

Uncertainty quantification using surrogate models

S. Adhikari*

Chair of Aerospace Engineering
College of Engineering, Swansea University, Swansea UK
S.Adhikari@swansea.ac.uk

*Director: [Flamingo Engineering Ltd](http://www.flamingoeng.com); <http://www.flamingoeng.com>

Uncertainty Quantification in High Value Manufacturing - Exploring the Opportunities
London, United Kingdom, 29 – 30 June 2015



Swansea University
Prifysgol Abertawe



KTN

the
Knowledge Transfer
Network



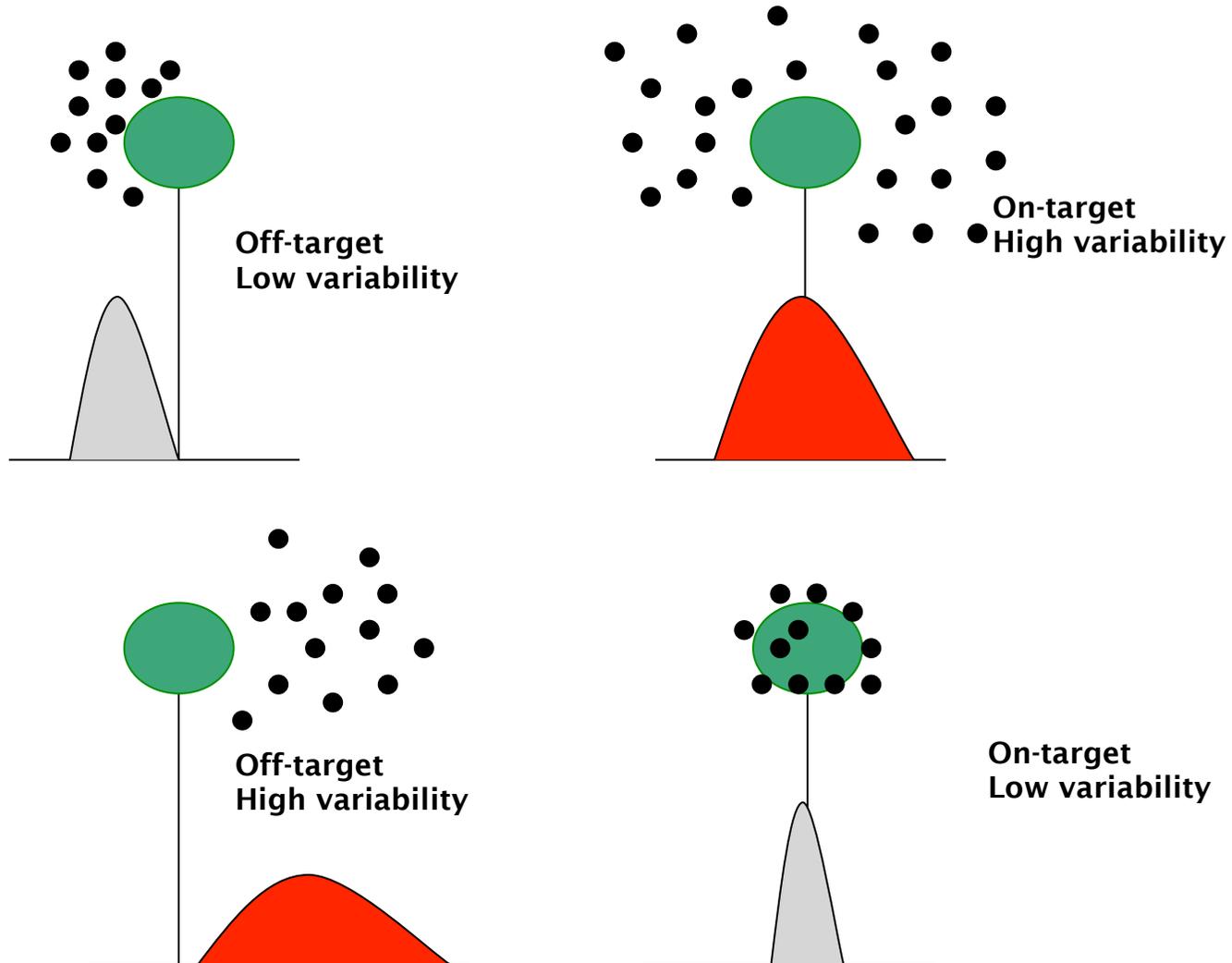
Outline

- **Introduction**
- **Uncertainty quantification**
- **Bottom up stochastic approach by Monte Carlo Simulation**
- **Surrogate modelling for uncertainty propagation**
 - **Random Sampling - High Dimensional Model Representation (RS-HDMR) model**
 - **D-optimal Design model**
 - **Kriging model**
 - **Central Composite Design (CCD) model**
 - **General high dimensional model representation (GHDMR)**
- ***Surrogate modelling and sampling – a comparative analysis***
- **Conclusions**

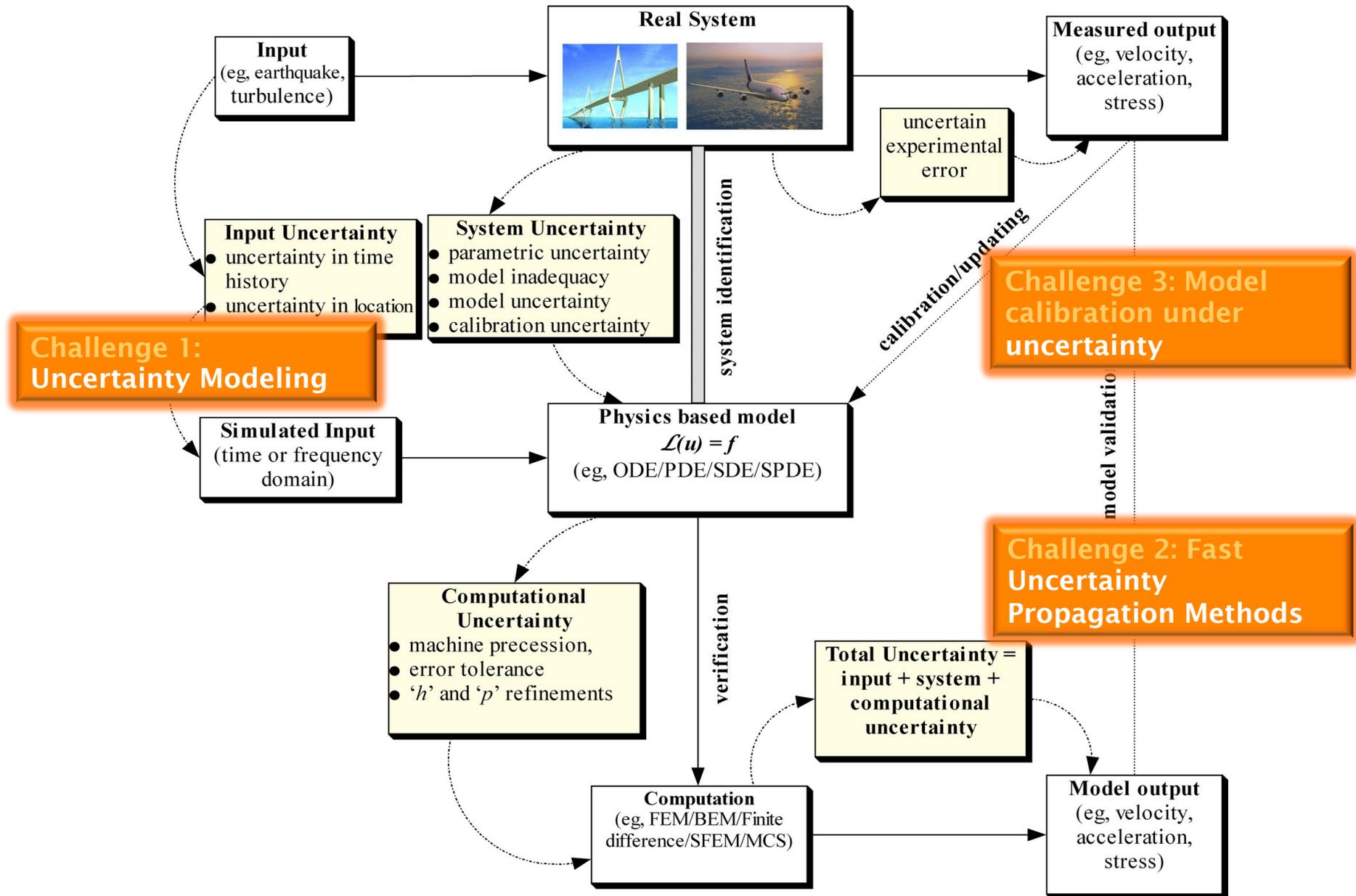


Uncertainty quantification – what is it?

Actual Performance of Engineering Designs



UQ in Computational Modeling



Why Uncertainty: The Sources

Experimental error

uncertain and unknown error percolate into the model when they are calibrated against experimental results

Parametric Uncertainty

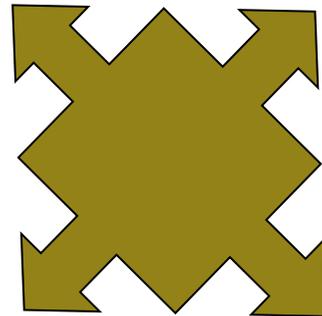
uncertainty in the geometric parameters, boundary conditions, forces, strength of the materials involved

Computational uncertainty

machine precession, error tolerance and the so called 'h' and 'p' refinements in finite element analysis

Model Uncertainty

arising from the lack of scientific knowledge about the model which is a-priori unknown (damping, nonlinearity, joints)



Uncertainty Modeling – A general overview

Parametric
Uncertainty

- Random variables
- Random fields

Non-parametric
Uncertainty

- Probabilistic Approach
 - Random matrix theory
- Possibilistic Approaches
 - Fuzzy variable
 - Interval algebra
 - Convex modeling

Equation of Motion of Dynamical Systems

- The Equation of motion of all these systems (and many other) about an equilibrium point can be expressed by:

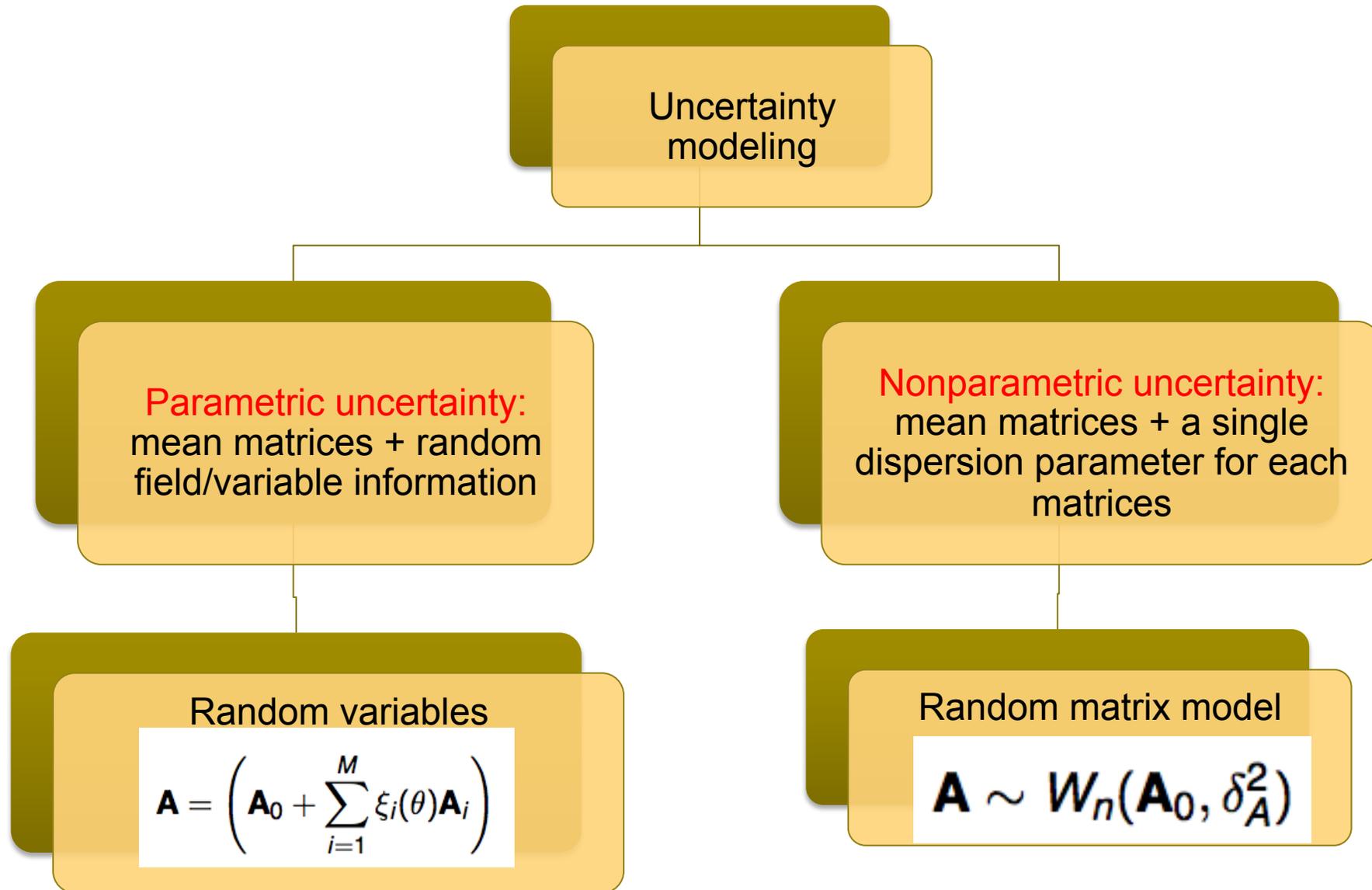
$$\mathbf{M}(\theta)\ddot{\mathbf{u}}(\theta, t) + \mathbf{C}(\theta)\dot{\mathbf{u}}(\theta, t) + \mathbf{K}(\theta)\mathbf{u}(\theta, t) = \mathbf{f}(t)$$

- $\mathbf{M}(\theta) \in \mathbb{R}^{n \times n}$ is the random mass matrix, $\mathbf{K}(\theta) \in \mathbb{R}^{n \times n}$ is the random stiffness matrix, $\mathbf{C}(\theta) \in \mathbb{R}^{n \times n}$ is the random damping matrix and $\mathbf{f}(t)$ is the forcing vector. We use (θ) to denote that the quantity is random.

The uncertainty propagation problem:

Given the stochastic description of the three systems matrices and the input forcing function, obtain the stochastic description of the response

Uncertainty modeling in structural dynamics





References on random matrix theory

1. Pascual, B. and Adhikari, S., "Combined parametric-nonparametric uncertainty quantification using random matrix theory and polynomial chaos expansion", *Computers & Structures*, 112-113[12] (2012), pp. 364-379.
2. Adhikari, S., Pastur, L., Lytova, A. and Du Bois, J. L., "Eigenvalue-density of linear stochastic dynamical systems: A random matrix approach", *Journal of Sound and Vibration*, 331[5] (2012), pp. 1042-1058.
3. Adhikari, S., "Uncertainty quantification in structural dynamics using non-central Wishart distribution", *International Journal of Engineering Under Uncertainty: Hazards, Assessment and Mitigation*, 2[3-4] (2010), pp. 123-139.
4. Adhikari, S. and Chowdhury, R., "A reduced-order random matrix approach for stochastic structural dynamics", *Computers and Structures*, 88[21-22] (2010), pp. 1230-1238.
5. Adhikari, S., "Generalized Wishart distribution for probabilistic structural dynamics", *Computational Mechanics*, 45[5] (2010), pp. 495-511.
6. Adhikari, S., "Wishart random matrices in probabilistic structural mechanics", *ASCE Journal of Engineering Mechanics*, 134[12] (2008), pp. 1029-1044.
7. Adhikari, S., "Matrix variate distributions for probabilistic structural mechanics", *AIAA Journal*, 45[7] (2007), pp. 1748-1762.

Broad approaches to UQ

UQ

Physics based UQ

- [1] Kundu, A., Adhikari, S., Friswell, M. I., "Transient response analysis of randomly parametrized finite element systems based on approximate balanced reduction", *Computer Methods in Applied Mechanics and Engineering*, 285[3] (2015), pp. 542-570.
- [2] Kundu, A. and Adhikari, S., "Dynamic analysis of stochastic structural systems using frequency adaptive spectral functions", *Probabilistic Engineering Mechanics*, 39[1] (2015), pp. 23-38.
- [3] DiazDelaO, F. A., Kundu, A., Adhikari, S. and Friswell, M. I., "A hybrid spectral and metamodeling approach for the stochastic finite element analysis of structural dynamic systems", *Computer Methods in Applied Mechanics and Engineering*, 270[3] (2014), pp. 201-209.
- [4] Kundu, A., Adhikari, S., "Transient response of structural dynamic systems with parametric uncertainty", *ASCE Journal of Engineering Mechanics*, 140[2] (2014), pp. 315-331.
- [5] Kundu, A., Adhikari, S. and Friswell, M. I., "Stochastic finite elements of discretely parametrized random systems on domains with boundary uncertainty", *International Journal for Numerical Methods in Engineering*, 100[3] (2014), pp. 183-221.

Black-box UQ

- [1] Dey, S., Mukhopadhyay, T., Sahu, S. K., Li, G., Rabitz, H. and Adhikari, S., "Thermal uncertainty quantification in frequency responses of laminated composite plates", *Composite Part B*, in press.
- [2] Dey, S., Mukhopadhyay, T., Adhikari, S. Khodaparast, H. H. and Kerfriden, P., "Rotational and ply-level uncertainty in response of composite conical shells", *Composite Structures*, in press.
- [3] Dey, S., Mukhopadhyay, T., Adhikari, S. and Khodaparast, H. H., "Stochastic natural frequency of composite conical shells", *Acta Mechanica*, in press.
- [4] Dey, S., Mukhopadhyay, T., and Adhikari, S., "Stochastic free vibration analyses of composite doubly curved shells - A Kriging model approach", *Composites Part B: Engineering*, 70[3] (2015), pp. 99-112.
- [5] Dey, S., Mukhopadhyay, T., and Adhikari, S., "Stochastic free vibration analysis of angle-ply composite plates - A RS-HDMR approach", *Composite Structures*, 122[4] (2015), pp. 526-536.

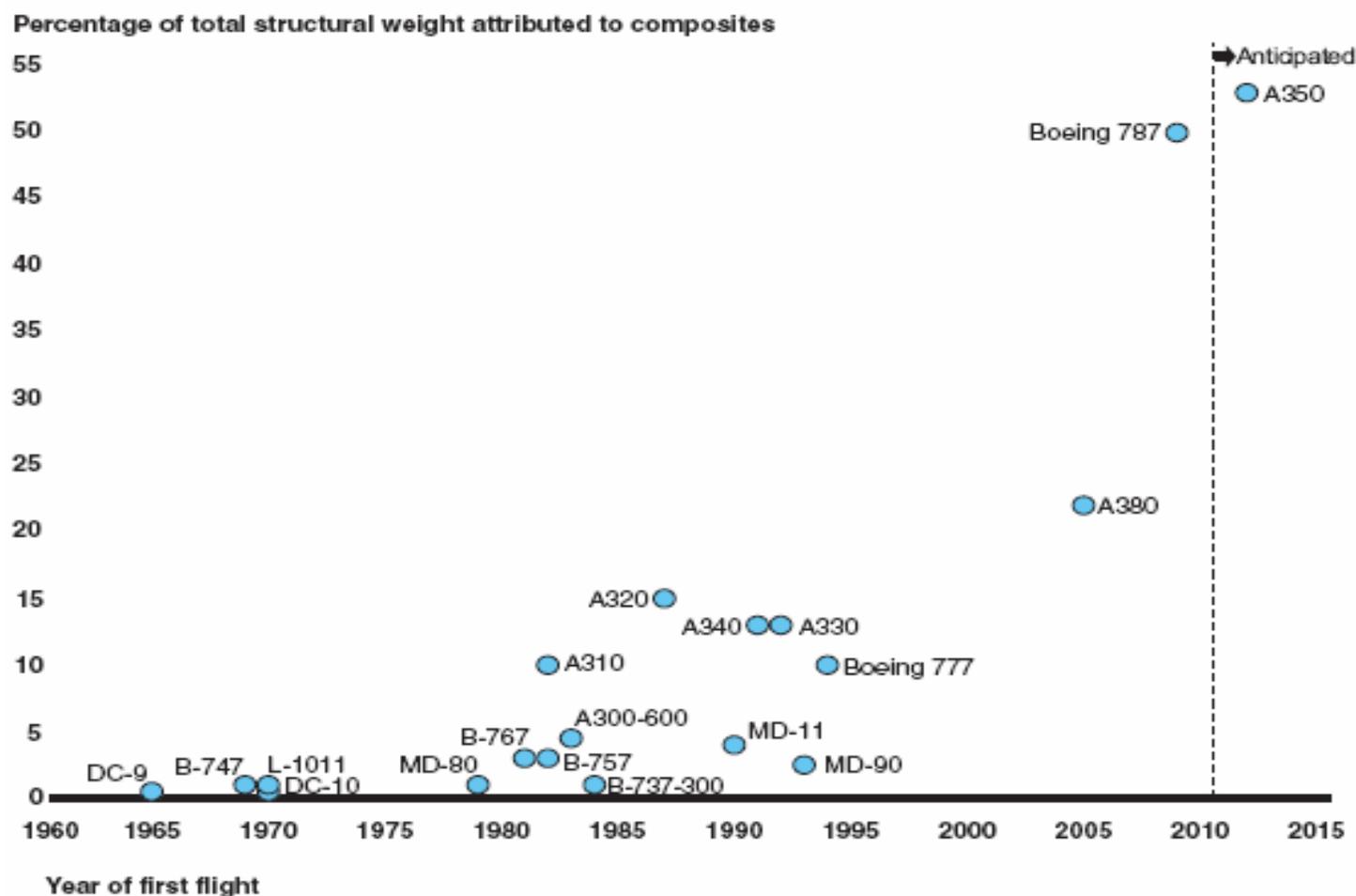


Bottom-up Approach for Composite Structures



Increasing use of composite materials

Figure 1: Commercial Airplane Models over Time by Percentage of Composites



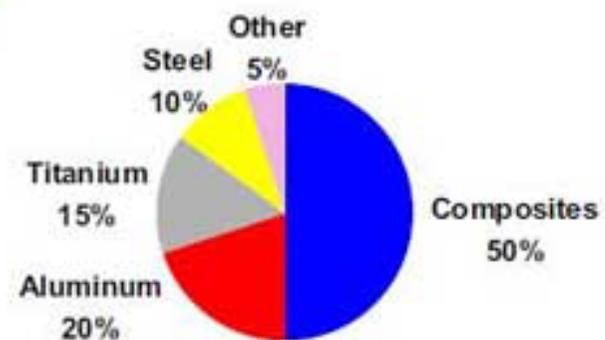
Sources: GAO analysis of information from FAA, NASA, Boeing Company, *Jane's All the World's Aircraft*, and *Jane's Aircraft Upgrades*.



