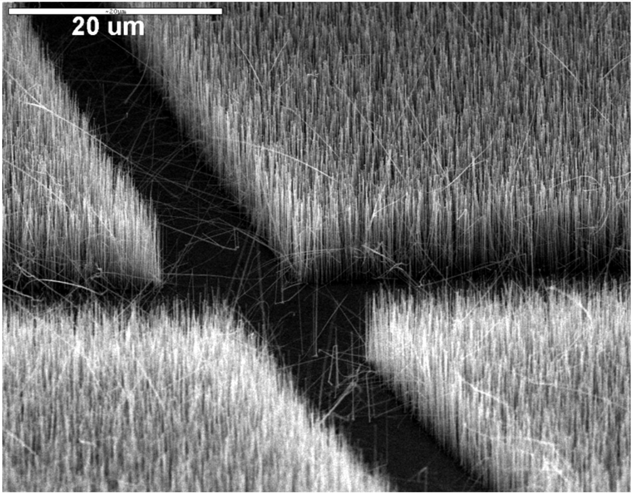
Close-up image shows a pair of entangled fibers that make up a microfiber nanogenerator. Both fibers are coated with zinc oxide nanowires; one fiber is additionally coated with gold. When rubbed together, they generate electrical current. (Credit: Georgia Tech Photo: Gary Meek)

See Also:

Matter & Energy
- Energy Technology
- Nanotechnology
- Materials Science
- Electricity
- Solar Energy
- Physics

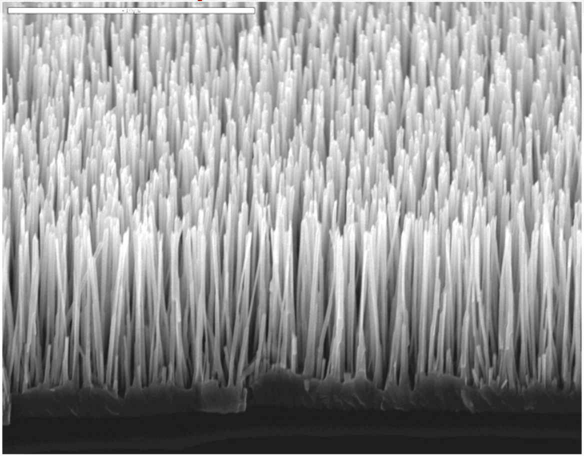
Reference
- Nanowire
- Electric power
- Electrical phenomena

Collection of ZnO



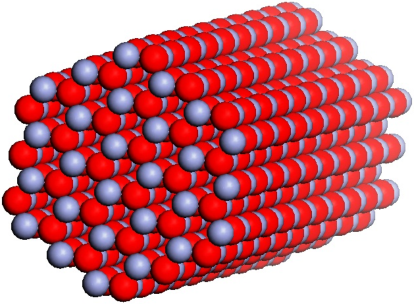
A collection of vertically grown ZnO NWs. This can be viewed as the sample space for the application of stochastic finite element method.

Collection of ZnO: Close up

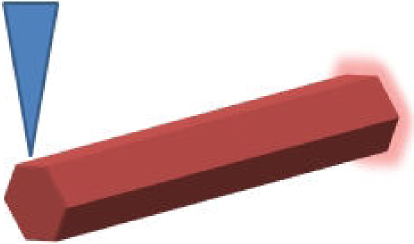


Uncertainties in ZnO NWs in the close up view. The uncertain parameter include geometric parameters such as the length and the cross sectional area along the length, boundary condition and material properties.

ZnO nanowires



(a) The atomistic model of a ZnO NW grown from a ZnO crystal in the $(0, 0, 0, 1)$ direction.