Composites in Boeing 787

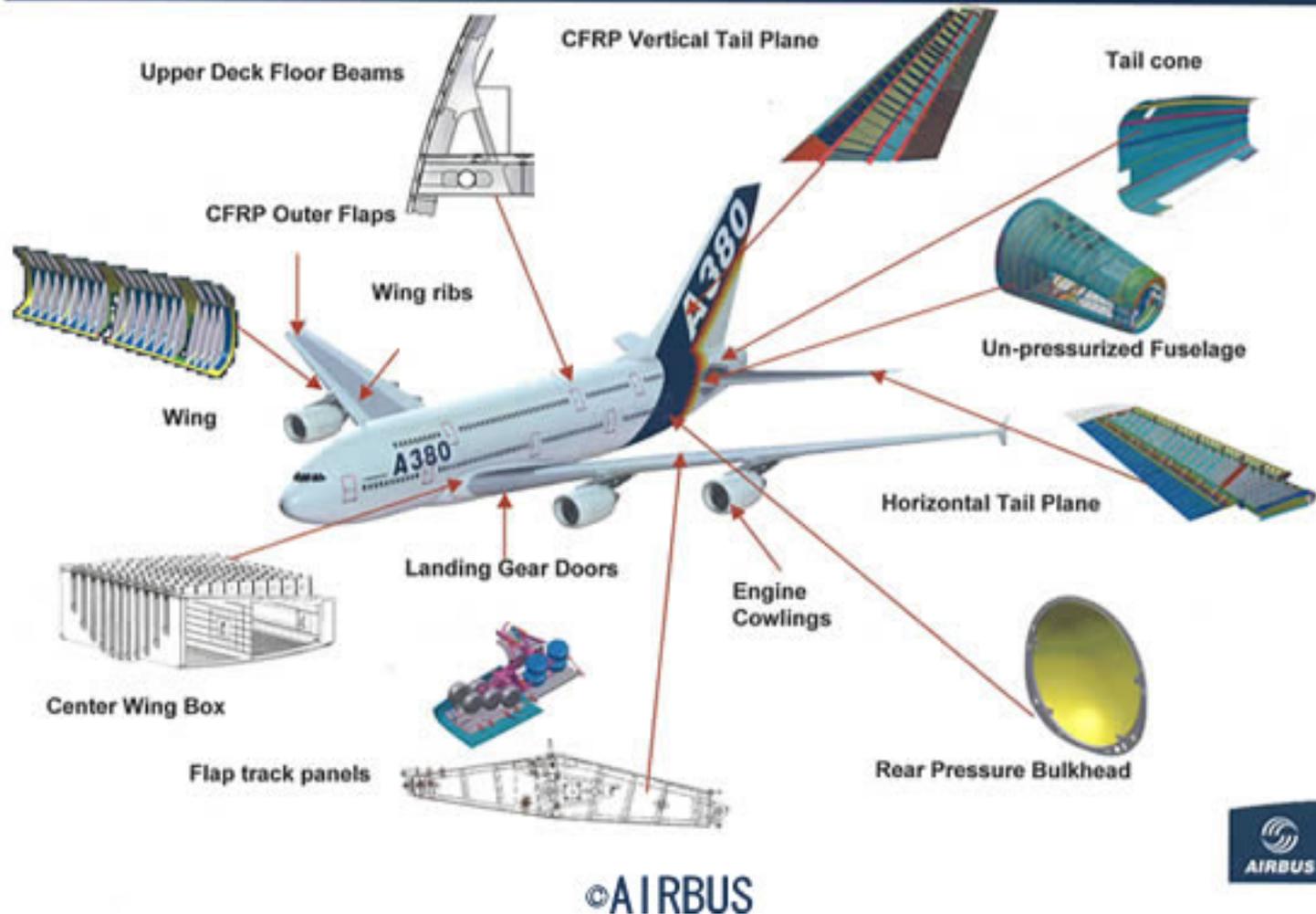


- Carbon laminate
- Carbon sandwich
- Fiberglass
- Aluminum
- Aluminum/steel/titanium pylons

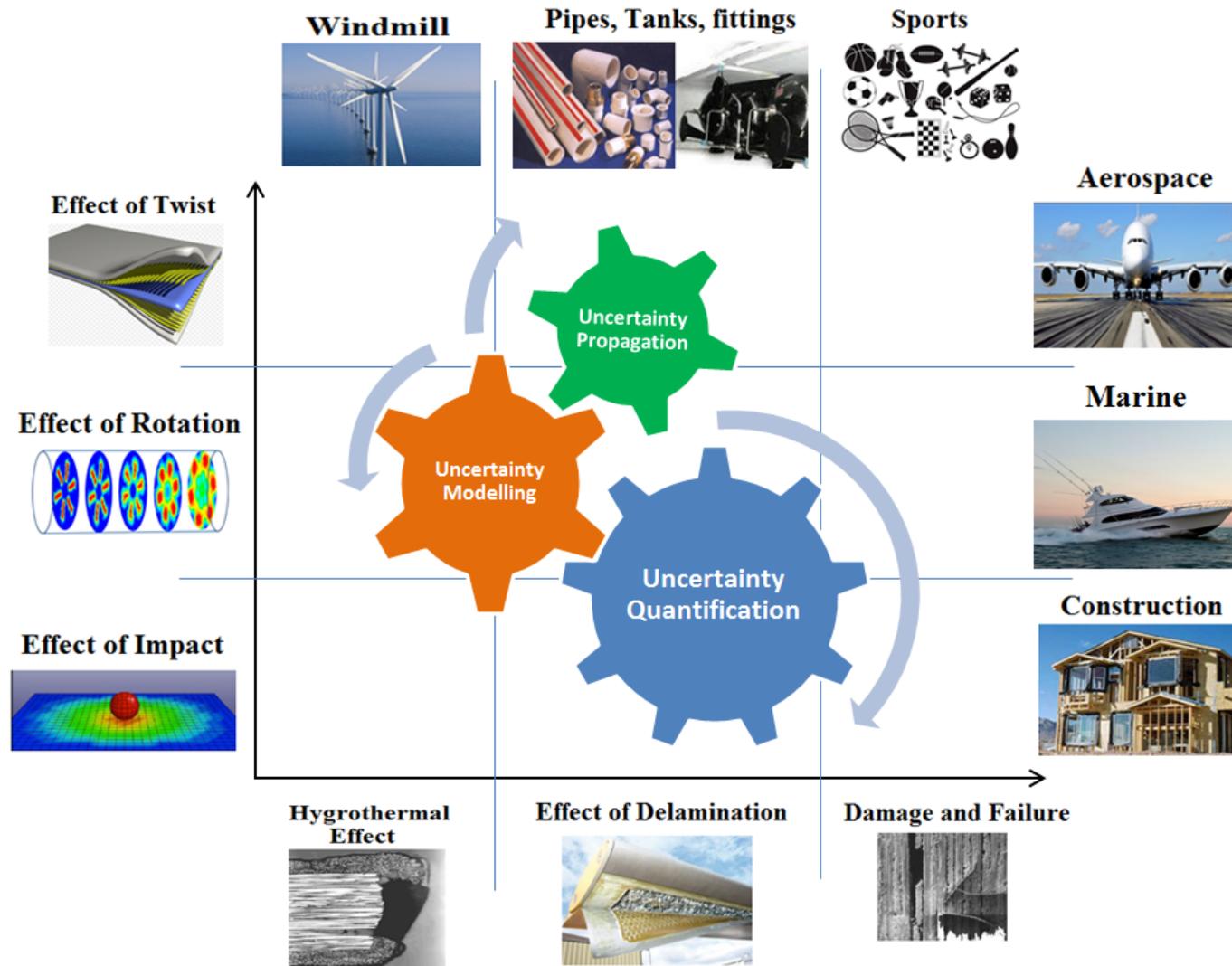


Composites in Airbus A380

Major monolithic Carbon Fiber Reinforced Plastic (CFRP) and Thermoplastics applications



Factors affecting uncertainty in composites



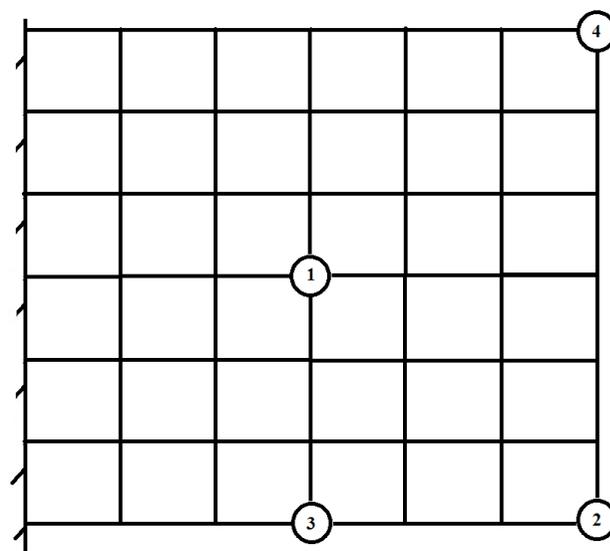
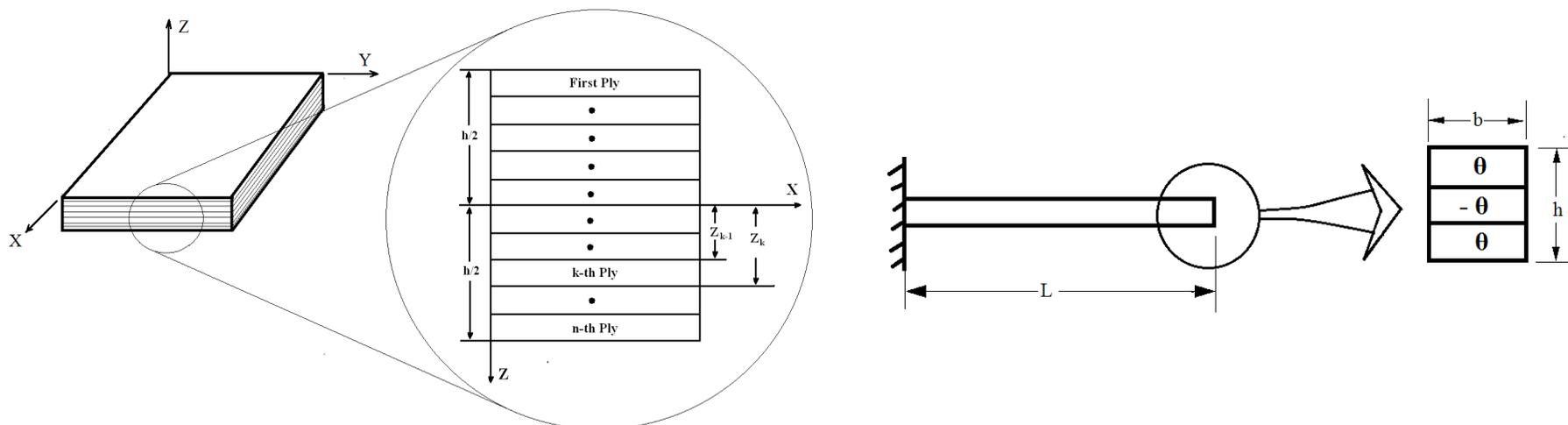


Uncertainty propagation

- The increasing use of composite materials requires more rigorous approach to uncertainty quantification for optimal, efficient and safe design. **Prime sources of uncertainties include:**
 - Material and Geometric uncertainties
 - Manufacturing uncertainties
 - Environmental uncertainties
- Suppose $f(\mathbf{x})$ is a computational intensive multidimensional nonlinear (smooth) function of a vector of parameters \mathbf{x} .
- We are interested in the statistical properties of $y=f(\mathbf{x})$, given the statistical properties of \mathbf{x} .
- The statistical properties include, mean, standard deviation, probability density functions and bounds
- This work develops computational methods for dynamics of composite structures with uncertain parameters by using Finite Element software



Composite Plate Model



Driving point (Point 2) and cross point (Point 1,3,4) for amplitude (in dB) of FRF

Governing Equations

- If mid-plane forms x-y plane of the reference plane, the displacements can be computed as

$$u(x, y, z) = u^0(x, y) - z\theta_x(x, y), \quad v(x, y, z) = v^0(x, y) - z\theta_y(x, y), \quad w(x, y, z) = w^0(x, y) = w(x, y)$$

- The strain-displacement relationships for small deformations can be expressed as

$$\varepsilon_{xx} = \varepsilon_x^0 + zk_x \quad \varepsilon_{yy} = \varepsilon_y^0 + zk_y \quad \gamma_{xy} = \gamma_{xy}^0 + zk_{xy} \quad \gamma_{xz} = w_{,x}^0 - \theta_x \quad \gamma_{yz} = w_{,y}^0 - \theta_y$$

$$\text{where } \varepsilon_x^0 = u_{,x}^0, \quad \varepsilon_y^0 = u_{,y}^0, \quad \gamma_{xy}^0 = u_{,y}^0 + v_{,x}^0$$

$$k_x = -\theta_{x,x} = -w_{,xx} + \gamma_{xz,x} \quad k_y = -\theta_{y,y} = -w_{,yy} + \gamma_{yz,y} \quad k_{xy} = -(\theta_{x,y} + \theta_{y,x}) = -2w_{,xy} + \gamma_{xz,y} + \gamma_{yz,x}$$

- The strains in the k -th lamina: $\{\varepsilon\}^k = \begin{Bmatrix} \varepsilon_x^0 \\ \varepsilon_y^0 \\ \gamma_{xy}^0 \end{Bmatrix} + z \begin{Bmatrix} k_x^0 \\ k_y^0 \\ k_{xy}^0 \end{Bmatrix} = \{\varepsilon^0\} + z\{k\}$ and $\{\gamma\}^k = \begin{Bmatrix} \gamma_{yz} \\ \gamma_{xz} \end{Bmatrix} = \{\gamma\}$

- In-plane stress resultant $\{N\}$, the moment resultant $\{M\}$, and the transverse shear resultants $\{Q\}$ can be expressed

$$\{N\} = [A]\{\varepsilon^0\} + [B]\{k\}, \quad \{M\} = [B]\{\varepsilon^0\} + [D]\{k\}, \quad \{Q\} = [A^*]\{\gamma\}$$

$$\text{where } [A_{ij}^*] = \int_{-h/2}^{h/2} \bar{Q}_{ij} dz \quad \text{where } i, j = 4, 5$$

Bottom Up Approach

All cases consider an eight noded isoparametric quadratic element with five degrees of freedom for graphite-epoxy composite plate / shells

Material properties (Graphite-Epoxy)**: $E_1=138.0$ GPa, $E_2=8.96$ GPa, $G_{12}=7.1$ GPa, $G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\nu=0.3$

$$[\bar{Q}_{ij}(\bar{\omega})] = \begin{bmatrix} m^4 & n^4 & 2m^2n^2 & 4m^2n^2 \\ n^4 & m^4 & 2m^2n^2 & 4m^2n^2 \\ m^2n^2 & m^2n^2 & (m^4 + n^4) & -4m^2n^2 \\ m^2n^2 & m^2n^2 & -2m^2n^2 & (m^2 - n^2) \\ m^3n & mn^3 & (mn^3 - m^3n) & 2(mn^3 - m^3n) \\ mn^3 & m^3n & (m^3n - mn^3) & 2(m^3n - mn^3) \end{bmatrix} [Q_{ij}]$$

$$\{N\} = [A] \{\varepsilon^0\} + [B] \{k\}$$

$$\{M\} = [B] \{\varepsilon^0\} + [D] \{k\}$$

$$m = \text{Sin} \theta(\bar{\omega}) \quad n = \text{Cos} \theta(\bar{\omega})$$

$$\theta(\bar{\omega}) = \text{Random ply orientation angle}$$

$$[D'(\bar{\omega})] = \begin{bmatrix} A_{ij}(\bar{\omega}) & B_{ij}(\bar{\omega}) & 0 \\ B_{ij}(\bar{\omega}) & D_{ij}(\bar{\omega}) & 0 \\ 0 & 0 & S_{ij}(\bar{\omega}) \end{bmatrix}$$

$$[A_{ij}(\bar{\omega}), B_{ij}(\bar{\omega}), D_{ij}(\bar{\omega})] = \sum_{k=1}^n \int_{z_{k-1}}^{z_k} [\bar{Q}_{ij}(\bar{\omega})]_k [1, z, z^2] dz \quad i, j = 1, 2, 6$$

$$[S_{ij}(\bar{\omega})] = \sum_{k=1}^n \int_{z_{k-1}}^{z_k} \alpha_s [\bar{Q}_{ij}(\bar{\omega})]_k dz \quad i, j = 4, 5$$

Equation of Motion and Eigenvalue Problem

- From Hamilton's principle:
$$\delta H = \int_{t_i}^{t_f} [\delta T - \delta U - \delta W] dt = 0$$
- Potential strain energy:
$$U = U_1 + U_2 = \frac{1}{2} \{\delta_e\}^T [K_e(\bar{\omega})] \{\delta_e\} + \frac{1}{2} \{\delta_e\}^T [K_{\sigma_e}(\bar{\omega})] \{\delta_e\}$$
- Kinetic energy:
$$T = \frac{1}{2} \{\dot{\delta}_e\}^T [M_e(\bar{\omega})] + [C_e(\bar{\omega})] \{\delta_e\}$$
- Mass matrix:
$$[M(\bar{\omega})] = \int_{Vol} [N][P(\bar{\omega})][N] d(vol) \quad \text{where } P(\bar{\omega}) = \sum_{k=1}^n \int_{z_{k-1}}^{z_k} \rho(\bar{\omega}) dz$$
- Stiffness matrix:
$$[K(\bar{\omega})] = \int_{-1}^1 \int_{-1}^1 [B(\bar{\omega})]^T [D(\bar{\omega})] [B(\bar{\omega})] d\xi d\eta$$
- Dynamic Equation:
$$[M(\bar{\omega})] \ddot{\delta}(t) + [C] \dot{\delta}(t) + [K(\bar{\omega})] \delta(t) = f(t)$$

For free vibration, the random natural frequencies are determined from the standard eigenvalue problem, solved by the QR iteration algorithm

$$[A(\bar{\omega})] \{\delta\} = \lambda(\bar{\omega}) \{\delta\} \quad \text{where } [A(\bar{\omega})] = ([K_e(\bar{\omega})] + [K_{\sigma_e}(\bar{\omega})])^{-1} [M(\bar{\omega})]$$

$$\lambda(\bar{\omega}) = \frac{1}{\{\omega_n(\bar{\omega})\}^2}$$

Modal Analysis

- The eigenvalues and eigenvectors satisfy the orthogonality relationship

$$\mathbf{x}_i^T [\mathbf{M}(\bar{\omega})] \mathbf{x}_j = \lambda_{ij} \quad \text{and} \quad \mathbf{x}_i^T [\mathbf{K}(\bar{\omega})] \mathbf{x}_j = \omega_j^2 \lambda_{ij} \quad \text{where } 1, j = 1, 2, \dots, n$$

$$\mathbf{X}^T [\mathbf{M}(\bar{\omega})] \mathbf{X} = \mathbf{I} \quad \text{and} \quad \mathbf{X}^T [\mathbf{K}(\bar{\omega})] \mathbf{X} = \Omega^2$$

- Using modal transformation, pre-multiplying by \mathbf{X}^T and using orthogonality relationships, equation of motion of a damped system in the modal coordinates is obtained as

$$\ddot{\mathbf{y}}(t) + \mathbf{X}^T \mathbf{C} \mathbf{X} \dot{\mathbf{y}}(t) + \Omega^2 \mathbf{y}(t) = \tilde{\mathbf{f}}(t)$$

- The damping matrix in the modal coordinate: $\mathbf{C}' = \mathbf{X}^T [\mathbf{C}] \mathbf{X}$
- The generalized proportional damping model expresses the damping matrix as a linear combination of the mass and stiffness matrices

$$\mathbf{C}(\bar{\omega}) = \alpha_1 \mathbf{M}(\bar{\omega}) + \alpha_2 (\mathbf{M}^{-1}(\bar{\omega}) \mathbf{K}(\bar{\omega})) \quad \text{where } \alpha_1 = 0.005 \text{ is constant damping factor}$$

- Transfer function matrix

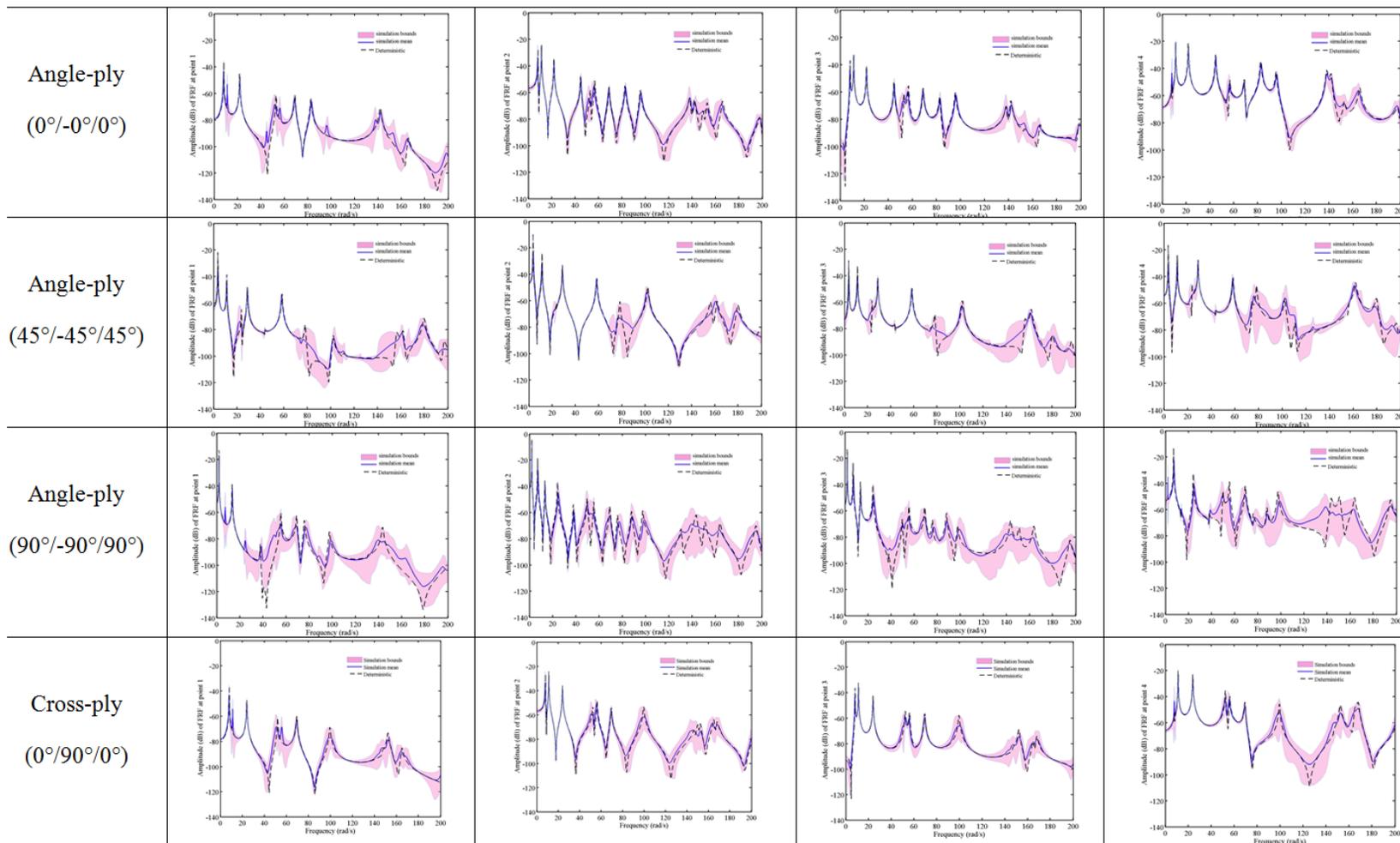
$$\mathbf{H}(i\omega)(\bar{\omega}) = \mathbf{X} [-\omega^2 \mathbf{I} + 2i\omega\boldsymbol{\zeta}\Omega + \Omega^2]^{-1} \mathbf{X}^T = \sum_{j=1}^n \frac{\mathbf{X}_j \mathbf{X}_j^T}{-\omega^2 + 2i\omega\zeta_j\omega_j + \omega_j^2}$$

- The dynamic response in the frequency domain with zero initial conditions:

$$\bar{\boldsymbol{\delta}}(i\omega)(\bar{\omega}) = \mathbf{H}(i\omega) \bar{\mathbf{f}}(i\omega) = \sum_{j=1}^n \frac{\mathbf{X}_j^T \bar{\mathbf{f}}(i\omega)}{-\omega^2 + 2i\omega\zeta_j\omega_j + \omega_j^2} \mathbf{X}_j$$

Amplitude (dB) Vs Frequency (rad/s)

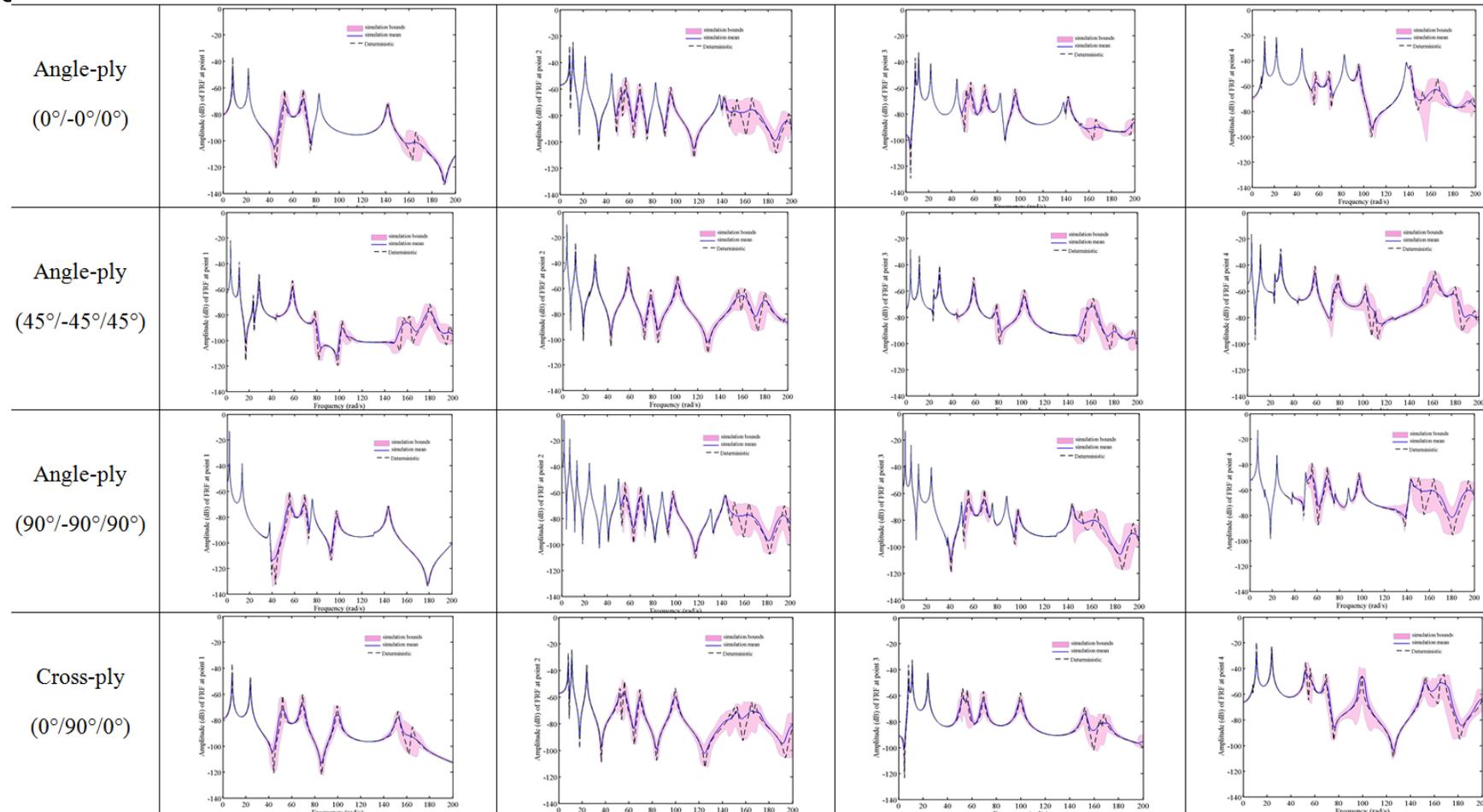
Variation of only ply-orientation angle (+/- 5 degrees) in each layer to plot the direct simulation bounds, direct simulation mean and deterministic values for amplitude (dB) with respect to frequency (rad/s) of points 1, 2, 3 and 4 considering graphite-epoxy composite laminated plate with $L=b=1$ m, $h=0.004$ m, $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\rho=1600$ Kg/m³, $\nu=0.3$.





Amplitude (dB) Vs Frequency (rad/s)

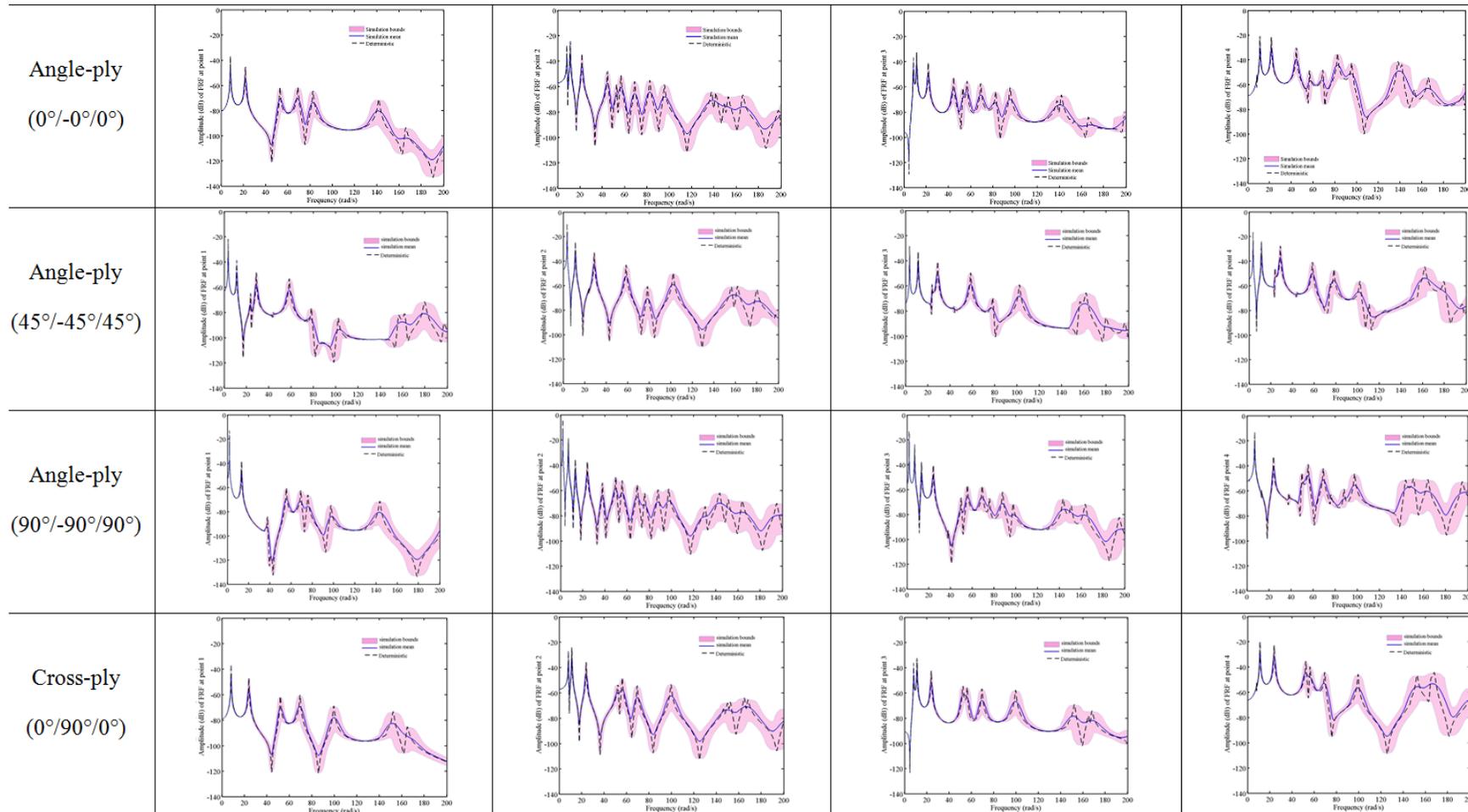
Variation of only elastic modulus (+/- 10%) in each layer to plot the direct simulation bounds, direct simulation mean and deterministic values for amplitude (dB) with respect to frequency (rad/s) of points 1, 2, 3 and 4 considering graphite-epoxy composite laminated plate with $L=b=1$ m, $h=0.004$ m, $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\rho=1600$ Kg/m³ $\nu=0.3$





Amplitude (dB) Vs Frequency (rad/s)

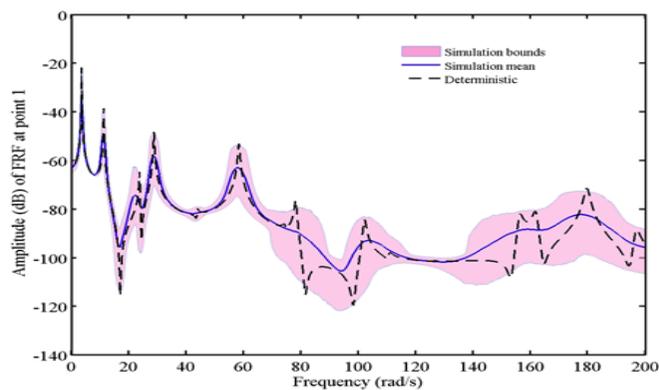
Variation of only mass density (+/- 10%) in each layer to plot the direct simulation bounds, direct simulation mean and deterministic values for amplitude (dB) with respect to frequency (rad/s) of points 1, 2, 3 and 4 considering graphite-epoxy composite laminated plate with $L=b=1$ m, $h=0.004$ m, $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\rho=1600$ Kg/m³, $\nu=0.3$.



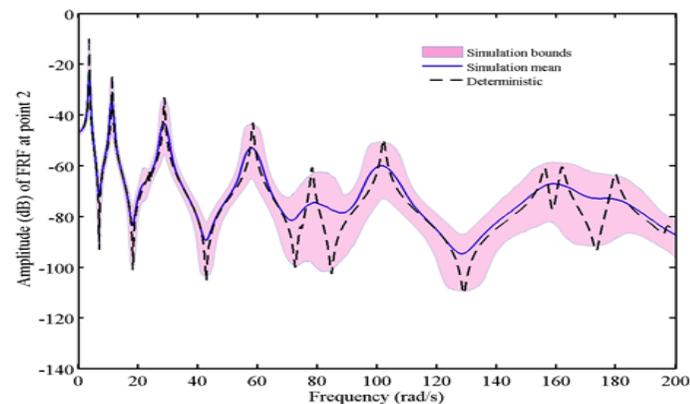


Combined Variation – Monte Carlo Simulation

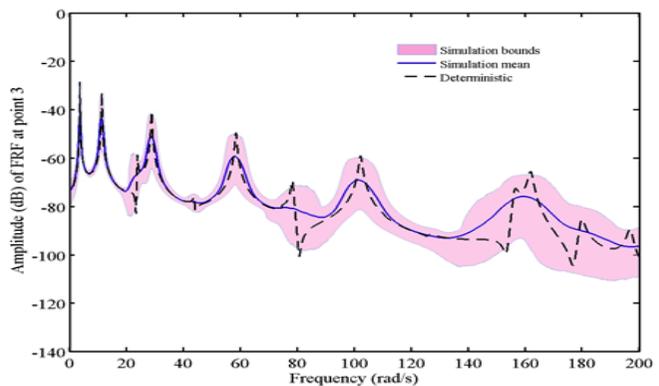
Combined variation of ply orientation angle, elastic modulus and mass density in each layer for the direct simulation bounds, direct simulation mean and deterministic values for the points of point 1, 2, 3 and 4 considering graphite-epoxy angle-ply ($45^\circ/-45^\circ/45^\circ$) composite laminated plate considering $L=b=1$ m, $h=0.004$ m, $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\nu=0.3$



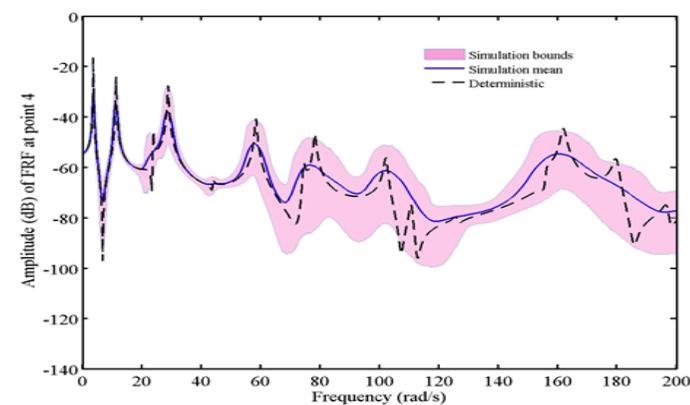
(a)



(b)



(c)



(d)



Uncertainty Quantification of Composites

- ❑ The bottom up approach is employed to quantify the volatility in natural frequency due to uncertainty in ply orientation angle, elastic modulus and mass density of the composite laminate.
- ❑ Monte Carlo Simulation is an expensive computational method for Uncertainty Quantification.
- ❑ If the model is “big”, this cost has cascading effect on the increase of cost of computation.
- ❑ To save computational iteration time and cost, the following metamodels are investigated:
 - 1) **Random Sampling-High Dimensional Model Representation (RS-HDMR)**
 - 2) **D-Optimal Design**
 - 3) **Kriging model**
 - 4) **Central composite Design (CCD) model**
 - 5) **General high dimensional model representation (GHDMR)**
- ❑ These metamodels can be employed to any such stochastic applications.



Random Sampling – High Dimensional Model Representation (RS-HDMR)

Random Sampling – High Dimensional Model Representation (RS-HDMR) Model

The mapping between the input variables x_1, x_2, \dots, x_n and the output $f(X) = f(x_1, x_2, \dots, x_n)$ in the domain R^n can be expressed in the following form:

$$f(X) = \underbrace{f_0}_{\text{constant term}} + \underbrace{\sum_{i=1}^n f_i(x_i)}_{\text{first order}} + \underbrace{\sum_{1 \leq i < j \leq n} f_{ij}(x_i, x_j)}_{\text{second order}} + \dots + f_{12\dots n}(x_1, x_2, \dots, x_n)_{n^{\text{th order}}$$

- Use of orthonormal polynomial for the computation of RS-HDMR component functions:

$$f_i(x_i) \approx \sum_{r=1}^k \alpha_r^i \varphi_r(x_i)$$

$$f_{ij}(x_i, x_j) \approx \sum_{p=1}^l \sum_{q=1}^{l'} \beta_{pq}^{ij} \varphi_p(x_i) \varphi_q(x_j)$$

- **Check for Coefficient of determination (R^2) and Relative Error (RE):**

$$R^2 = \frac{SS_R}{SS_T} = 1 - \frac{SS_E}{SS_T} \quad (0 \leq R^2 \leq 1)$$

$$RE(\%) = \frac{|F - F'|}{F} \times 100$$

where, $SS_T = SS_E + SS_R$



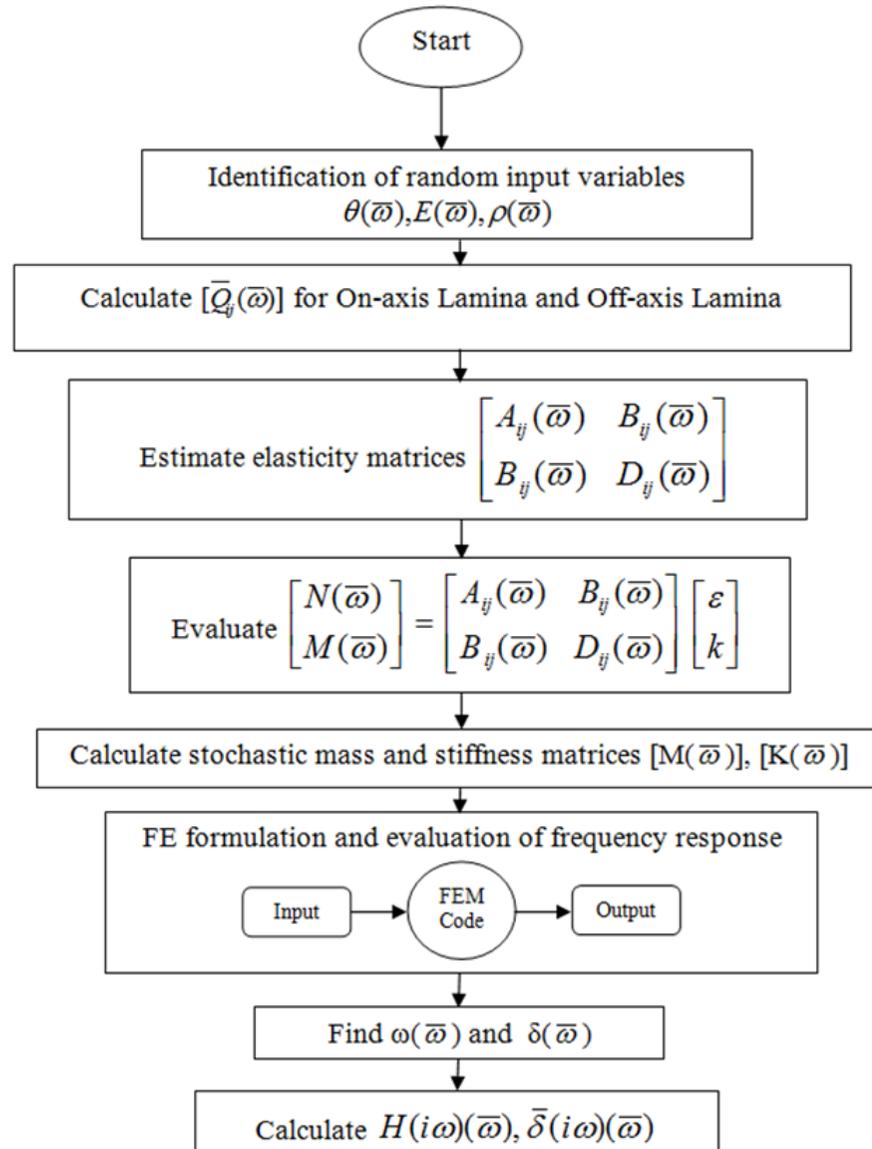
Global Sensitivity Analysis based on RS-HDMR

- The orthogonal relationship between the component functions of **Random Sampling – High Dimensional Model Representation (RS-HDMR)** expression implies that the component functions are independent and contribute their effects independently to the overall output response.
- Sensitivity Index

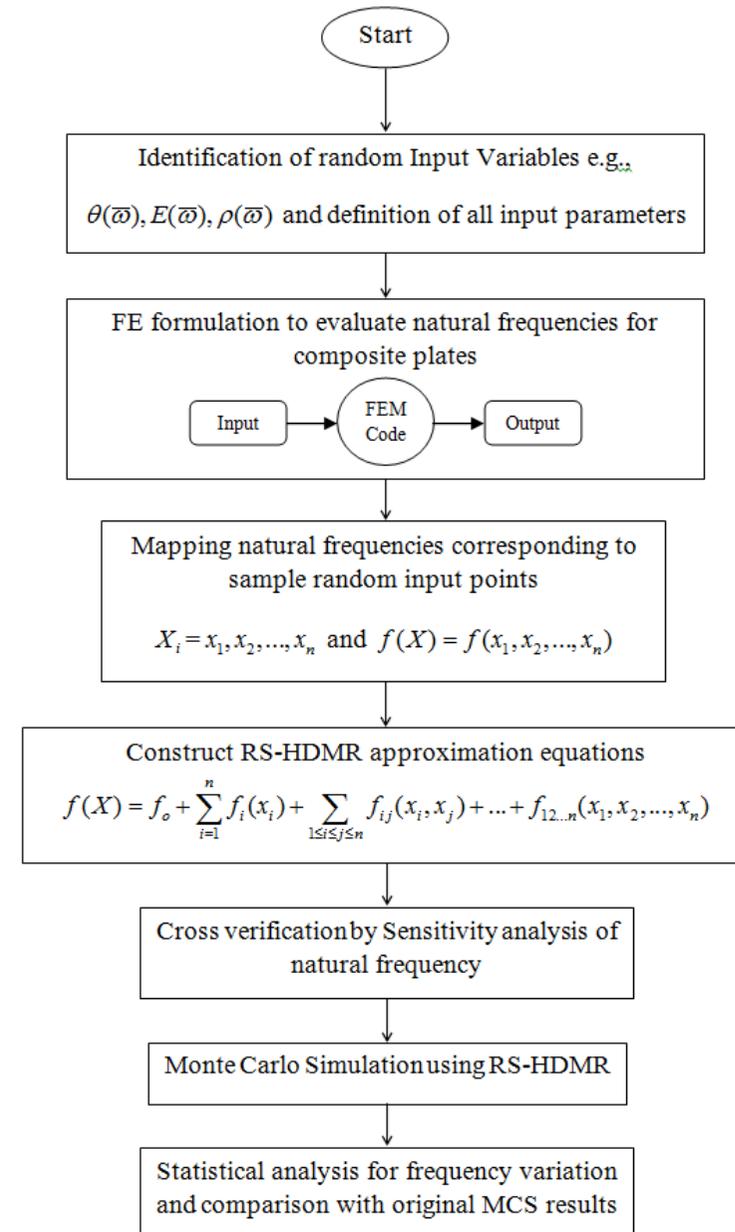
Sensitivity index an input parameter (S_i) = $\frac{\text{partial variance of the input parameter}}{\text{total variance}}$

$$\text{Such that, } \sum_{i=1}^n S_i + \sum_{1 \leq i < j \leq n} S_{ij} + \dots + S_{1,2,\dots,n} = 1$$

Monte Carlo Simulation



Random Sampling – High Dimensional Model Representation (RS-HDMR) Model





Validation – Random Sampling – High Dimensional Model Representation (RS-HDMR) Model

Figure : Probability distribution function (PDF) with respect to model response of first three natural frequencies for variation of ply-orientation angle of graphite-epoxy angle-ply (45°/-45°/45°) composite cantilever plate, considering $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\rho=1600$ Kg/m³, $t=0.004$ m, $\nu=0.3$

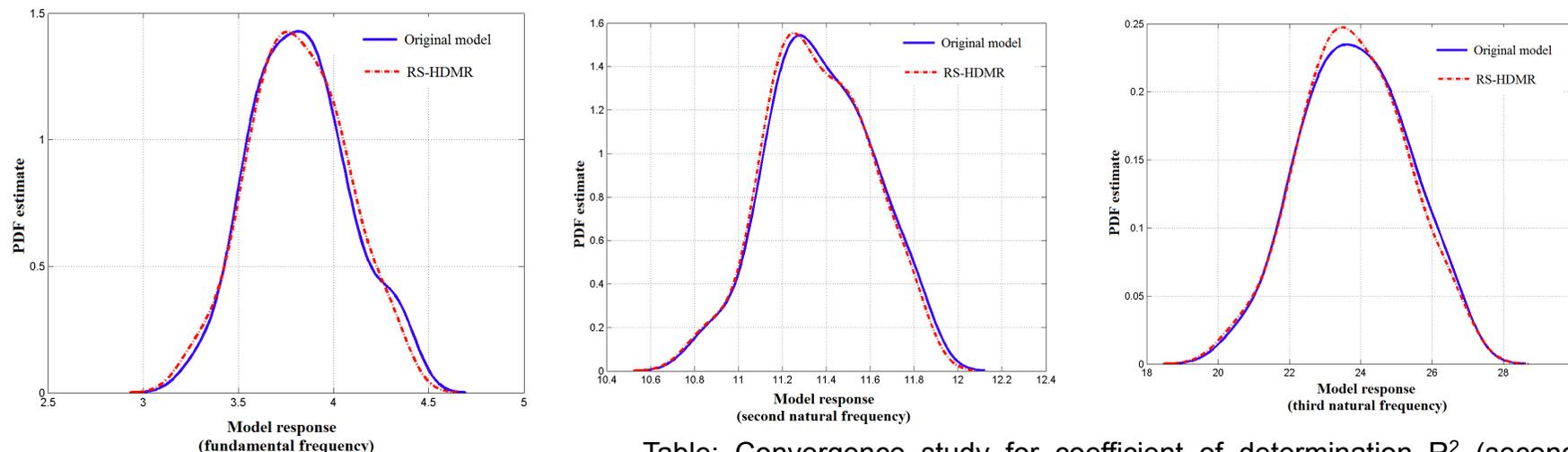


Figure: Scatter plot for fundamental frequencies for variation of ply-orientation angle of angle-ply (45°/-45°/45°) composite cantilever plate

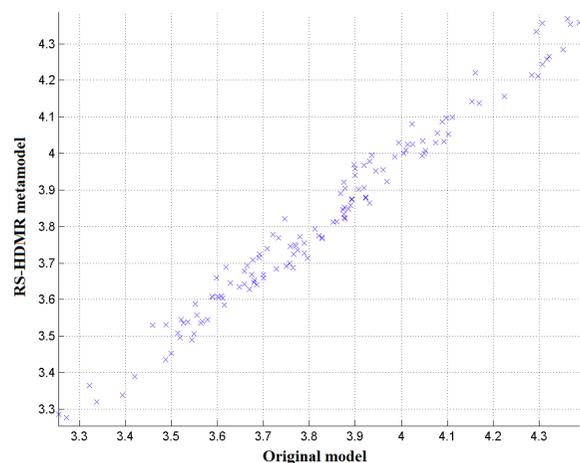


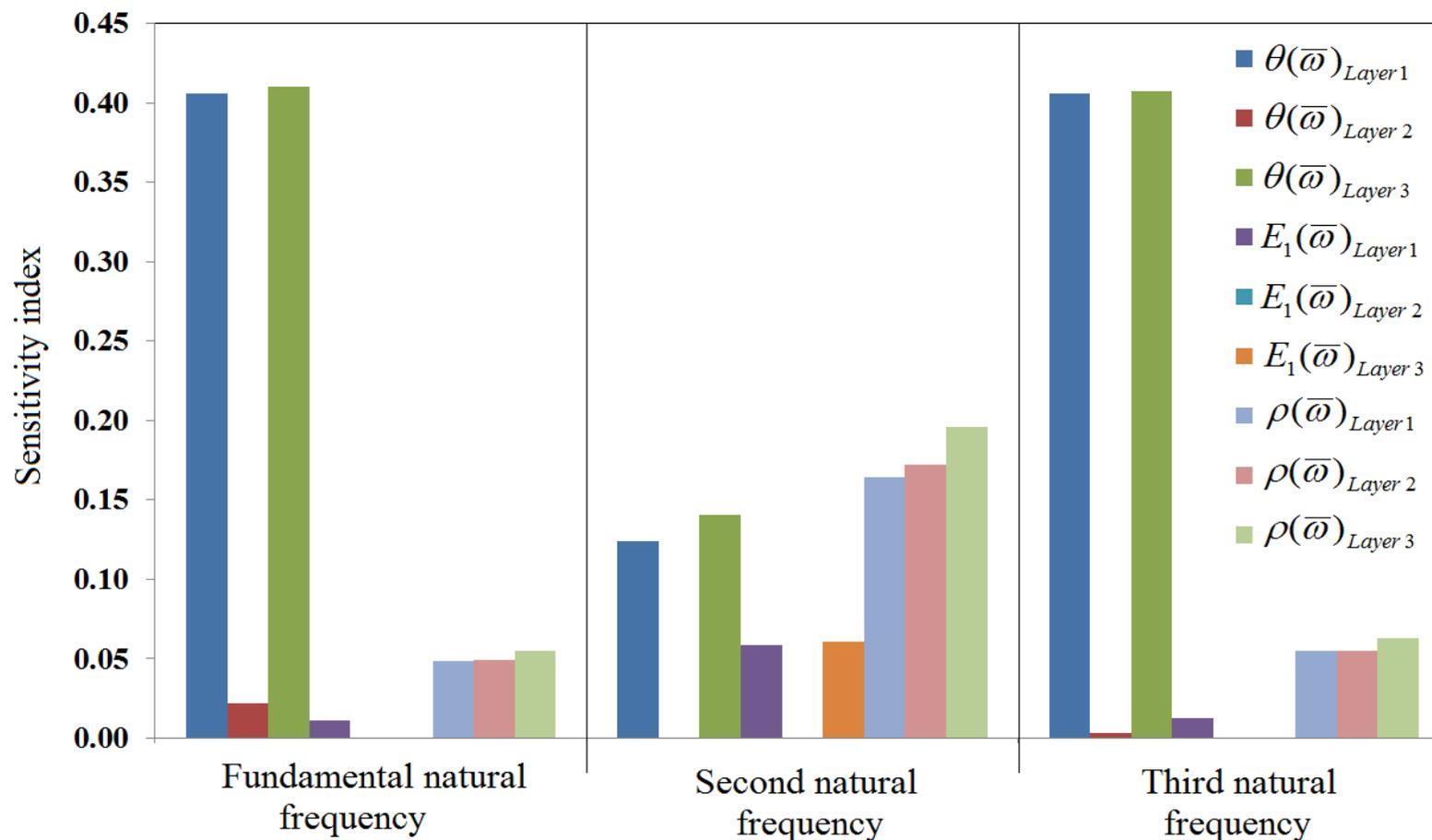
Table: Convergence study for coefficient of determination R^2 (second order) of the RS-HDMR expansions with different sample sizes for variation of only ply-orientation angle of graphite-epoxy angle-ply (45°/-45°/45°) composite cantilever plate, considering $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $t=0.004$ m, $\nu=0.3$

Frequency	Sample Size				
	32	64	128	256	512
FF	65.68	93.48	99.60	99.95	99.96
SF	69.67	93.74	99.47	96.38	97.81
TF	66.44	97.85	99.40	98.86	99.61



Sensitivity Analysis

Figure: Sensitivity index for combined variation (10,000 samples) of ply-orientation angle, elastic modulus and mass density for graphite-epoxy angle-ply (45°/-45°/45°) composite cantilever plate, considering $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\rho=1600$ Kg/m³, $t=0.004$ m, $\nu=0.3$





D-Optimal Design Model



D-Optimal Design Model

On the basis of statistical and mathematical analysis RSM gives an approximate equation which relates the input features ξ and output features y for a particular system.

$$y = f(\xi_1, \xi_2, \dots, \xi_k) + \varepsilon$$

where ε is the statistical error term.

$$Y = X\beta + \varepsilon, \quad X \text{ denotes the design matrix}$$

where,

$$\beta = (X^T X)^{-1} X^T Y$$

D-optimality is achieved if the determinant of $(X^T X)^{-1}$ is minimal

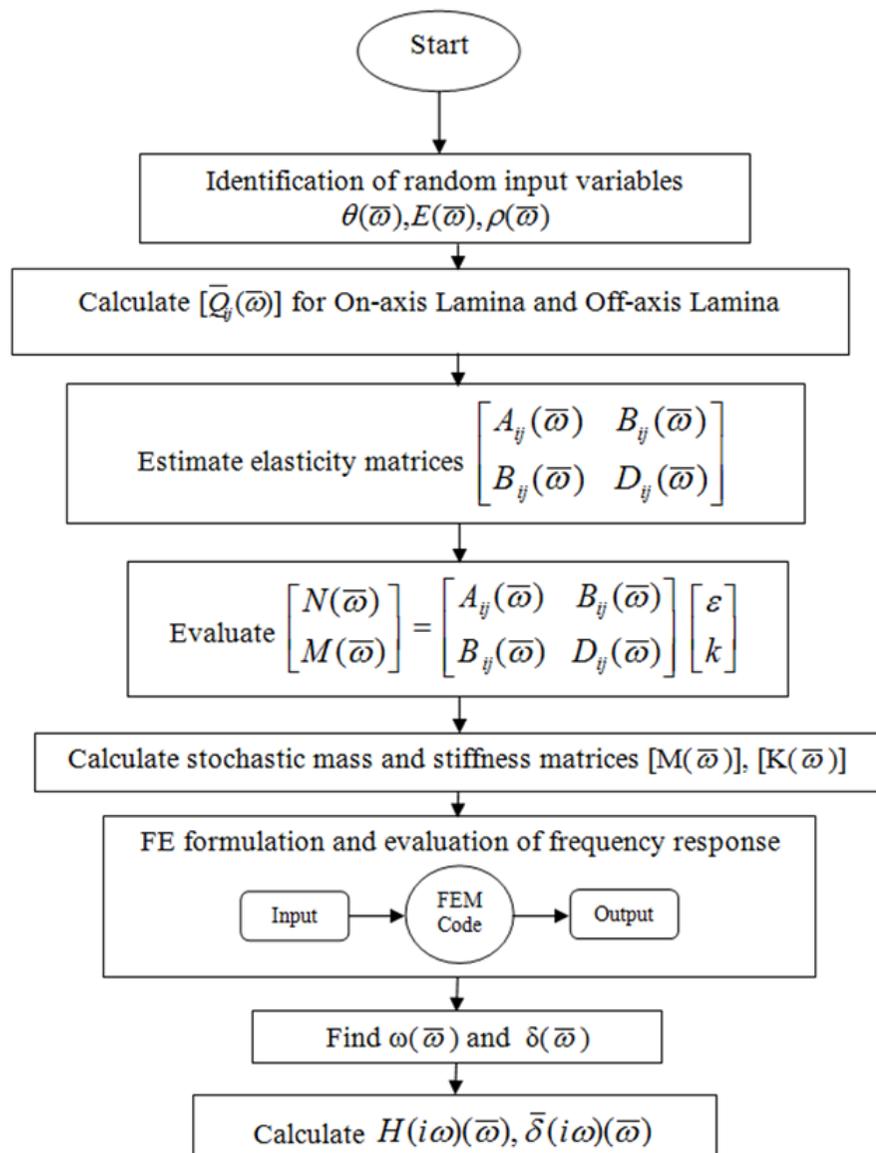
Check for quality of constructed model: R^2 , R_{adj}^2 , R_{pred}^2

$$R^2 = \left(\frac{SS_R}{SS_T} \right) = 1 - \left(\frac{SS_E}{SS_T} \right) \quad \text{where } 0 \leq R^2 \leq 1$$