(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

$$EI(x,\theta) = EI_0(1 + a(x,\theta)) \tag{55}$$

  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

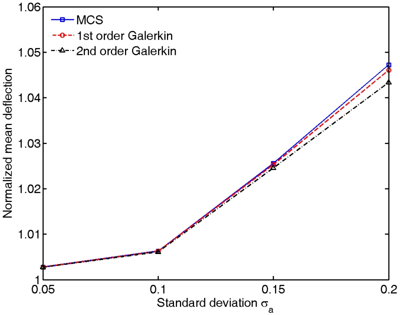
$$C_a(x_1,x_2) = \sigma_a^2 e^{-(|x_1-x_2|)/\mu_a} \tag{56}$$

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

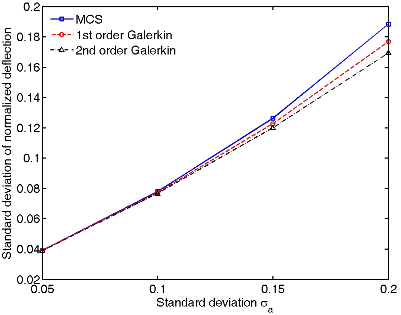
Problem details

- 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 $L = 600$nm, diameter $d = 50$nm and the lateral point force at the tip $f_T = 80$nN.
- Using these data, the baseline deflection can be obtained as $\delta_0 = 145$nm. We normalize our results with this baseline value for convenience.
- Two correlation lengths are considered in the numerical studies: $\mu_a = L/3$ and $\mu_a = L/10$.
- The number of terms M in the KL expansion becomes 24 and 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: larger correlation length



(c) Mean of the normalized deflection.



(d) Standard deviation of the normalized deflection.

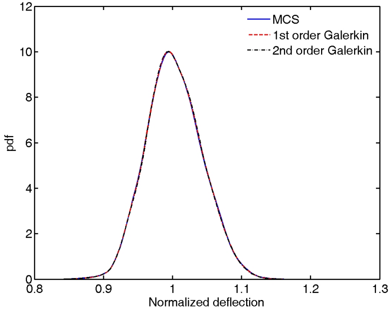
Figure: The number of random variable used: $M = 24$. The number of degrees of freedom: $n = 100$.

Error in moments: larger correlation length

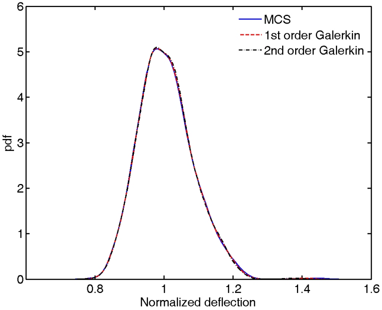
Statistics	Methods	$\sigma_a = 0.05$	$\sigma_a = 0.10$	$\sigma_a = 0.15$	$\sigma_a = 0.20$
Mean	1st order Galerkin	0.1027	0.4240	1.0104	1.9749
	2nd order Galerkin	0.0003	0.0045	0.0283	0.1321
Standard deviation	1st order Galerkin	1.8693	3.0517	5.2490	11.3447
	2nd order Galerkin	0.2201	1.0425	2.7690	8.2712

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 $M = 24$, if the second-order PC was used, one would need to solve a linear system of equation of size 32400. The results shown here are obtained by solving a linear system of equation of size 6 using the proposed Galerkin approach.

Pdf: larger correlation length



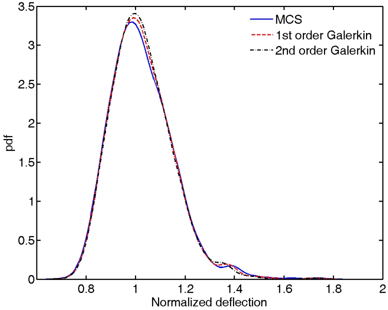
(a) Probability density function for $\sigma_a = 0.05$.



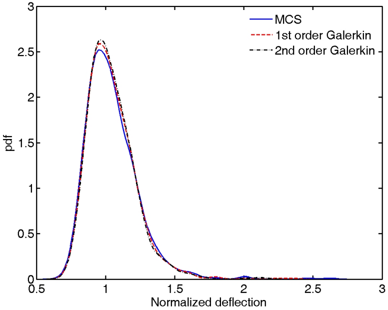
(b) Probability density function for $\sigma_a = 0.1$.

The probability density function of the normalized deflection δ/δ_0 of the ZnO NW under the AFM tip ($\delta_0 = 145$nm).