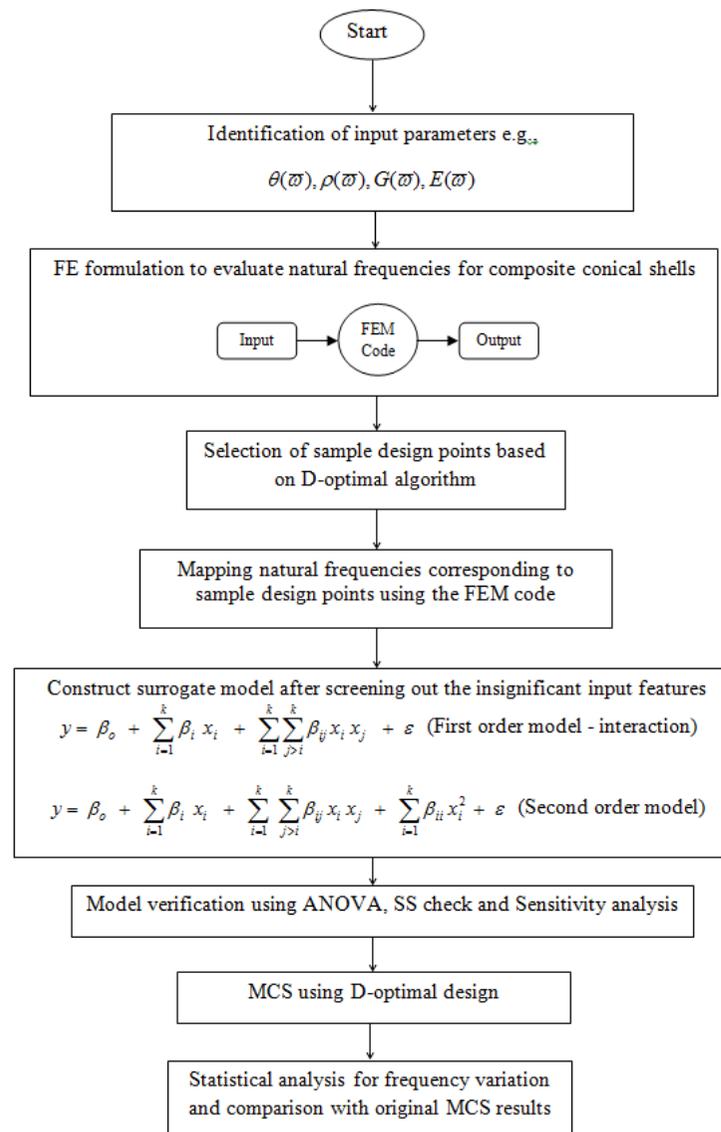
$$R_{adj}^2 = 1 - \frac{\left(\frac{SS_E}{n-k-1} \right)}{\left(\frac{SS_T}{n-1} \right)} = 1 - \left(\frac{n-1}{n-k-1} \right) (1 - R^2) \quad \text{where } 0 \leq R_{adj}^2 \leq 1$$

$$R_{pred}^2 = 1 - \left(\frac{PRESS}{SS_T} \right) \quad \text{where } 0 \leq R_{pred}^2 \leq 1$$

MCS Model



D-Optimal Design Model





Validation – D-optimal

Probability density function obtained by original MCS and D-optimal design with respect to first three natural frequencies indicating for combined variation of mass density, longitudinal shear modulus, Transverse shear modulus and longitudinal elastic modulus for graphite-epoxy angle-ply ($45^\circ/-45^\circ/-45^\circ/45^\circ$) composite conical shells, considering sample size=10,000, $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\rho=1600$ kg/m³, $t=0.002$ m, $\nu=0.3$, $L_0/s=0.7$, $\theta = 45^\circ$, $\phi = 20^\circ$

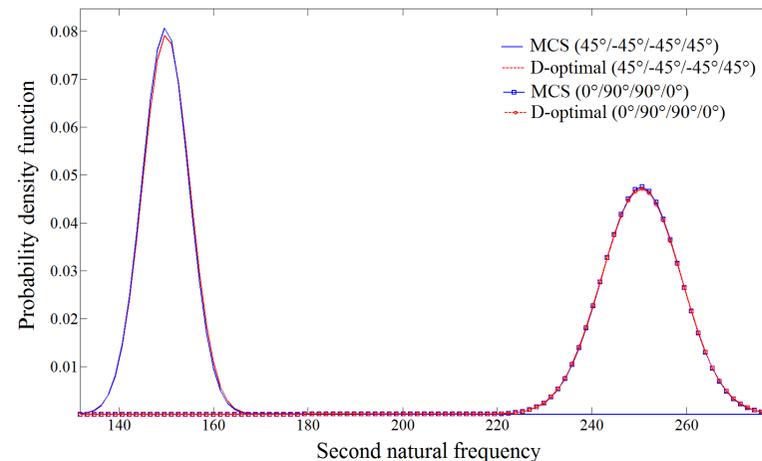
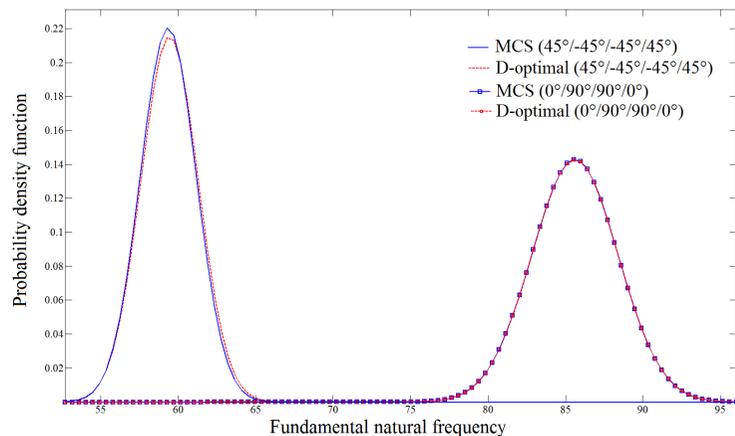
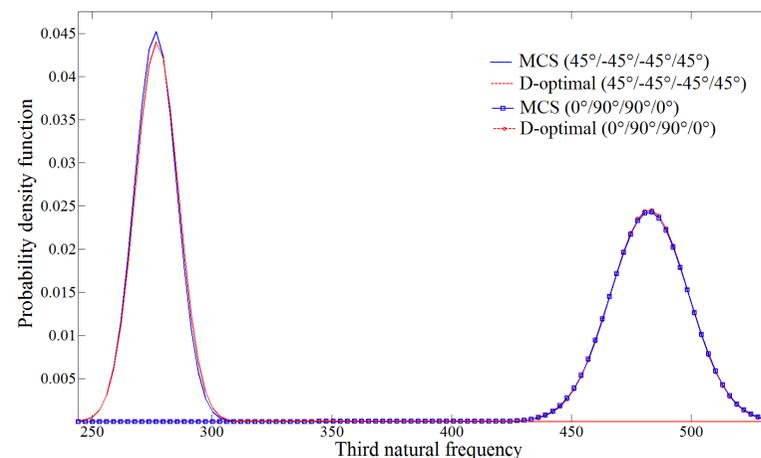
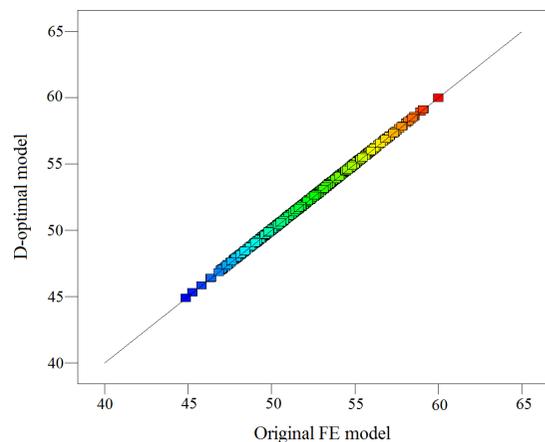


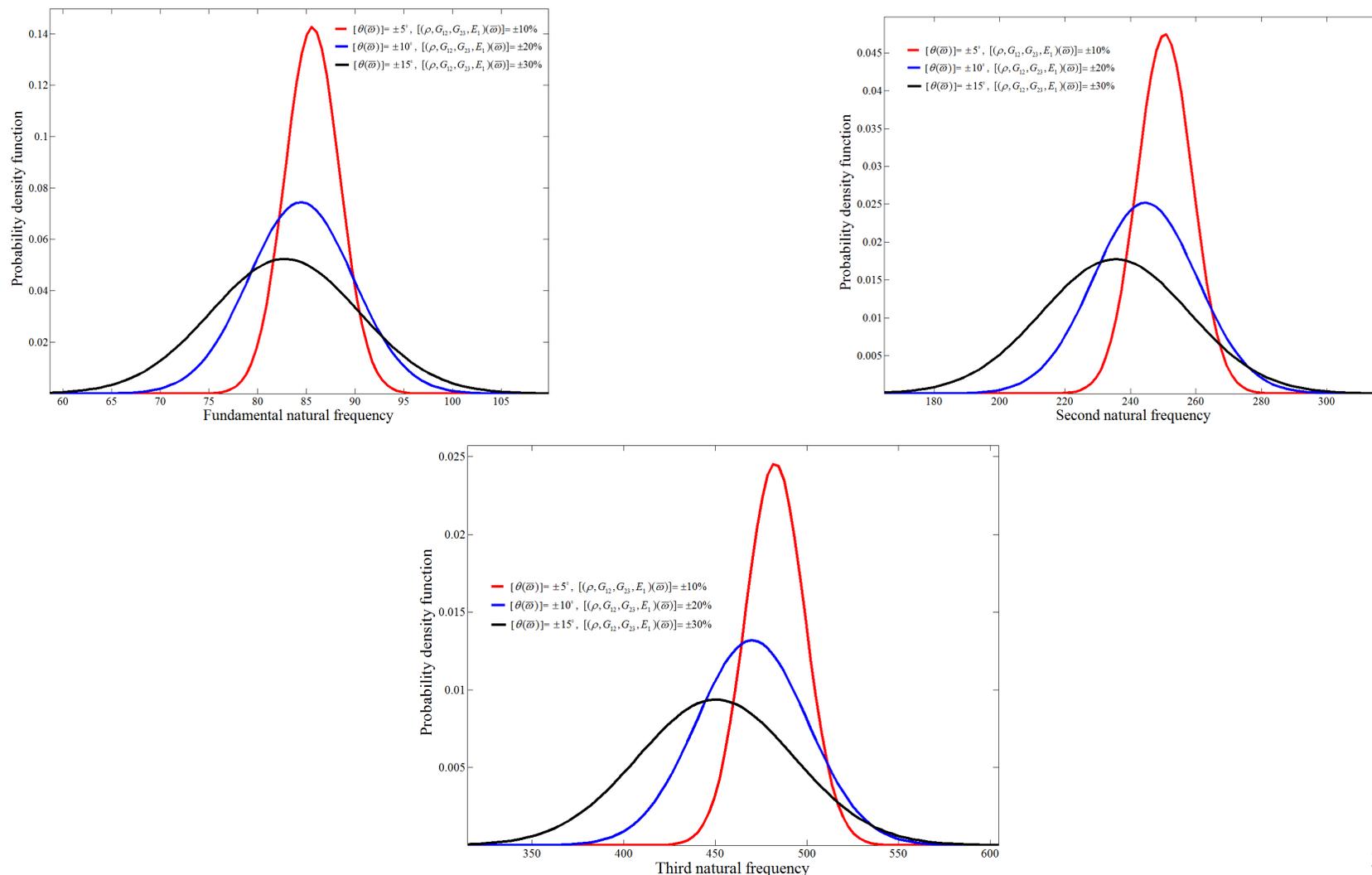
Figure: D-optimal design model with respect to original FE model of fundamental natural frequencies for variation of only ply-orientation angle of angle-ply ($45^\circ/-45^\circ/-45^\circ/45^\circ$) composite cantilever conical shells





Combined Variation

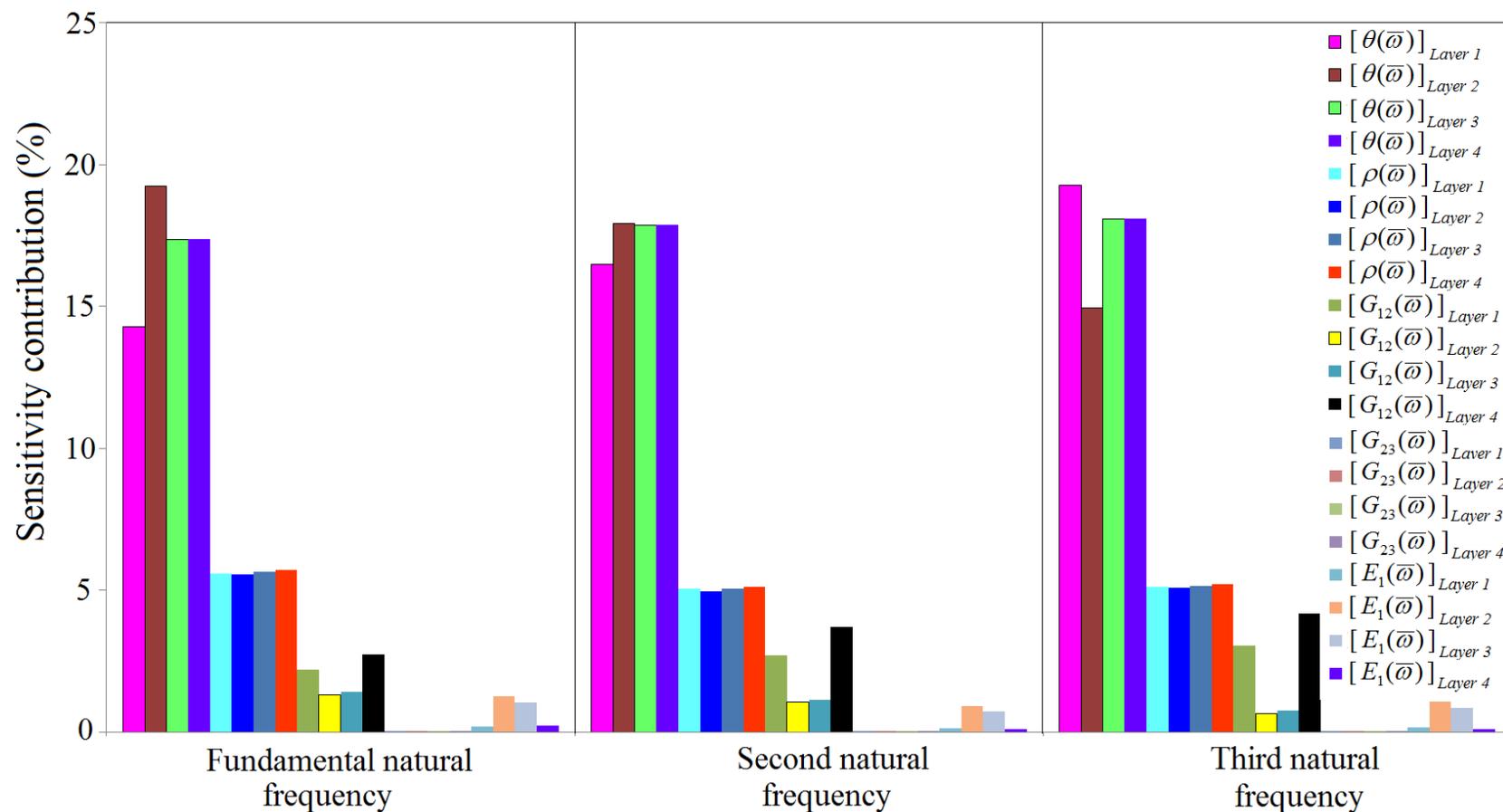
Figure: Probability density function with respect to first three natural frequencies due to combined variation for cross-ply ($0^\circ/90^\circ/90^\circ/0^\circ$) conical shells considering sample size=261, $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\rho=1600$ kg/m³, $t=0.002$ m, $\nu=0.3$, $L_0/s=0.7$, $\alpha = 45^\circ$, $\beta = 20^\circ$.





Sensitivity – Angle-ply

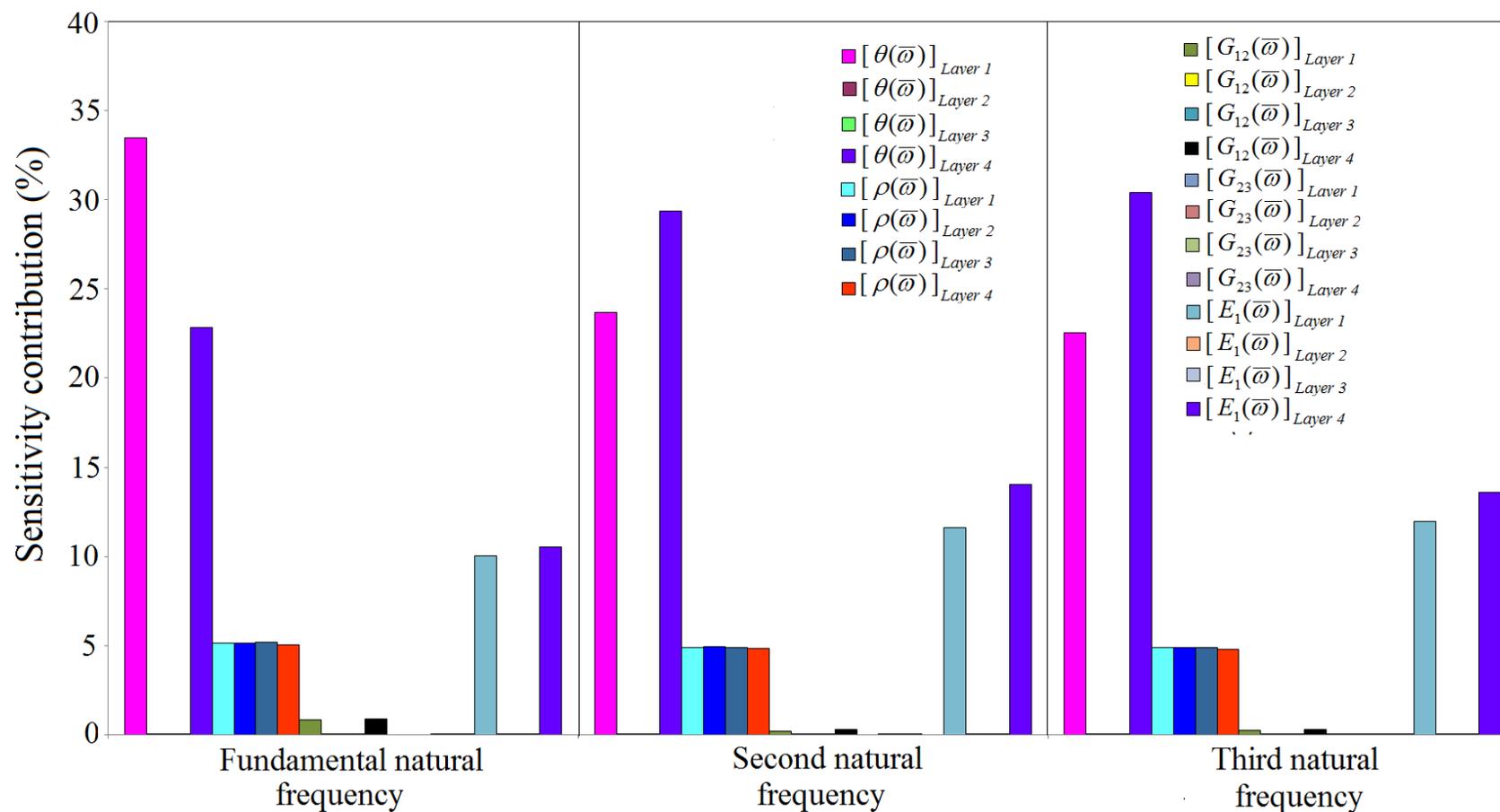
Sensitivity contribution in percentage for **combined variation in ply orientation angle, mass density, longitudinal shear modulus, Transverse shear modulus and longitudinal elastic modulus** for four layered graphite-epoxy **angle-ply (45°/45°/45°/45°)** composite conical shells, considering sample size=261, $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\rho=1600$ kg/m³, $t=0.002$ m, $\nu=0.3$, $L_0/s=0.7$, $\alpha = 45^\circ$, $\beta = 20^\circ$





Sensitivity – Cross-ply

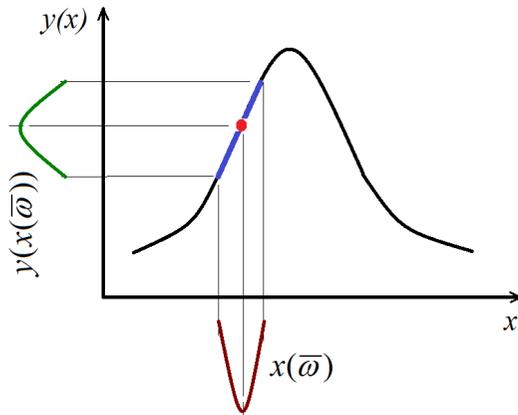
Sensitivity contribution in percentage for **combined variation in ply orientation angle, mass density, longitudinal shear modulus, Transverse shear modulus and longitudinal elastic modulus** for four layered graphite-epoxy **cross-ply (0°/90°/90°/0°)** composite conical shells, considering sample size=261, $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\rho=1600$ kg/m³, $t=0.002$ m, $\nu=0.3$, $L_0/s=0.7$, $\alpha = 45^\circ$, $\beta = 20^\circ$





Kriging Model

Kriging Model



- Kriging model for simulation of required output $y(x) = y_0(x) + Z(x)$

Where $y(x)$ is the unknown function of interest, x is an m dimensional vector (m design variables), $y_0(x)$ is the known approximation (usually polynomial) function and $Z(x)$ represents is the realization of a stochastic process with mean zero, variance, and nonzero covariance.

- Kriging predictor: $\hat{y}(x) = \hat{\beta} + r^T(x) R^{-1} [y - f \hat{\beta}]$

$$\hat{\beta} = (f^T R^{-1} f)^{-1} f^T R^{-1} y$$

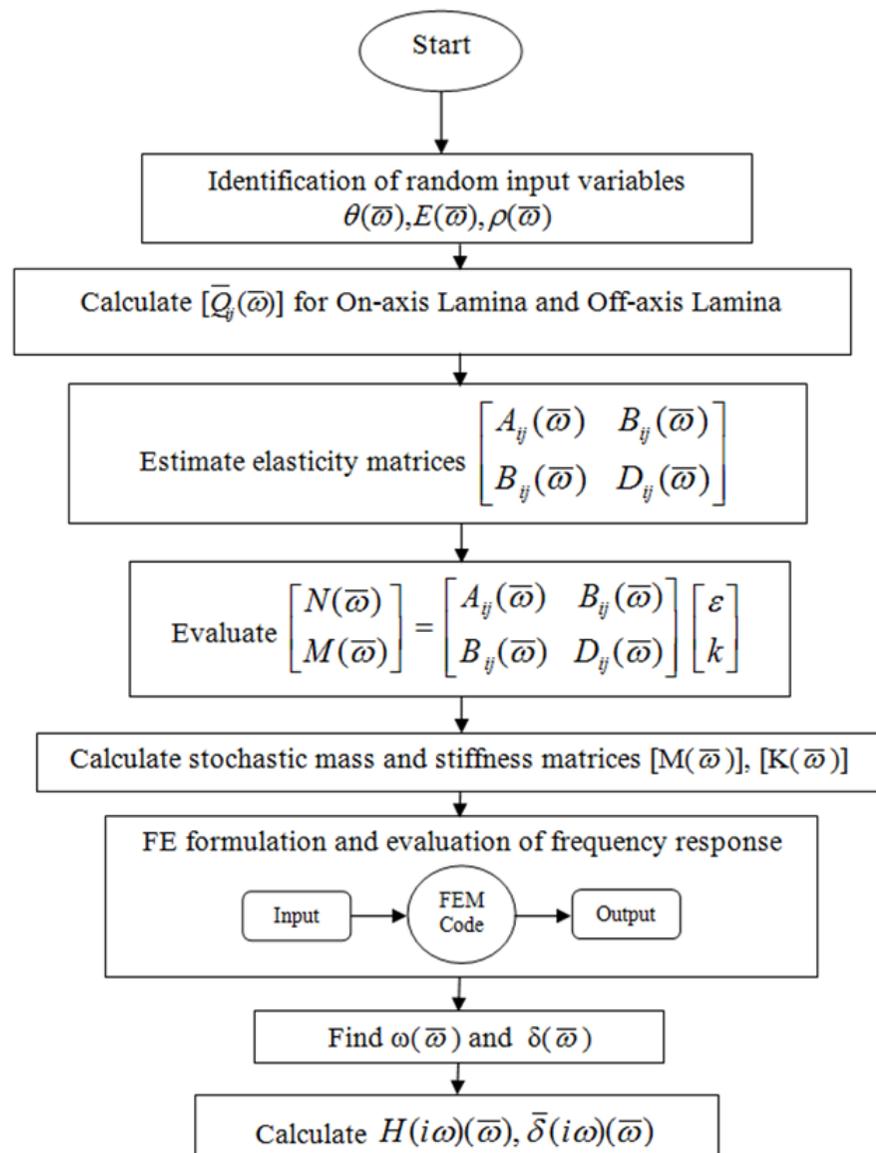
where y is the column vector of length p that contains the sample values of the frequency responses and f is a column vector of length p that is filled with ones when $y_0(x)$ is taken as constant. $r^T(x)$ is the correlation vector of length p between the random x and the sample data points $\{x^1, x^2, \dots, x^p\}$ and R is correlation matrix.

- **Check for maximum error (ME) and maximum mean square error (MMSE):**

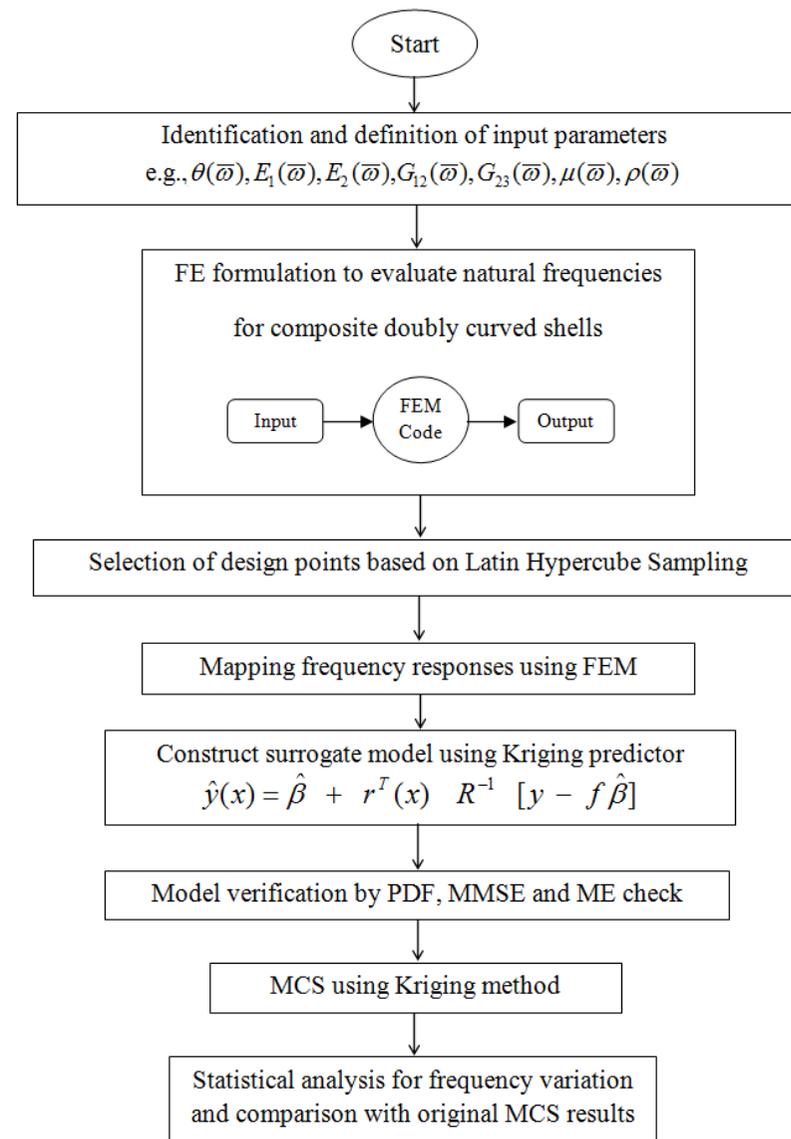
$$ME (\%) = \text{Max} \left[\frac{y_{i,MCS} - y_{i,Kriging}}{Y_{i,MCS}} \right] \quad MMSE = \max \left[\frac{1}{k} \sum_{i=1}^k (\bar{y}_i - y_i)^2 \right]$$

where y_i and \bar{y}_i are the vector of the true values and the vector corresponding to i -th prediction, respectively.

MCS Model



Kriging Model





Validation – Kriging Model

Table: Non-dimensional fundamental frequencies $[\omega = \omega_n a^2 \sqrt{(12 \rho (1 - \mu^2) / E_1 t^2)}a/b=1$, $a'/a=1$, $a/t = 100$, $a/R = 0.5$, $\mu = 0.3$

R_x/R_y	Shell Type	Present FEM	Leissa and Narita [48]	Chakravorty et al. [39]
1	Spherical	50.74	50.68	50.76
-1	Hyperbolic paraboloid	17.22	17.16	17.25

Figure: Scatter plot for Kriging model for combined variation of ply orientation angle, longitudinal elastic modulus, transverse elastic modulus, longitudinal shear modulus, Transverse shear modulus, Poisson's ratio and mass density for composite cantilevered spherical shells

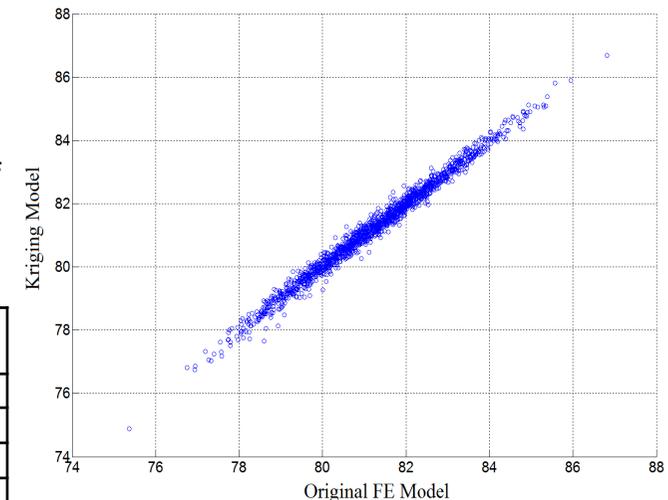


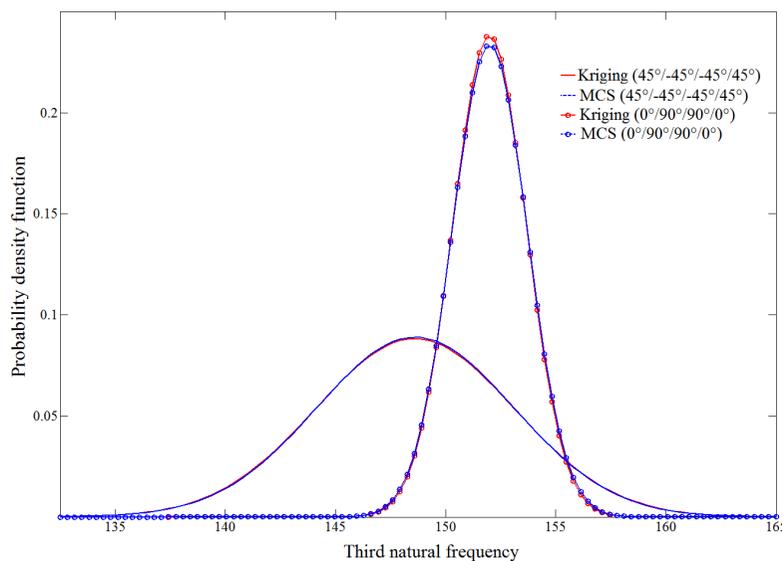
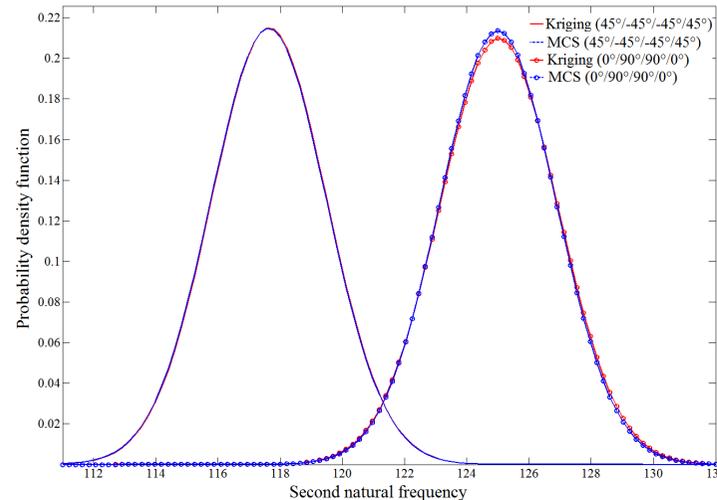
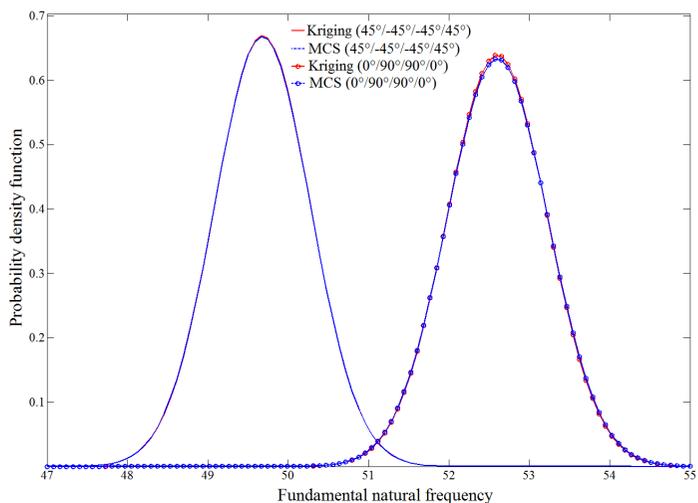
Table: Convergence study for maximum mean square error (MMSE) and maximum error (in percentage) using Kriging model compared to original MCS with different sample sizes for combined variation of 28 nos. input parameters of graphite-epoxy angle-ply (45°/-45°/-45°/45°) composite cantilever spherical shells, considering $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $t=0.005$ m, $\mu=0.3$

Sample size	Parameter	Fundamental frequency	Second natural frequency	Third natural frequency
450	MMSE	0.0289	0.1968	0.2312
	Max Error (%)	2.4804	7.6361	6.5505
500	MMSE	0.0178	0.1466	0.2320
	Max Error (%)	1.6045	2.6552	3.0361
550	MMSE	0.0213	0.1460	0.2400
	Max Error (%)	1.2345	2.0287	1.8922
575	MMSE	0.0207	0.1233	0.2262
	Max Error (%)	1.1470	1.8461	1.7785
600	MMSE	0.0177	0.1035	0.2071
	Max Error (%)	1.1360	1.7208	1.7820
625	MMSE	0.0158	0.0986	0.1801
	Max Error (%)	1.0530	1.7301	1.6121
650	MMSE	0.0153	0.0966	0.1755
	Max Error (%)	0.9965	1.8332	1.6475



Individual variation : Kriging Model

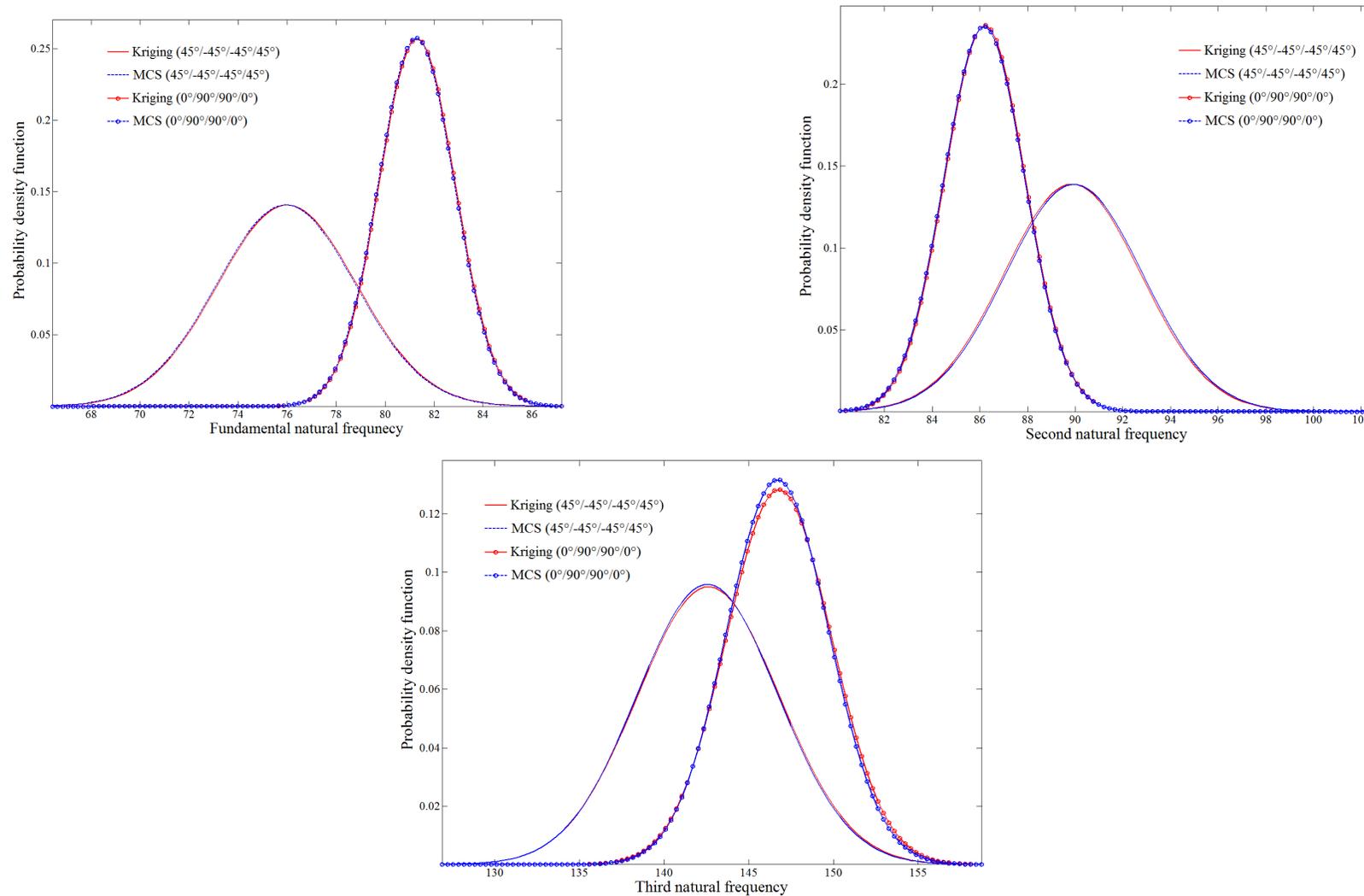
Figure: Probability density function obtained by original MCS and Kriging model with respect to first three natural frequencies for **individual variation of ply orientation angle** for composite elliptical paraboloid shells, considering sample size=10,000, $R_x R_y, R_{xy}=\alpha$, $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\rho=1600$ kg/m³, $t=0.005$ m, $\mu=0.3$





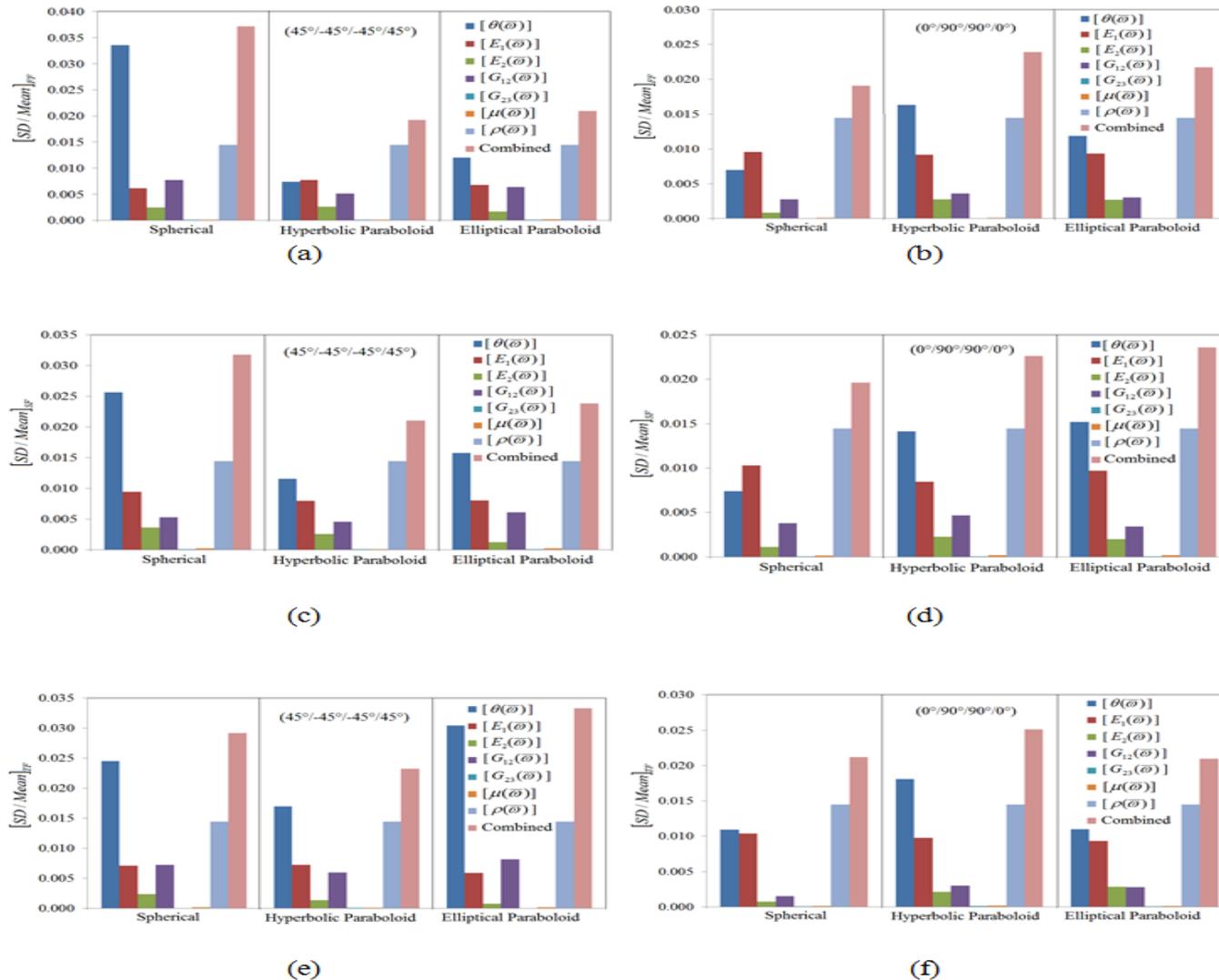
Combined Variation : Kriging Model

Figure: Probability density function obtained by original MCS and Kriging model with respect to first three natural frequencies for **combined variation of ply orientation angle, elastic modulus (longitudinal and transverse), shear modulus (longitudinal and transverse), poisson's ratio and mass density** for composite elliptical paraboloid shells, considering sample size=10,000, $R_x R_y, R_{xy}=\alpha$, $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\rho=1600$ kg/m³, $t=0.005$ m, $\mu=0.3$



Comparative Sensitivity – Angle-ply Vs Cross-ply

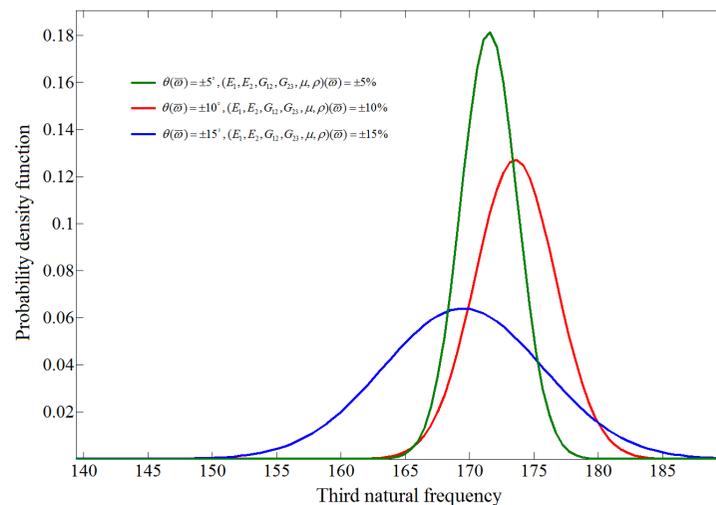
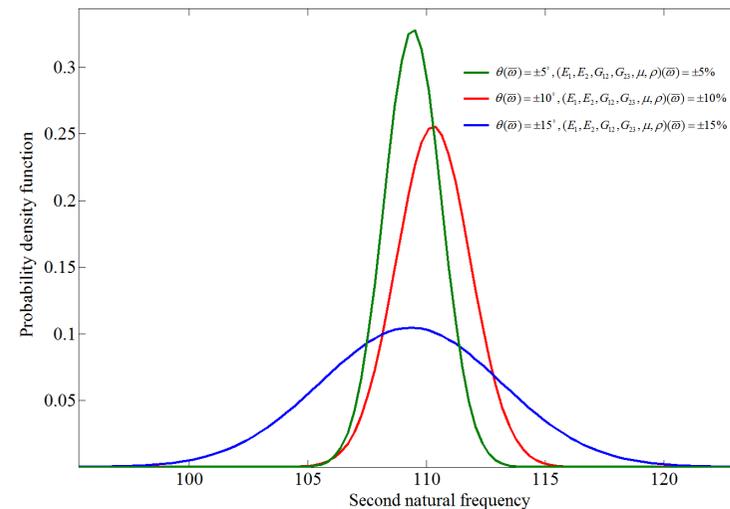
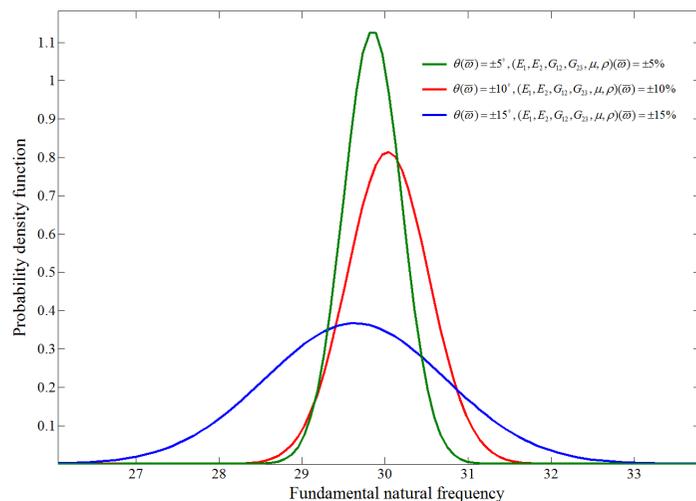
Figure: [SD/Mean]_{1st} of first three natural frequencies for individual variation of input parameters and combined variation for angle-ply (45°/-45°/-45°/45°) and cross-ply (0°/90°/90°/0°) composite shallow doubly curved shells (spherical, hyperbolic paraboloid and elliptical paraboloid), considering deterministic values as $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\rho=1600$ kg/m³, $t=0.005$ m, $\mu=0.3$





Combined Variation - Kriging Model

Probability density function with respect to first three natural frequencies with different combined variation for cross-ply ($0^\circ/90^\circ/90^\circ/0^\circ$) composite hyperbolic paraboloid shallow doubly curved shells considering $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\rho=1600$ kg/m³, $t=0.005$ m, $\mu=0.3$

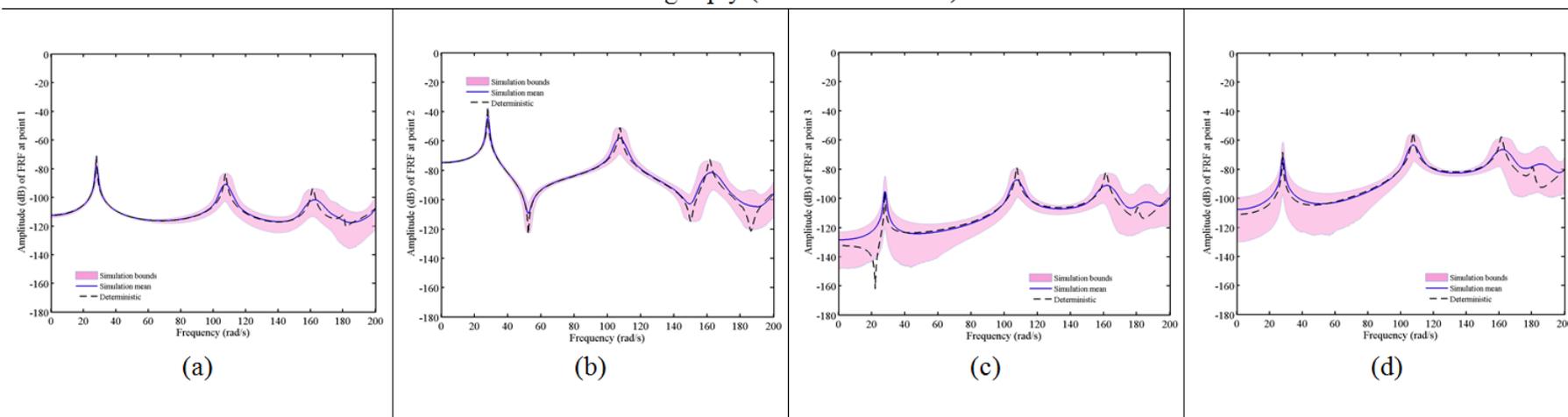




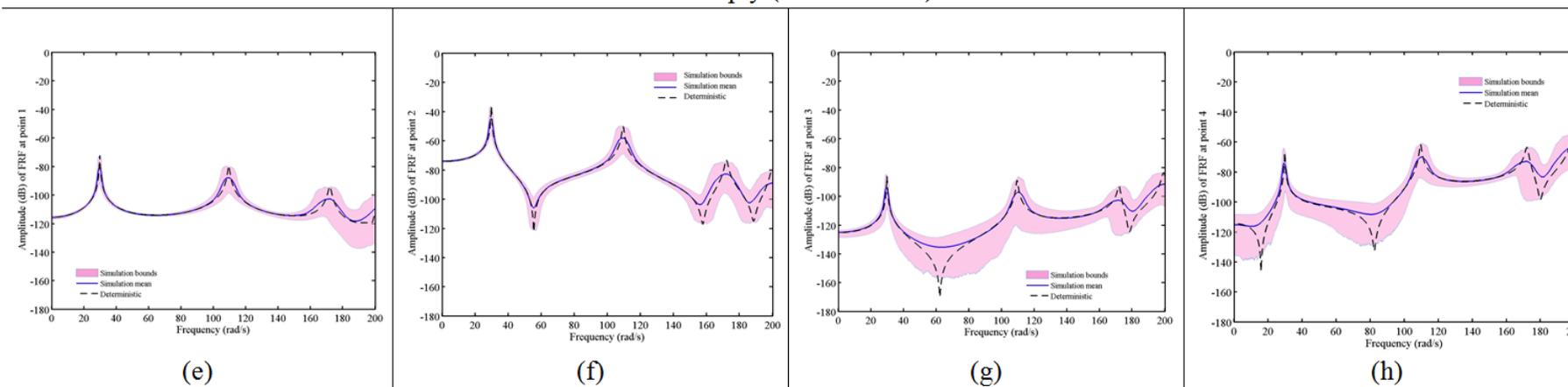
Frequency Response Function - Kriging Model

Figure: Frequency response function (FRF) plot of simulation bounds, simulation mean and deterministic mean for combined stochasticity with four layered graphite epoxy composite cantilever elliptical paraboloid shells considering $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\rho=1600$ Kg/m³, $t=0.005$ m, $\mu=0.3$

Angle-ply ($45^\circ/-45^\circ/-45^\circ/45^\circ$)



Cross-ply ($0^\circ/90^\circ/90^\circ/0^\circ$)





Central Composite Design (CCD) Model

Central Composite Design (CCD) Model

On the basis of statistical and mathematical analysis RSM gives an approximate equation which relates the input features ξ and output features y for a particular system.