Pdf: larger correlation length



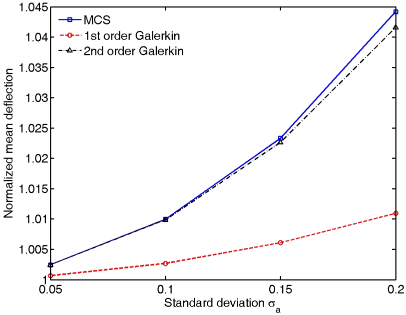
(c) Probability density function for $\sigma_a = 0.15$.



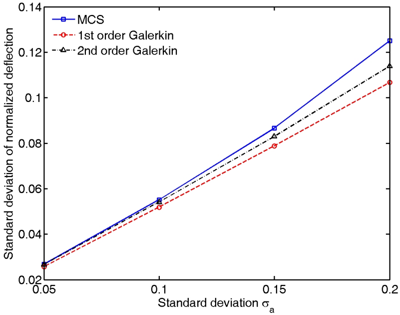
(d) Probability density function for $\sigma_a = 0.2$.

The probability density function of the normalized deflection δ/δ_0 of the ZnO NW under the AFM tip ($\delta_0 = 145$nm).

Moments: smaller correlation length



(e) Mean of the normalized deflection.



(f) Standard deviation of the normalized deflection.

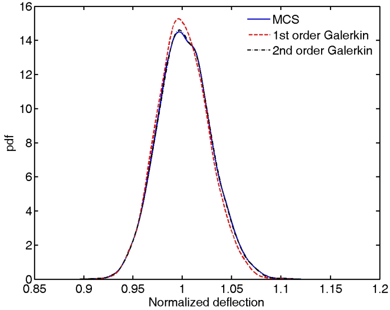
Figure: The number of random variable used: $M = 67$. The number of degrees of freedom: $n = 100$.

Error in moments: smaller correlation length

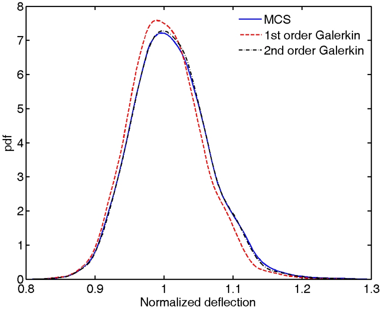
Statistics	Methods	$\sigma_a = 0.05$	$\sigma_a = 0.10$	$\sigma_a = 0.15$	$\sigma_a = 0.20$
Mean	1st order Galerkin	0.1761	0.7206	1.6829	3.1794
	2nd order Galerkin	0.0007	0.0113	0.0642	0.6738
Standard deviation	1st order Galerkin	3.9543	5.9581	9.0305	14.6568
	2nd order Galerkin	0.3222	1.8425	4.6781	8.9037

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 6 using the proposed Galerkin approach.

Pdf: smaller correlation length



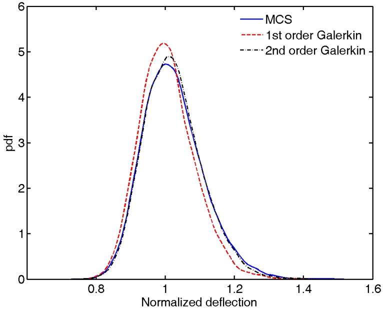
(a) Probability density function for $\sigma_a = 0.05$.



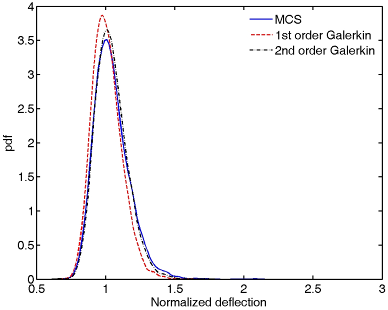
(b) Probability density function for $\sigma_a = 0.1$.

The probability density function of the normalized deflection δ/δ_0 of the ZnO NW under the AFM tip ($\delta_0 = 145$nm).

Pdf: smaller correlation length



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



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

The probability density function of the normalized deflection δ/δ_0 of the ZnO NW under the AFM tip ($\delta_0 = 145$nm).

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 $p < n$ 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 24 and 67 random variables and $n = 100$ degrees of freedom. A second-order PC would require the solution of equations of dimension 32,400 and 234,500 respectively. In comparison, the proposed Galerkin approach requires the solution of algebraic equations of dimension 6 only.

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