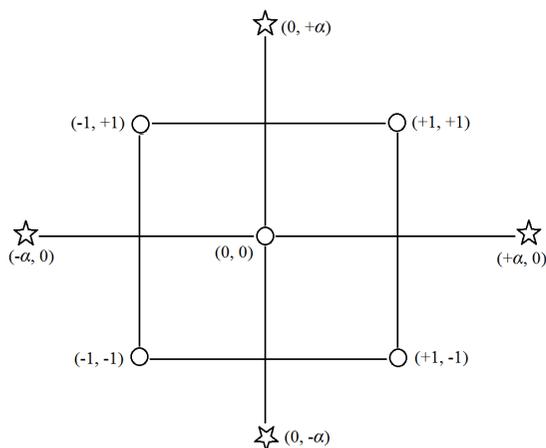
$$y = f(\xi_1, \xi_2, \dots, \xi_k) + \varepsilon$$

ε is the statistical error term.

First order model (interaction),
$$y = \beta_o + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \sum_{j>i}^k \beta_{ij} x_i x_j + \varepsilon$$

Second order model,

$$y = \beta_o + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \sum_{j>i}^k \beta_{ij} x_i x_j + \sum_{i=1}^k \beta_{ii} x_i^2 + \varepsilon$$



Check for quality of constructed model: $R^2, R_{adj}^2, R_{pred}^2$

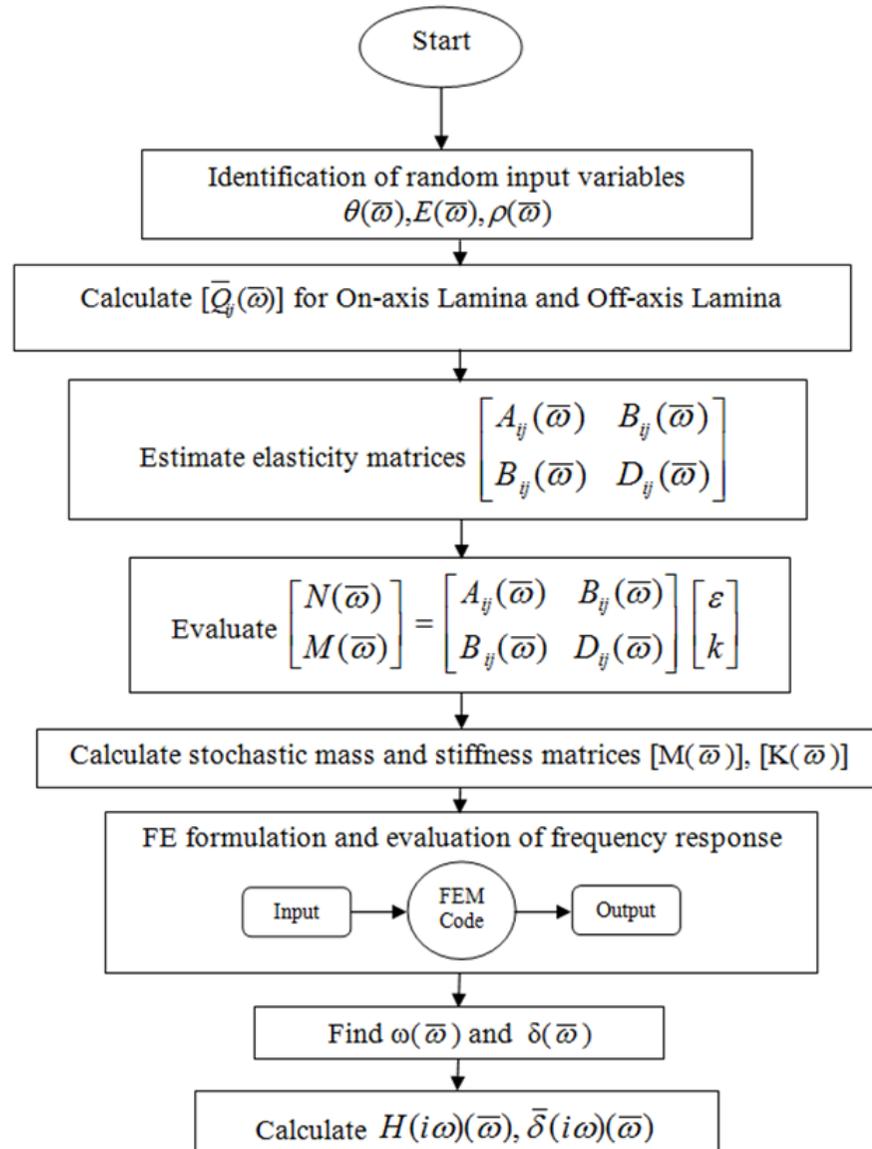
$$R^2 = \left(\frac{SS_R}{SS_T} \right) = 1 - \left(\frac{SS_E}{SS_T} \right) \quad \text{where } 0 \leq R^2 \leq 1$$

$$R_{adj}^2 = 1 - \frac{\left(\frac{SS_E}{n-k-1} \right)}{\left(\frac{SS_T}{n-1} \right)} = 1 - \left(\frac{n-1}{n-k-1} \right) (1 - R^2) \quad \text{where } 0 \leq R_{adj}^2 \leq 1$$

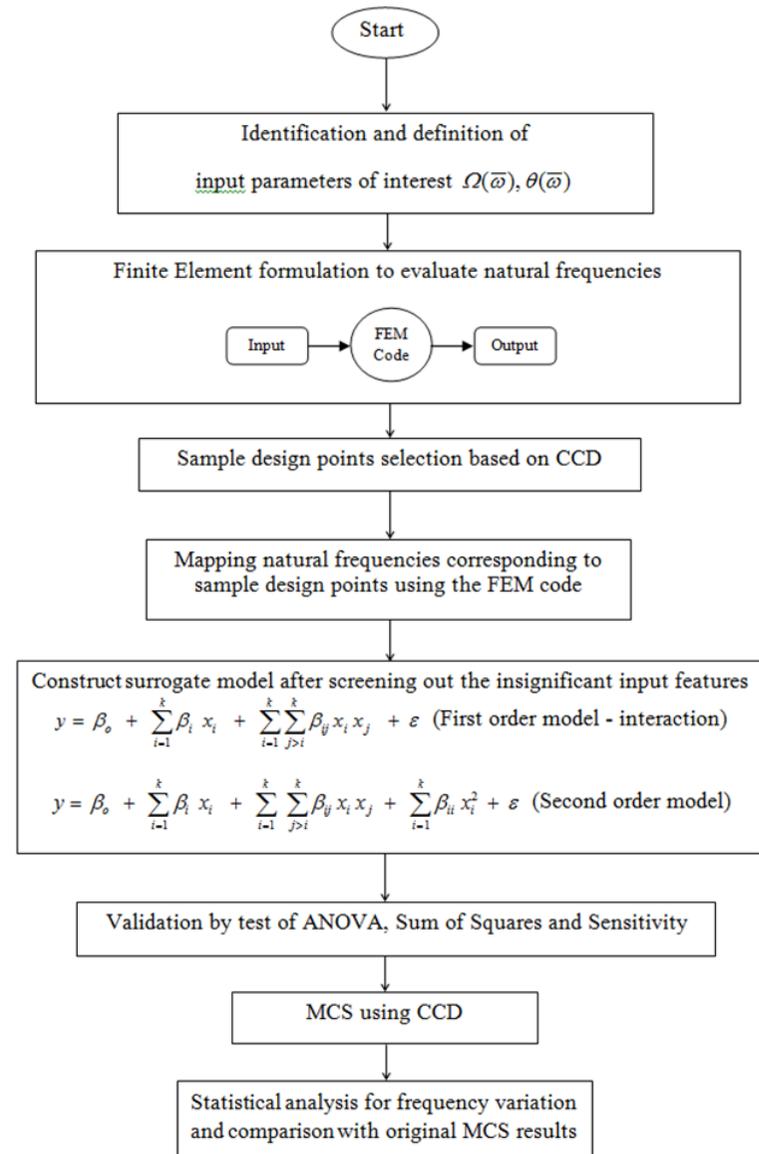
Figure: Sampling scheme for two factor Central composite design

$$R_{pred}^2 = 1 - \left(\frac{PRESS}{SS_T} \right) \quad \text{where } 0 \leq R_{pred}^2 \leq 1$$

Monte Carlo Simulation Model



Central Composite Design Model



Validation - Central Composite Design (CCD) Model

Figure: Central composite design (CCD) model with respect to Original FE model of fundamental natural frequencies for combined variation of rotational speed and ply-orientation angle of angle-ply $[(45^\circ/-45^\circ/45^\circ/-45^\circ)_s]$ composite cantilever conical shells

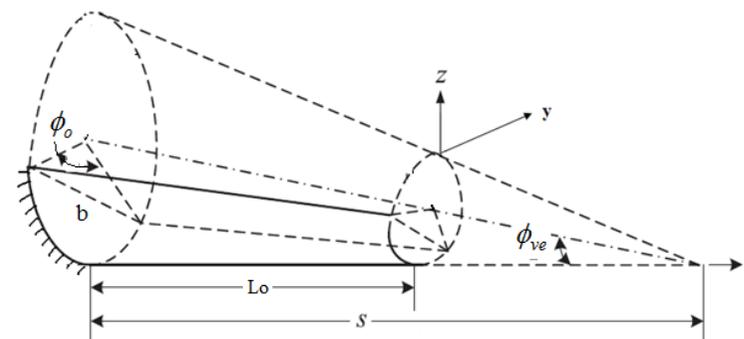
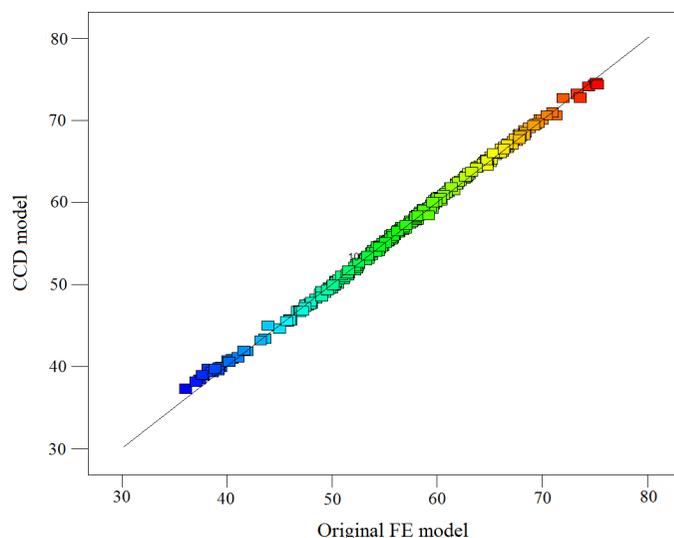


Table: Non-dimensional fundamental frequencies $[\omega = \omega_n L^2 \sqrt{(\rho t/D)}]$ of graphite-epoxy composite rotating cantilever plate, $L/b_0=1$, $t/L=0.12$, $D=Et^3/12(1-\nu^2)$, $\nu=0.3$

Ω	Present FEM	Sreenivasamurthy and Ramamurti (1981)
0.0	3.4174	3.4368
1.0	4.9549	5.0916

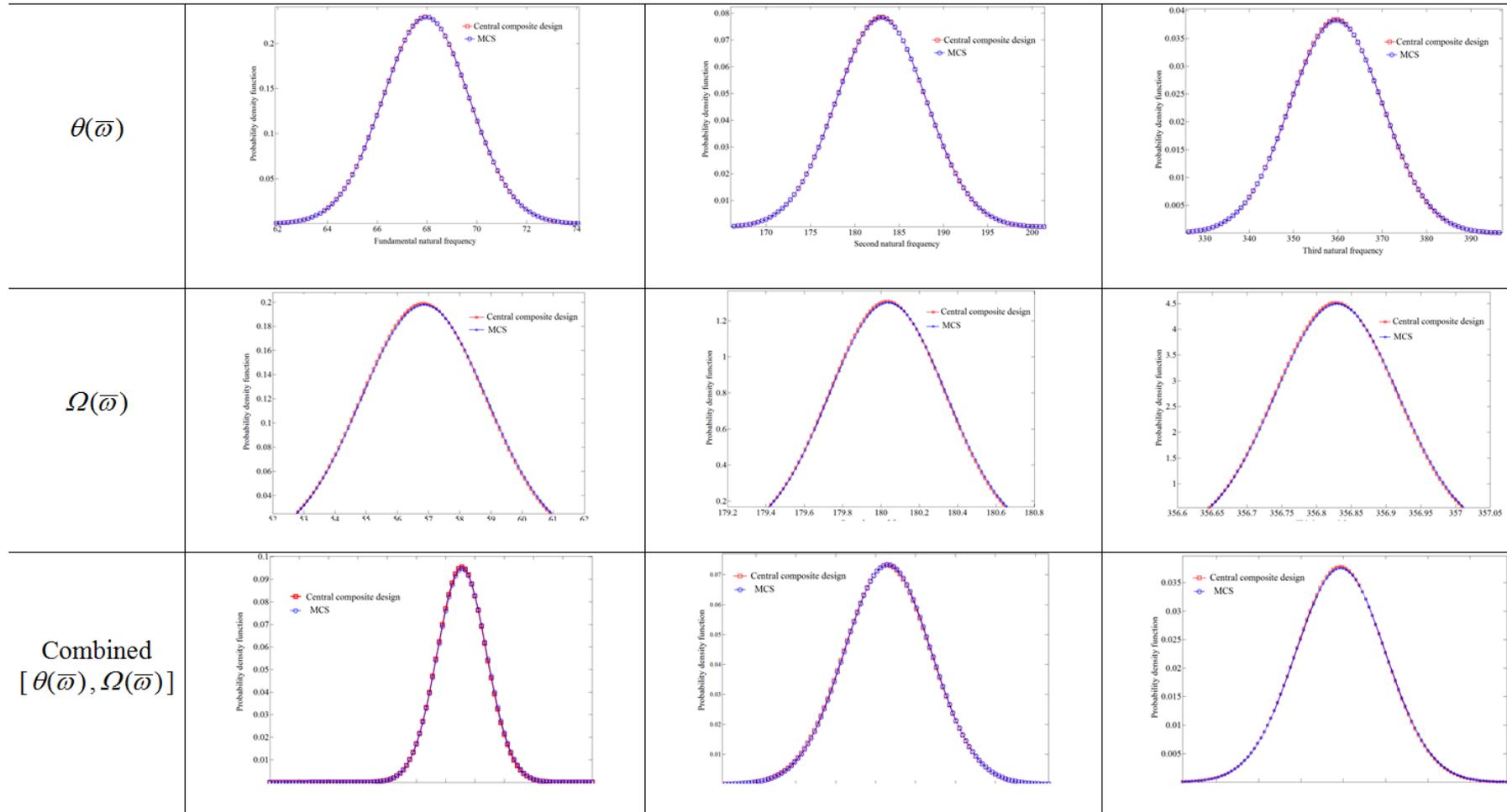
Table: Non-dimensional fundamental frequencies $[\omega = \omega_n b^2 \sqrt{(\rho t/D)}, D=Et^3/12(1-\nu^2)]$ for the untwisted shallow conical shells with $\nu=0.3$, $s/t=1000$, $\phi_0 = 30^\circ$, $\phi_{ve} = 15^\circ$.

Aspect Ratio (L/s)	Present FEM (8 x 8) (Deterministic mean)	Present FEM (6 x 6) (Deterministic mean)	Liew et al. (1991)
0.6	0.3524	0.3552	0.3599
0.7	0.2991	0.3013	0.3060
0.8	0.2715	0.2741	0.2783



Validation – Central Composite Design model

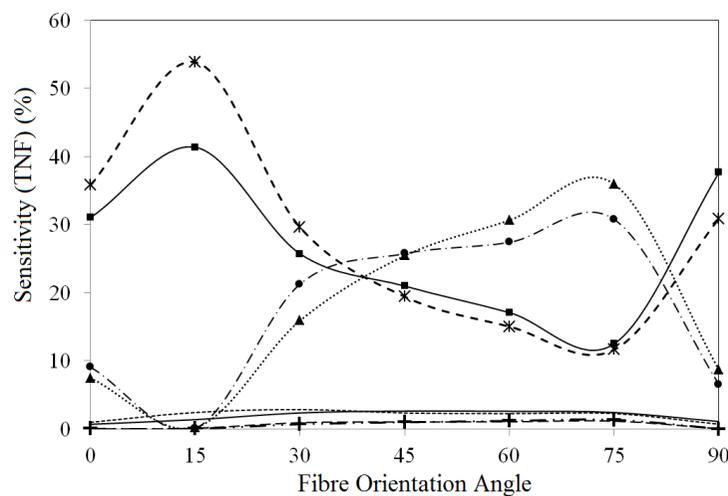
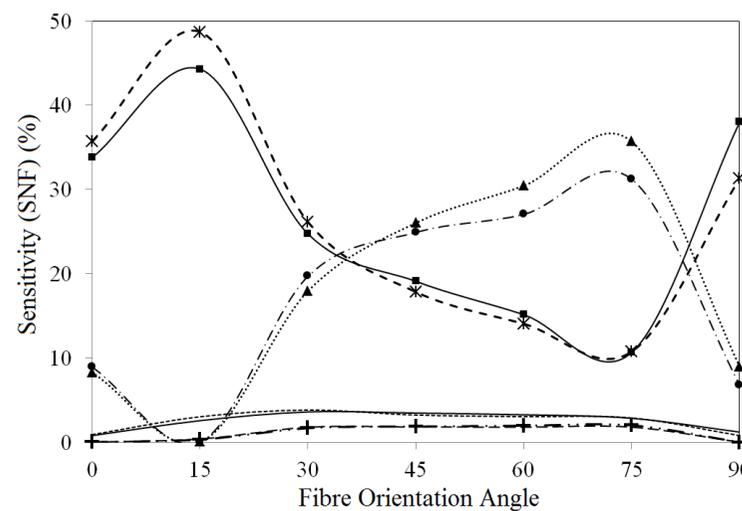
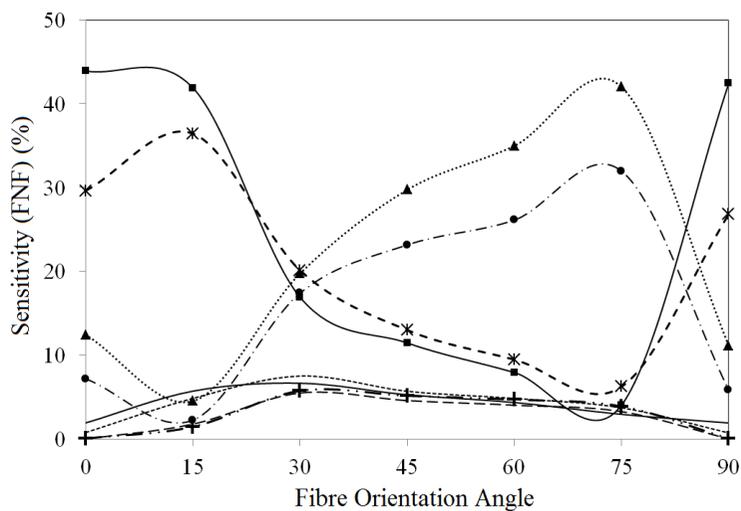
Figure: Probability density function obtained by original MCS and Central composite design (CCD) with respect to first three natural frequencies (Hz) indicating for variation of only ply orientation angle, only rotational speeds, and combined variation for graphite-epoxy angle-ply $[(\theta^\circ/-\theta^\circ/\theta^\circ/-\theta^\circ)_s]$ composite conical shells, considering sample size=10,000, $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\rho=1600$ kg/m³, $\theta=45^\circ \pm 5^\circ$ variation), $\Omega=100$ rpm ($\pm 10\%$ variation), $t=0.003$ m, $\nu=0.3$, $L_o/s=0.7$, $\alpha=45^\circ$, $\beta=20^\circ$.





Central Composite Design Model - Sensitivity

Sensitivity in percentage for variation in only fibre orientation angle [] (5° variation) for eight layered graphite-epoxy angle-ply $[(\theta^\circ/-\theta^\circ/\theta^\circ/-\theta^\circ)_s]$ composite conical shells, considering $E_1=138$ GPa, $E_2=8.9$ GPa, $G_{12}=G_{13}=7.1$ GPa, $G_{23}=2.84$ GPa, $\rho=1600$ kg/m³, $t=0.003$ m, $\nu=0.3$, $L_0/s=0.7$, $\alpha = 45^\circ$, $\phi_o = 20^\circ$ (ϕ_{ve} – fundamental natural frequency, SNF – second natural frequency and TNF – Third natural frequency)





**General high dimensional model
representation (GHDMR) with D-MORPH**



General high dimensional model representation (GHDMR) with D-MORPH

For different input parameters, the output is calculated as

$$\lambda(x) = \lambda_0 + \sum_{i=1}^k \lambda_i(S_i) + \sum_{1 \leq i < j \leq k} \lambda_{ij}(S_i, S_j) + \dots + \lambda_{12\dots k}(S_1, S_2, \dots, S_k)$$

Hilbert space $\bar{H} = H \oplus H^\perp$

Second order HDMR expansion

$$\lambda_{ij}(S_i, S_j) \approx \sum_{r=1}^k [\alpha_r^{(ij)i} \varphi_r^i(S_i) + \alpha_r^{(ij)j} \varphi_r^j(S_j)] + \sum_{p=1}^l \sum_{q=1}^l \beta_{pq}^{(0)ij} \varphi_p^i(S_i) \varphi_q^j(S_j)$$

The regression equation for least squares of the algebraic equation

$$\frac{1}{N_{\text{camp}}} \Gamma^T \Gamma J = \frac{1}{N_{\text{camp}}} \Gamma^T \hat{R}$$

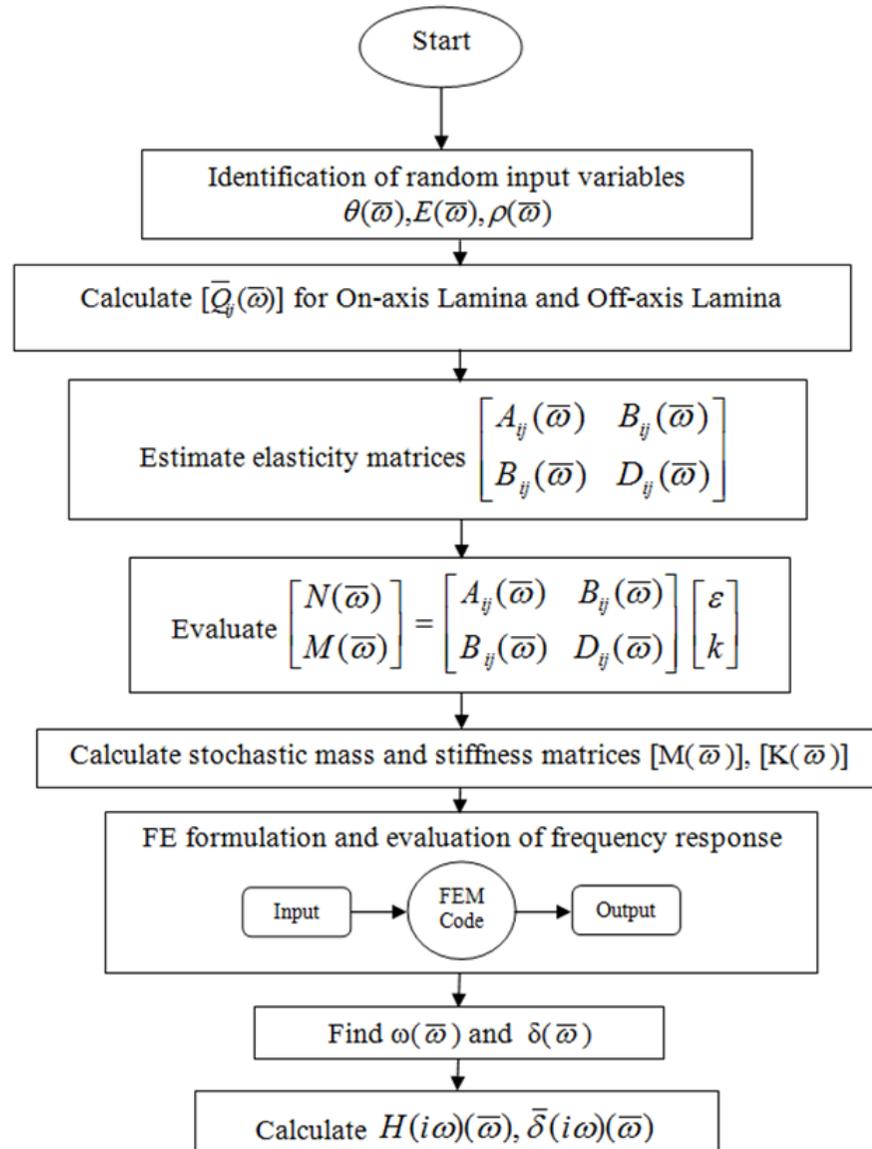
some rows of the above equation are identical and can be removed to give an underdetermined algebraic equation system $AJ = \hat{V}$

D-MORPH regression provides a solution to ensure additional condition of exploration path represented by differential equation

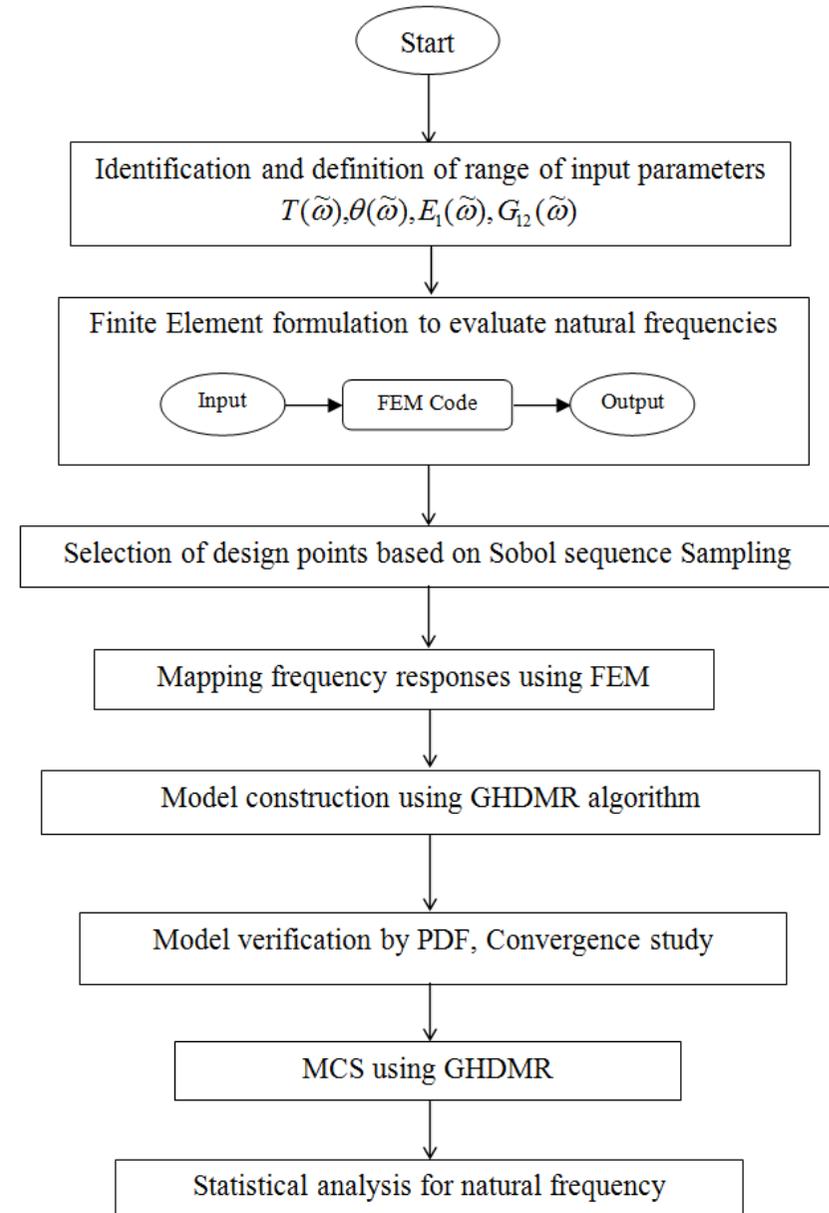
$$\frac{dJ(l)}{dl} = \chi v(l) = (I_t - A^+ A) v(l)$$



Monte Carlo Simulation Model



GHDMR Model





Validation - GHDMR Model

Figure: Central composite design (CCD) model with respect to Original FE model of fundamental natural frequencies for combined variation of rotational speed and ply-orientation angle of angle-ply [(45°/-45°/45°/-45°)s] composite cantilever conical shells

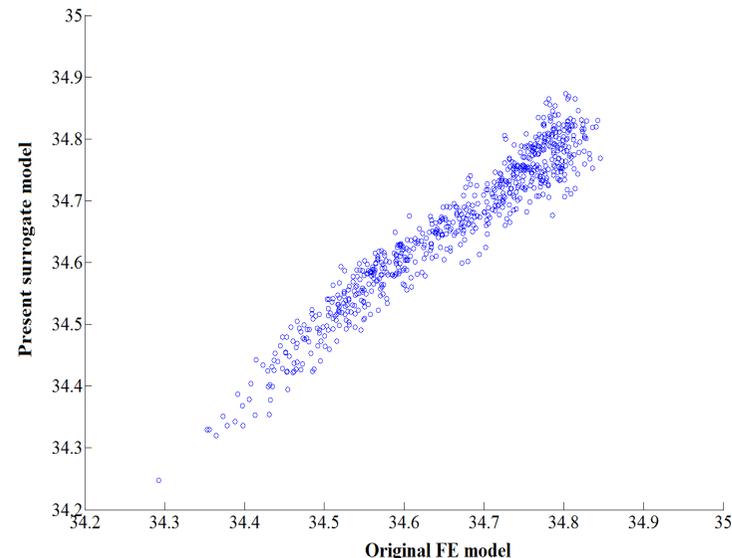


Table: Convergence study for non-dimensional fundamental natural frequencies [$\omega = \omega_n L^2 \sqrt{(\rho/E_1 t^2)}$] of three layered ($\theta^\circ/-\theta^\circ/\theta^\circ$) graphite-epoxy untwisted composite plates, $a/b=1$, $b/t=100$, considering $E_1 = 138$ GPa, $E_2 = 8.96$ GPa, $G_{12} = 7.1$ GPa, $\nu_{12} = 0.3$.

Ply Angle	Present FEM (4 x4)	Present FEM (6 x6)	Present FEM (8x8)	Present FEM (10 x10)	Qatu and Leissa (1991)
0°	1.0112	1.0133	1.0107	1.004	1.0175
45°	0.4556	0.4577	0.4553	0.4549	0.4613
90°	0.2553	0.2567	0.2547	0.2542	0.2590

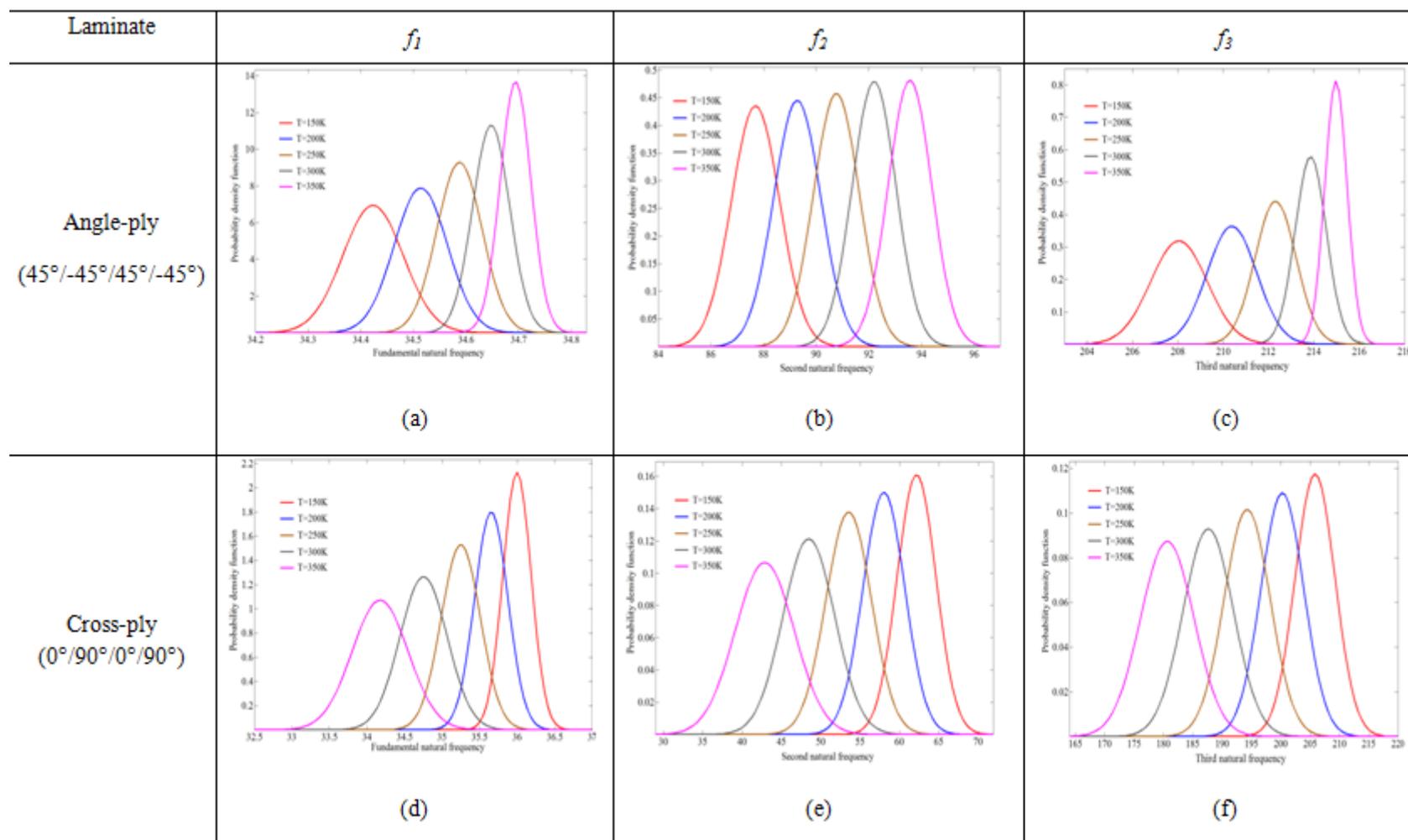
Table: Non-dimensional natural frequencies [$\omega = \omega_n a^2 \sqrt{(\rho/E_2 t^2)}$] for simply-supported graphite-epoxy symmetric cross-ply (0°/90°/90°/0°) composite plates considering $a/b=1$, $T=325K$, $a/t=100$

Frequency	Present FEM (4 x4)	Present FEM (6 x6)	Present FEM (8x8)	Present FEM (10 x10)	Sai Ram and Sinha (1991)
1	8.041	8.061	8.023	8.001	8.088
2	18.772	19.008	18.684	18.552	19.196
3	38.701	38.981	38.597	38.443	39.324



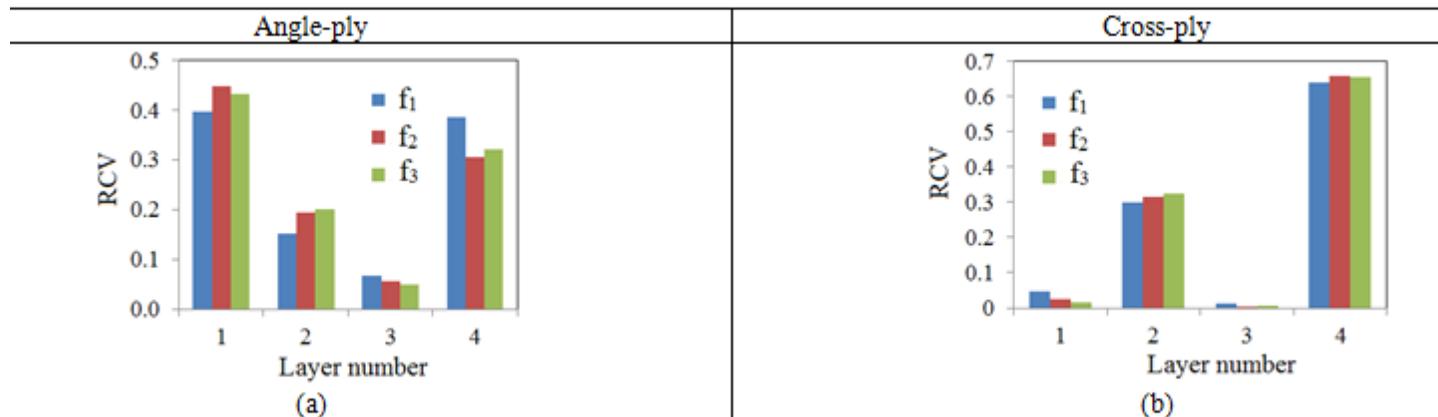
Thermal Uncertainty Quantification

Probability density function with respect to first three natural frequencies (Hz) due to individual variation of temperature of angle-ply ($45^\circ/-45^\circ/45^\circ/-45^\circ$) and cross-ply ($0^\circ/90^\circ/0^\circ/90^\circ$) composite cantilever plate

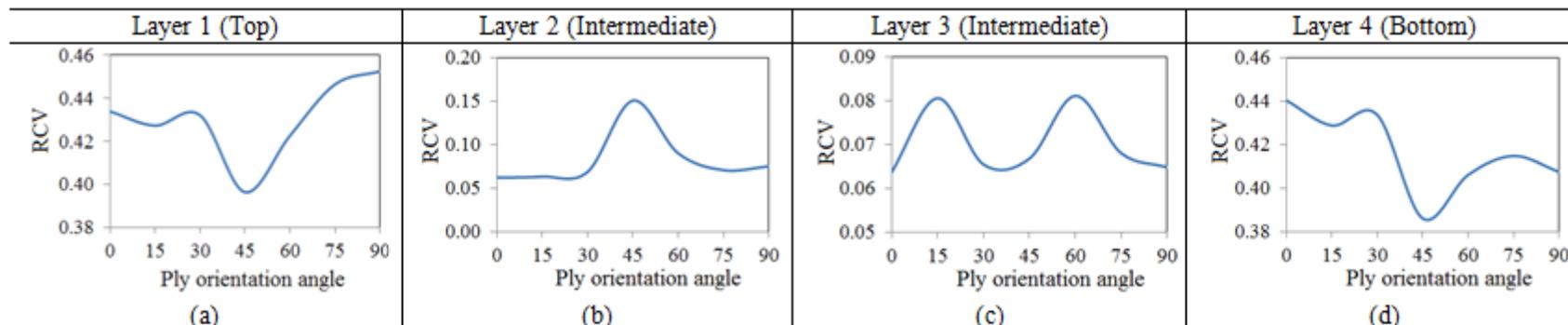


GHDMR – Relative Co-efficient of Variance (RCV)

Relative coefficient of variance (RCV) of first three natural frequencies due to variation of temperature (layerwise) for angle-ply ($45^\circ/-45^\circ/45^\circ/-45^\circ$) and cross-ply ($0^\circ/90^\circ/0^\circ/90^\circ$) composite cantilever plate at mean temperature ($T_{\text{mean}}=300\text{K}$)



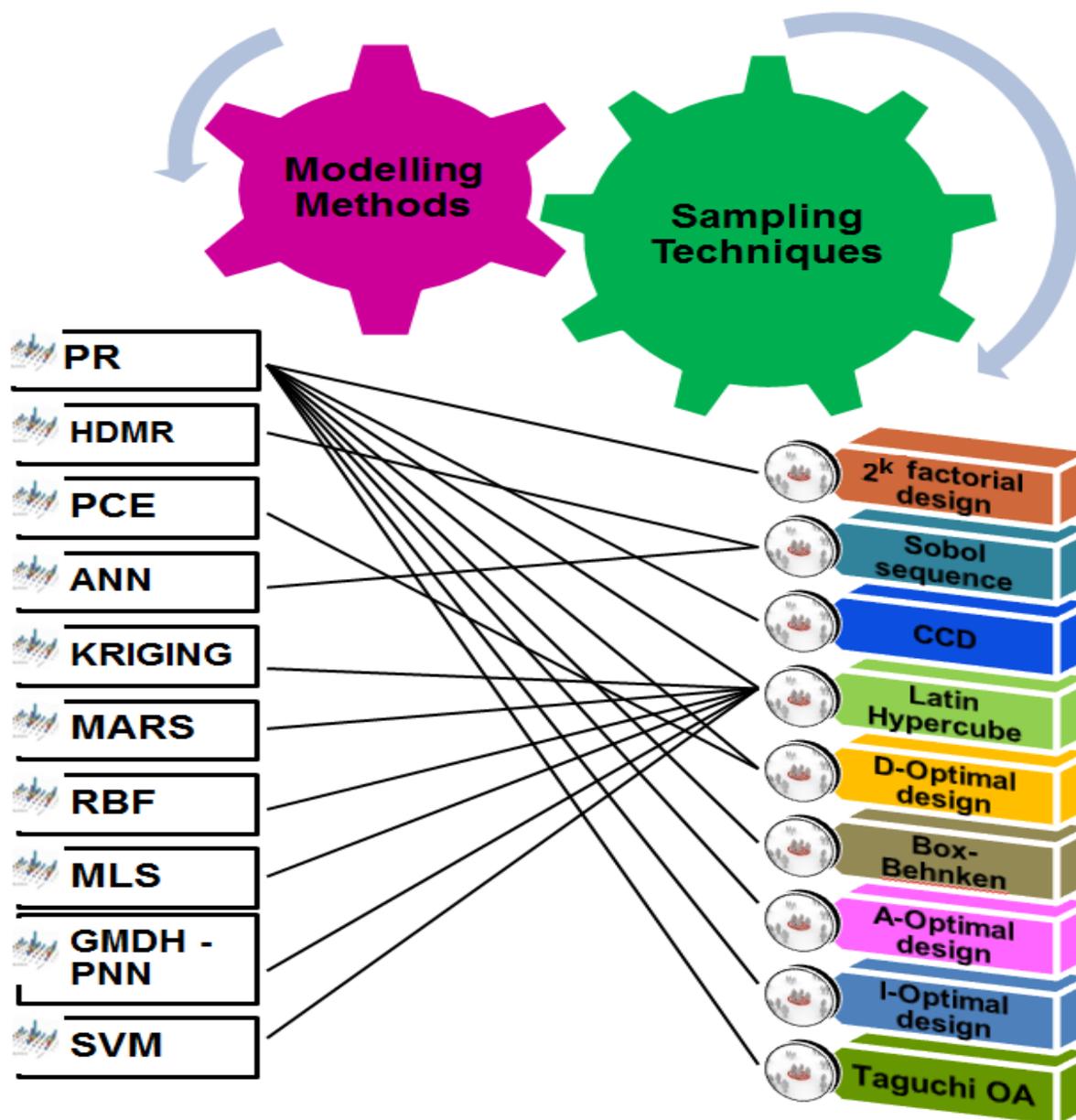
Relative coefficient of variance (RCV) of fundamental mode due to variation of temperature (layerwise) for angle-ply ($\theta^\circ/-\theta^\circ/\theta^\circ/-\theta^\circ$) (=Ply orientation angle) composite cantilever plate at mean temperature ($T_{\text{mean}}=300\text{K}$)





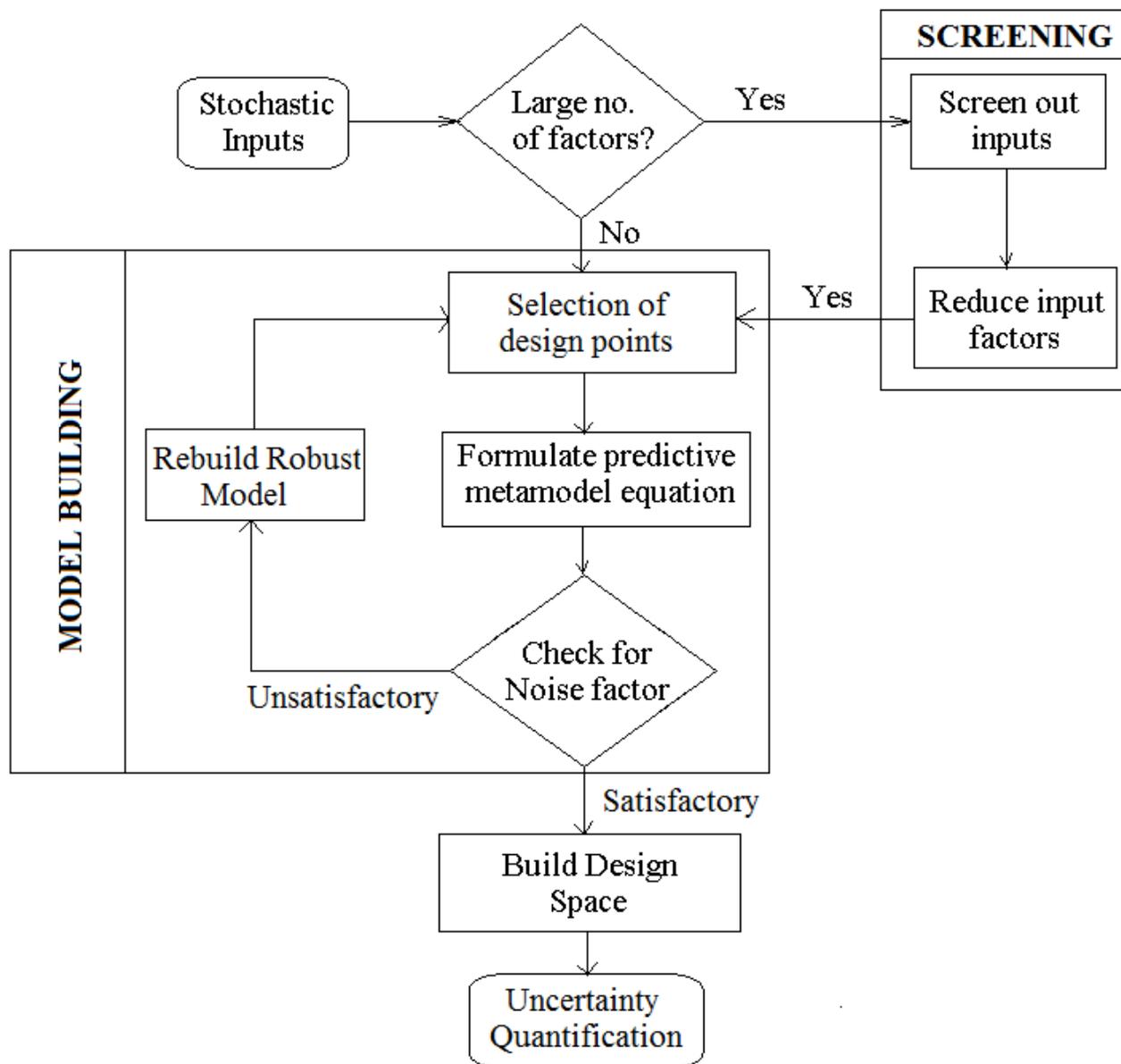
Comparative Study

Modelling methods and Sampling techniques

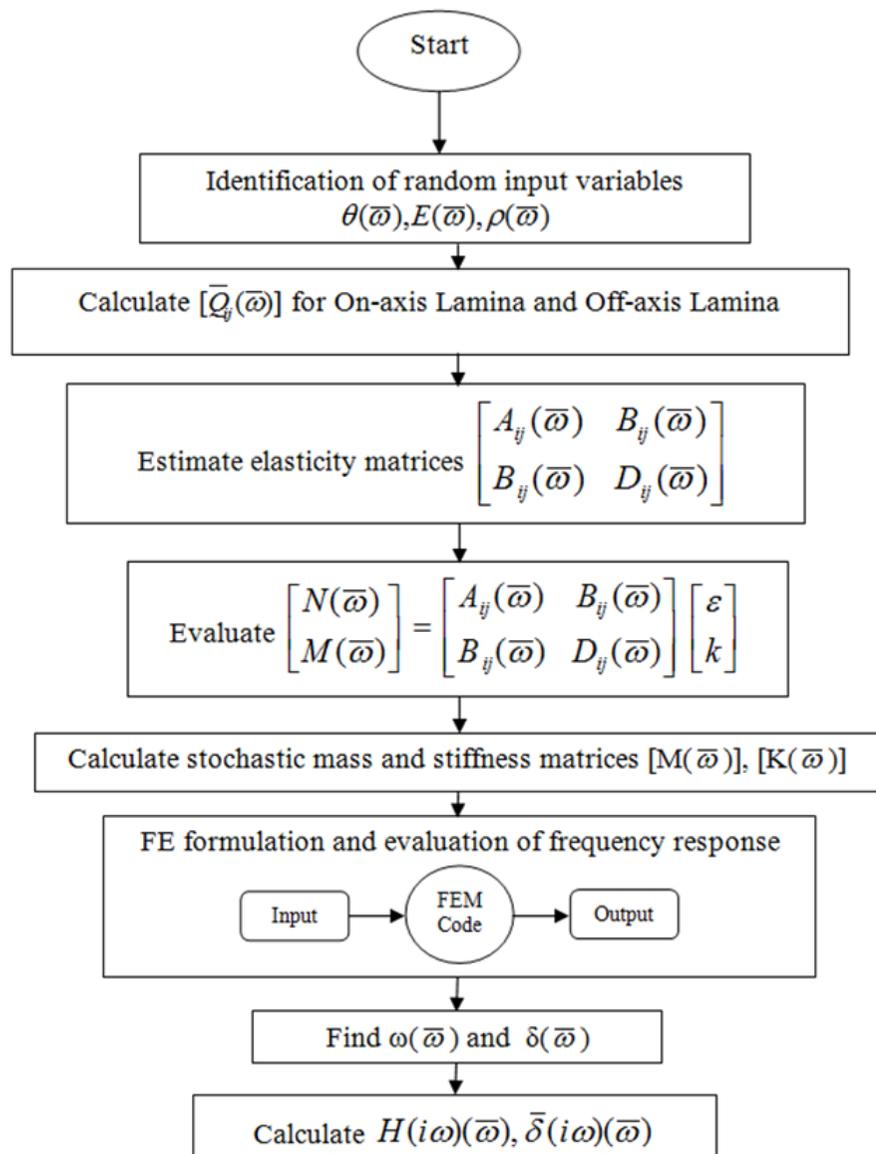




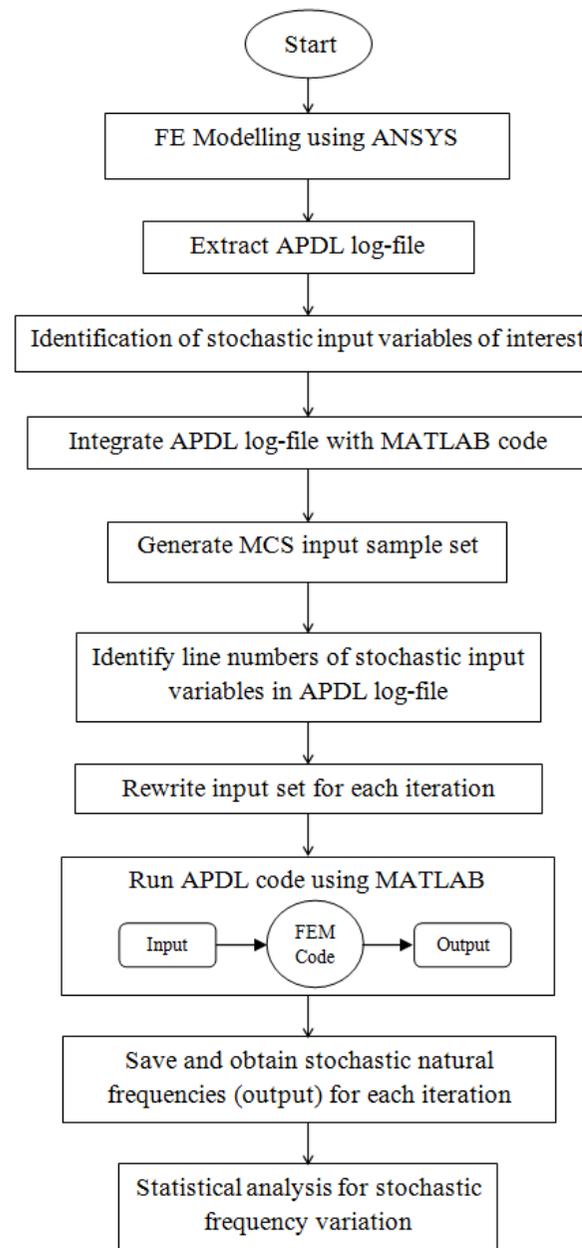
Flowchart : Uncertainty Quantification (UQ) using metamodel



Monte Carlo Simulation Model



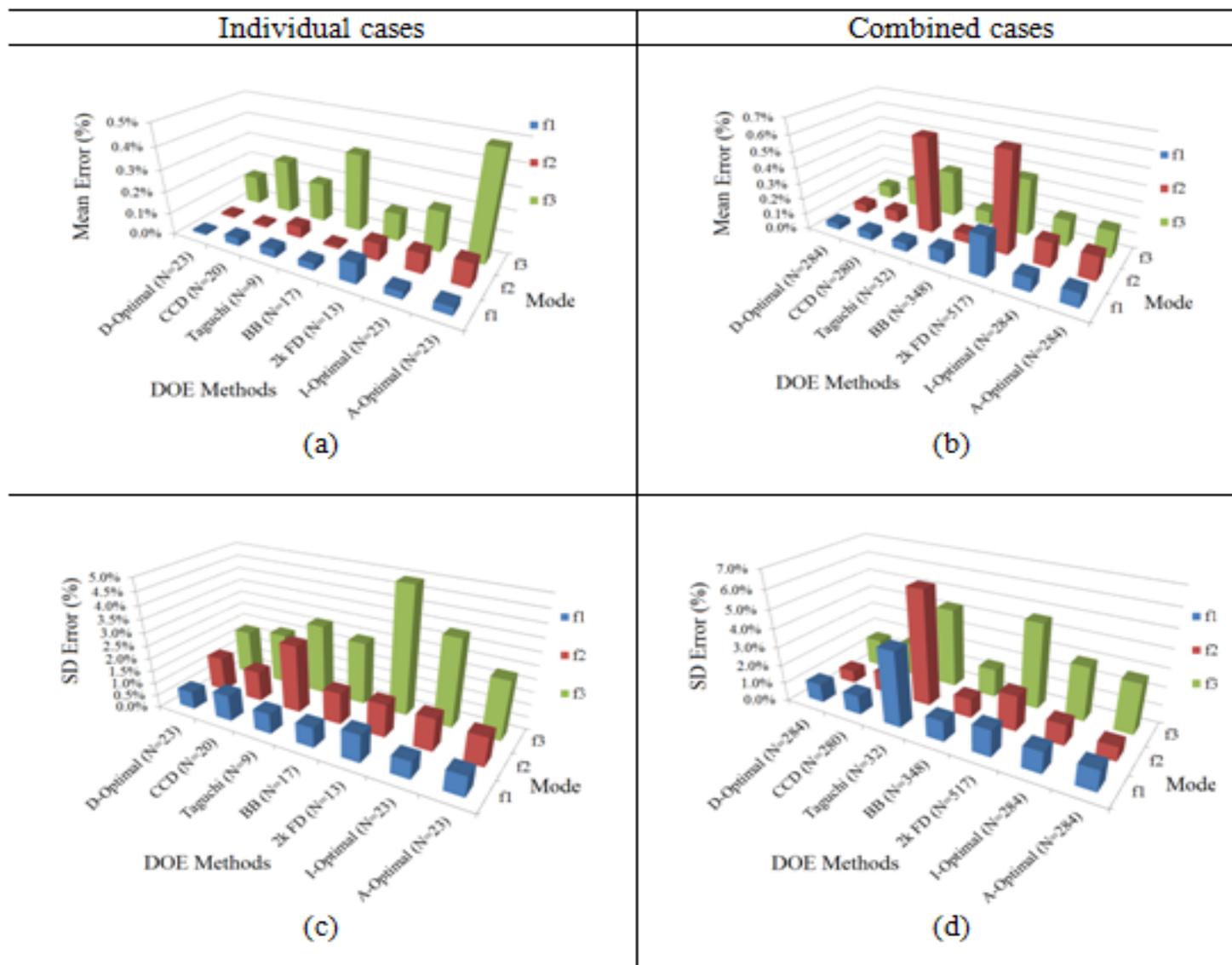
Response Surface Model





Sampling techniques – A Comparative study

Error (%) of mean and standard deviation of first three natural frequencies between polynomial regression method with different sampling techniques and MCS results for individual variation and combined variation for angle-ply (45°/-45°/45°) composite plates





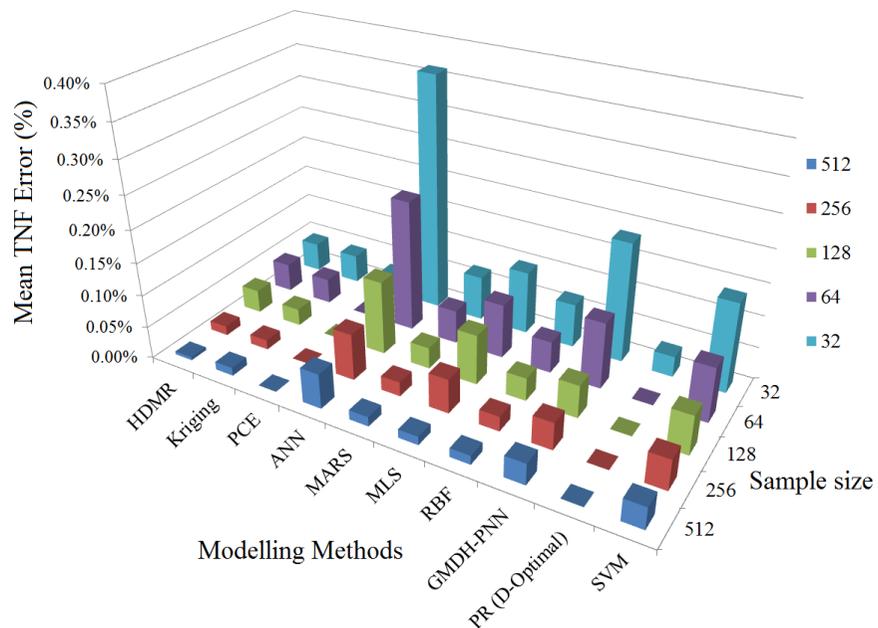
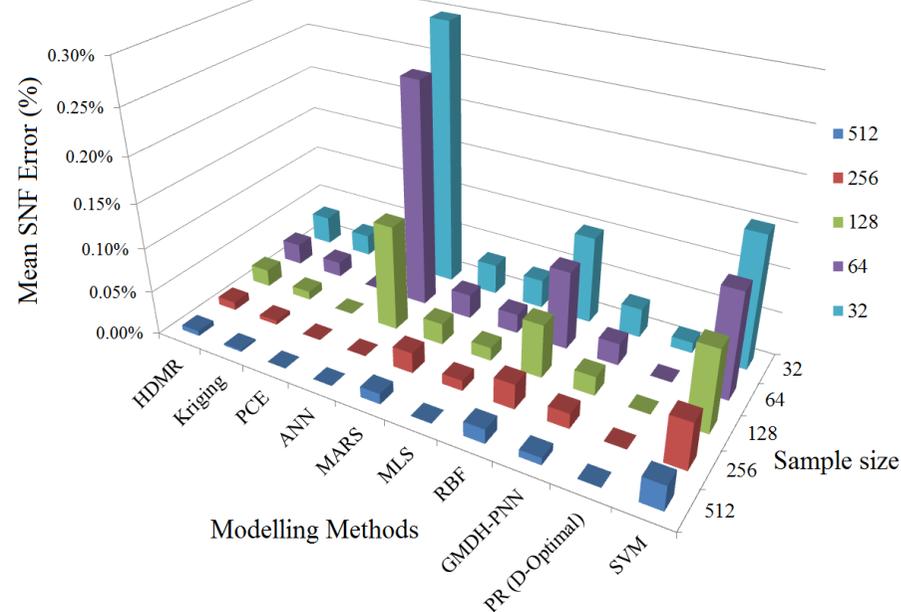
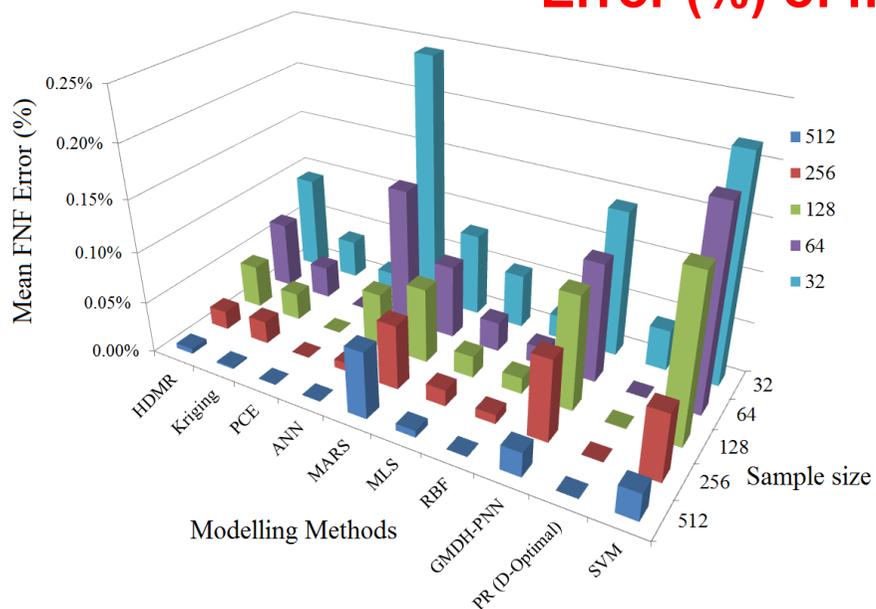
Modelling methods – A Comparative study

Minimum sample size required for modelling methods (21 and 63 random variables respectively)

Sl. No.	Modelling method	Minimum number of samples required for model formation	
		Individual variation	Combined variation
1.	Polynomial Regression (by D-optimal)	32	64
2.	High dimensional model representation (HDMR)	256	512
3.	Kriging method	128	256
4.	Polynomial chaos expansion (PCE)	64	128
5.	Artificial neural network (ANN)	256	2048
6.	Multivariate adaptive regression splines (MARS)	64	128
7.	Moving Least Square (MLS)	128	512
8.	Radial basis function (RBF)	64	1024
9.	Group method of data handling - Polynomial neural network (GMDH-PNN)	512	1024
10.	Support Vector Regression (SVR)	512	1024



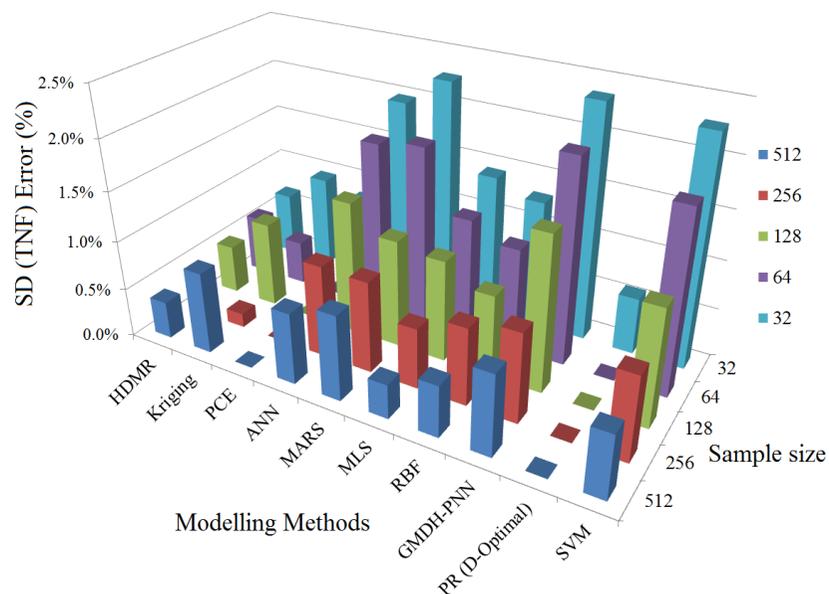
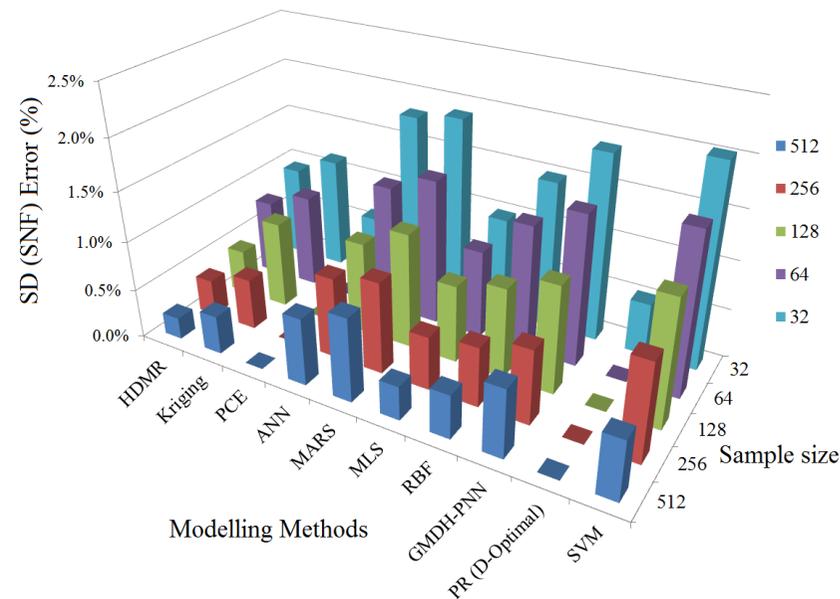
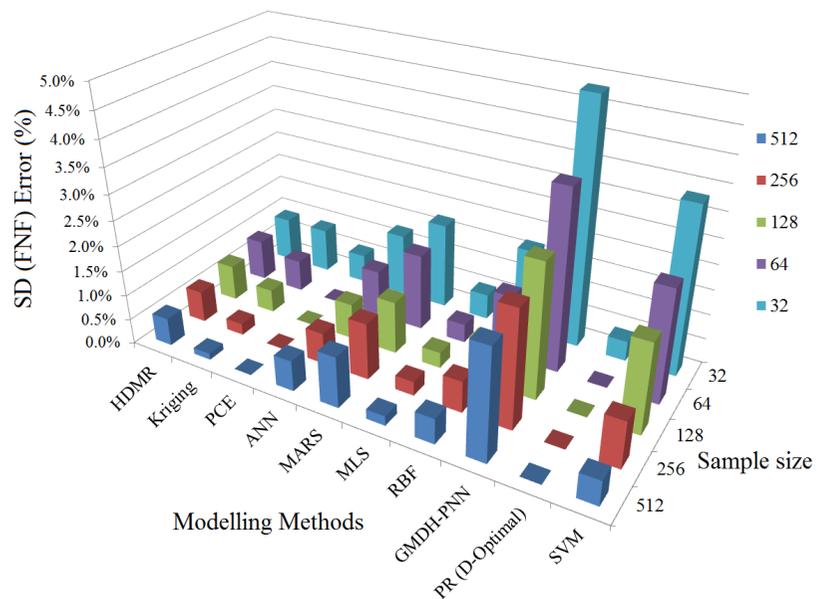
Individual (only ply angle) Variation Error (%) of mean with MCS





Individual (only ply angle) Variation

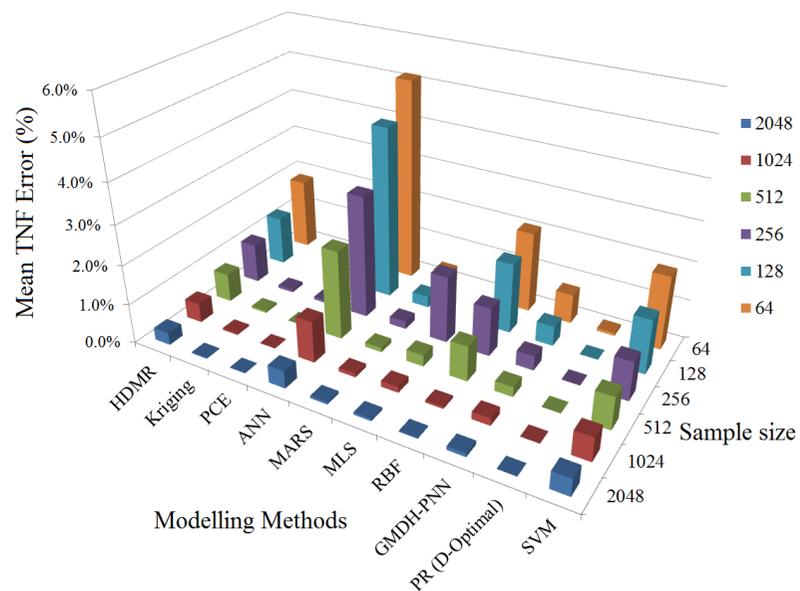
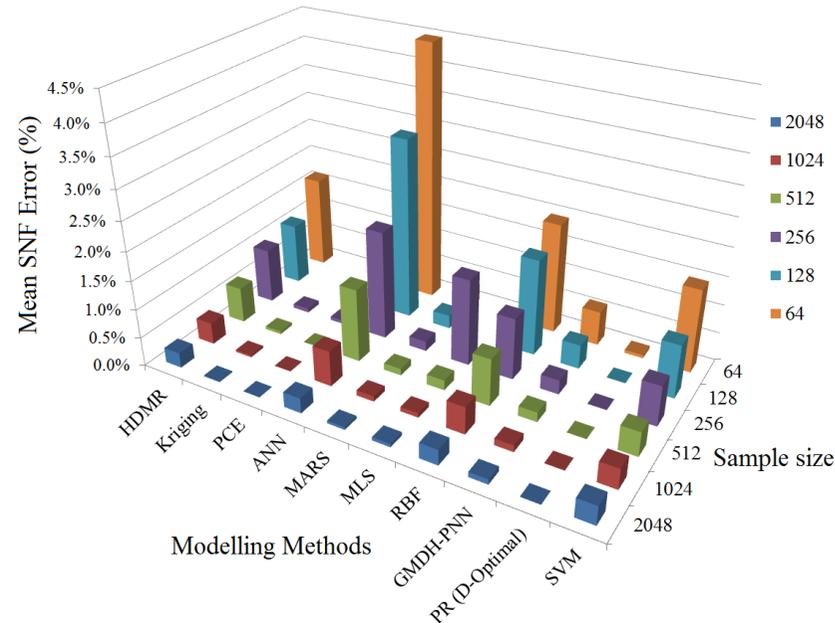
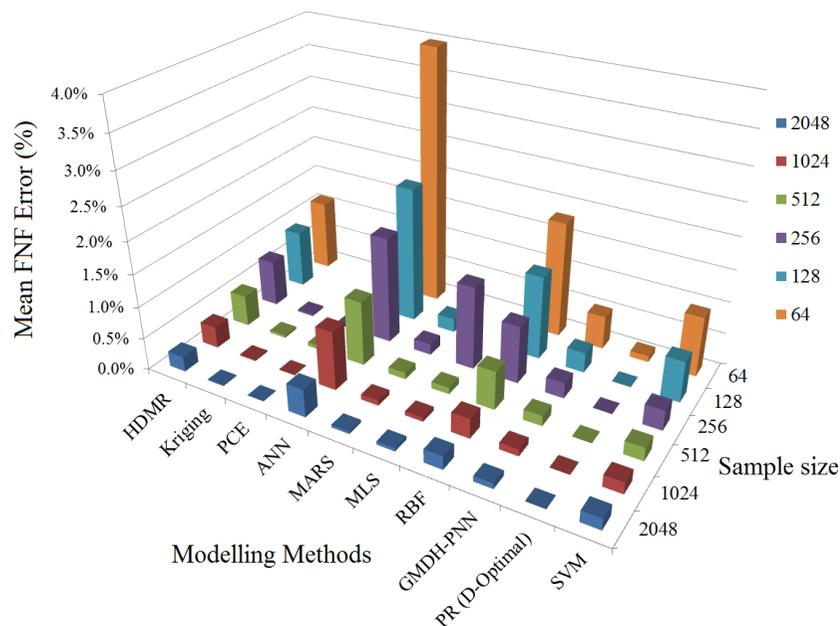
Error (%) of SD with MCS





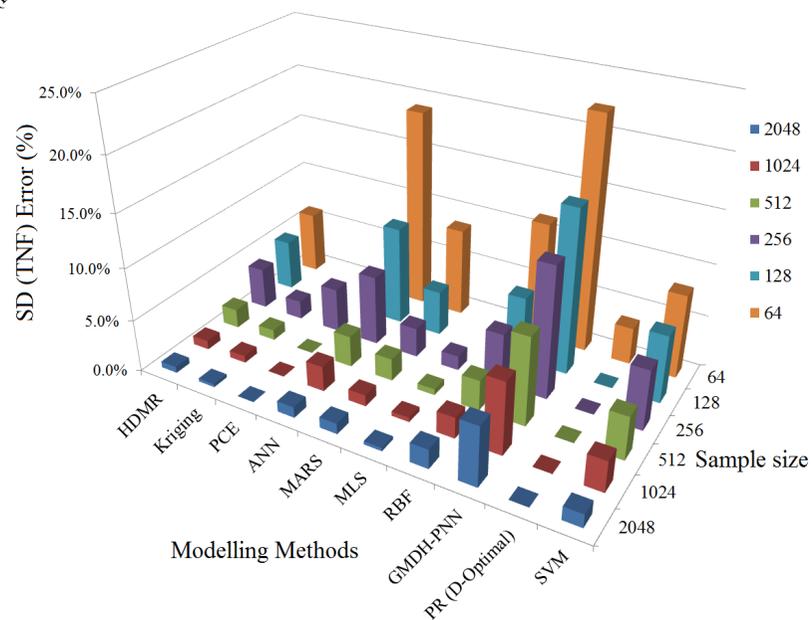
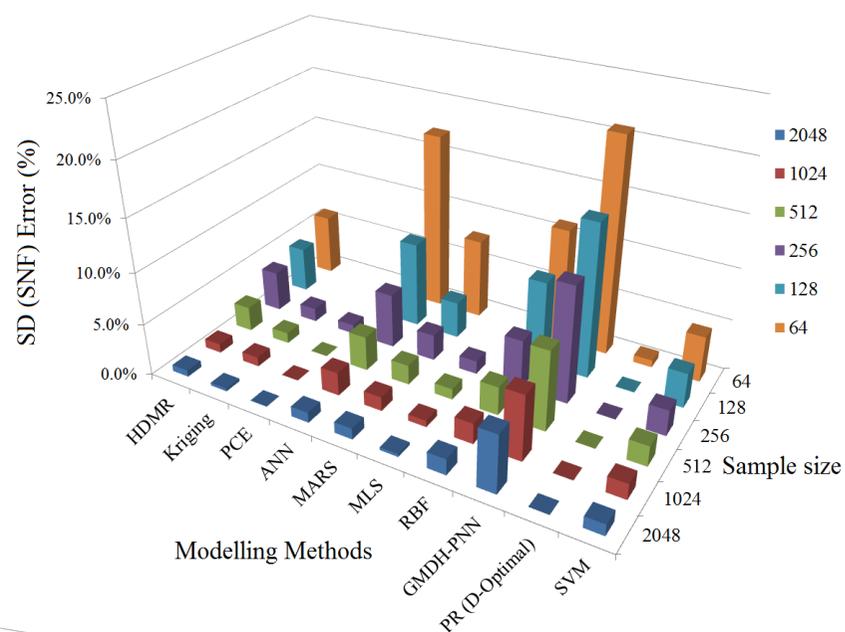
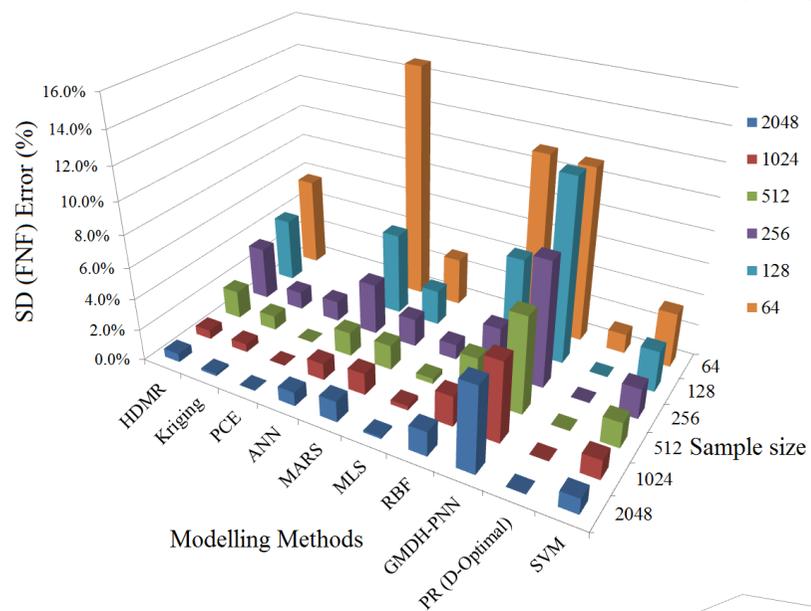
Combined Variation

Error (%) of mean with MCS





Combined Variation Error (%) of SD with MCS





Summary – Comparative Study

- ❑ As the sample size increases, error (%) of mean and standard deviation are found to reduce irrespective of all modelling methods.
- ❑ Polynomial regression with D-optimal design method is found to be most computationally cost effective for both individual as well as combined variation cases.
- ❑ Group method of data handling - Polynomial neural network (GMDH-PNN) method and Support Vector Regression (SVR) are observed to be least computationally efficient for individual variation.
- ❑ Artificial neural network (ANN) method is found to be most computationally expensive for combined variation.



Conclusions

- ❑ Several approaches for investigation on the effect of variation in input parameters on the **dynamics of composite plates / shells** were developed.
- ❑ The focus has been of the efficient generation of a **surrogate model** with limited use of the computational intensive finite element computations
- ❑ The UQ methods are validated with results from direct MCS with original model.
- ❑ Sensitivity methods can be used to reduce the number of random variables in the model
- ❑ The techniques can be integrated with **general purpose finite element software (NASTRAN / ABACUS)** to solve complex problems.