Polynomial Chaos Decomposition with Differentiation and Applications

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Outline

- Introduction
- Theory and Methodology
- Applications

  A. Analytical Problems

  i. One-dimensional problem

  ii. Two-dimensional problem

  B. Composite Laminate Problems

  i. Macroscale Modeling of a CFRP Composite Laminate

  ii. Multiscale Modeling of a CFRP Composite Laminate
- Conclusion
- Future work

Introduction

- Why Uncertainty Quantification (UQ)?
- PC expansion:- spectral method for Uncertainty Quantification (L_2 Convergence)
- Methods for PC expansion:

  i) Intrusive, and ii) Non-intrusive
- PCDD is a new non-intrusive technique that involves differentiation of the multivariate polynomials and sensitivity calculation
- Number of samples equal to number of PC expansion coefficients

Polynomial Chaos Expansion

- PC expansion (introduced by Norbert Weiner, 1938) of uncertain response, *y=f(x)*:

$$y(\vec{\xi}) = \sum_{k=0}^{P} a_k \psi_k(\vec{\xi}); \quad Using\ NQ: a_k = \frac{\langle y, \psi_k(\vec{\xi})\rangle}{\langle \psi_k(\vec{\xi}), \psi_k(\vec{\xi})\rangle}$$

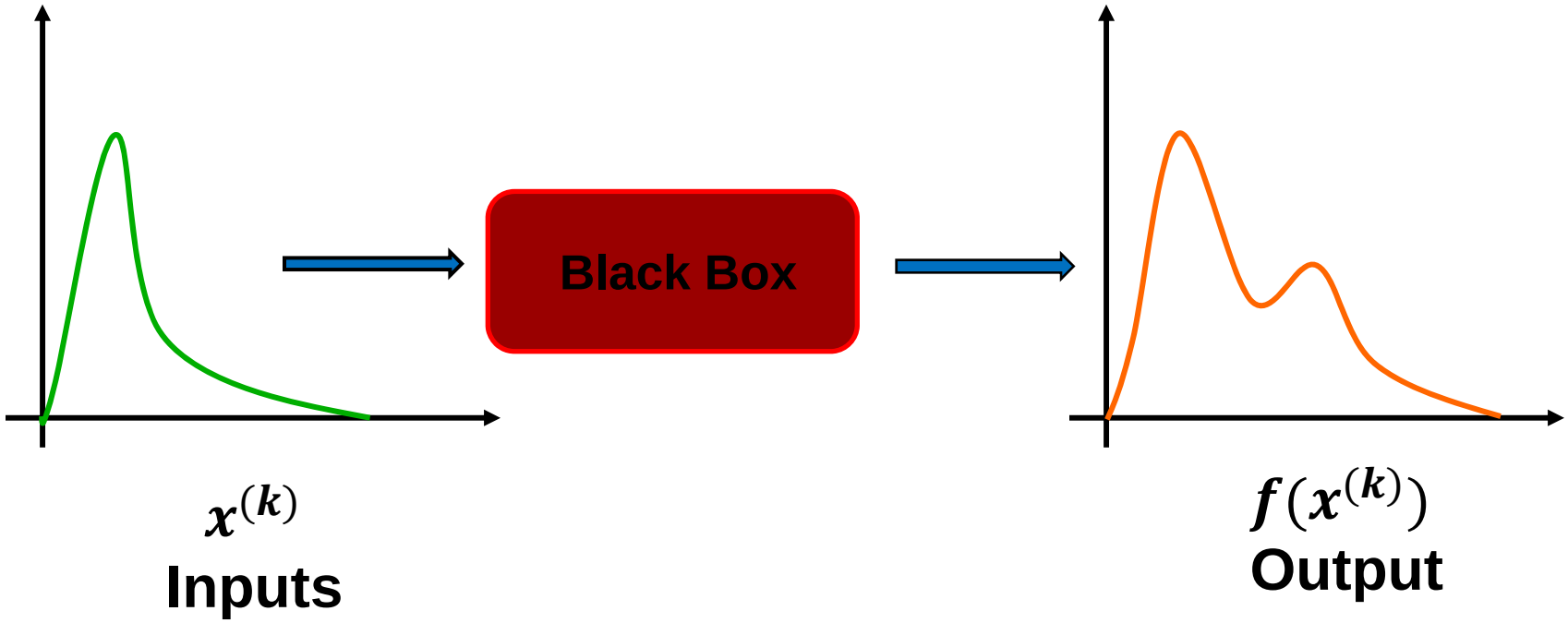
- To obtain *y*, find PC expansion coefficients, a_k
- Express input and response random variables in PC expansion form:

$$y(\vec{x}) = y(\vec{\xi}) = \sum_{k=0}^{P} a_k \psi_k(\vec{\xi}); \qquad x_i = \sum_{j=0}^{t} \lambda_{j1} \psi_i(\xi_i)$$

- Substitute in $y = f(\vec{x})$:

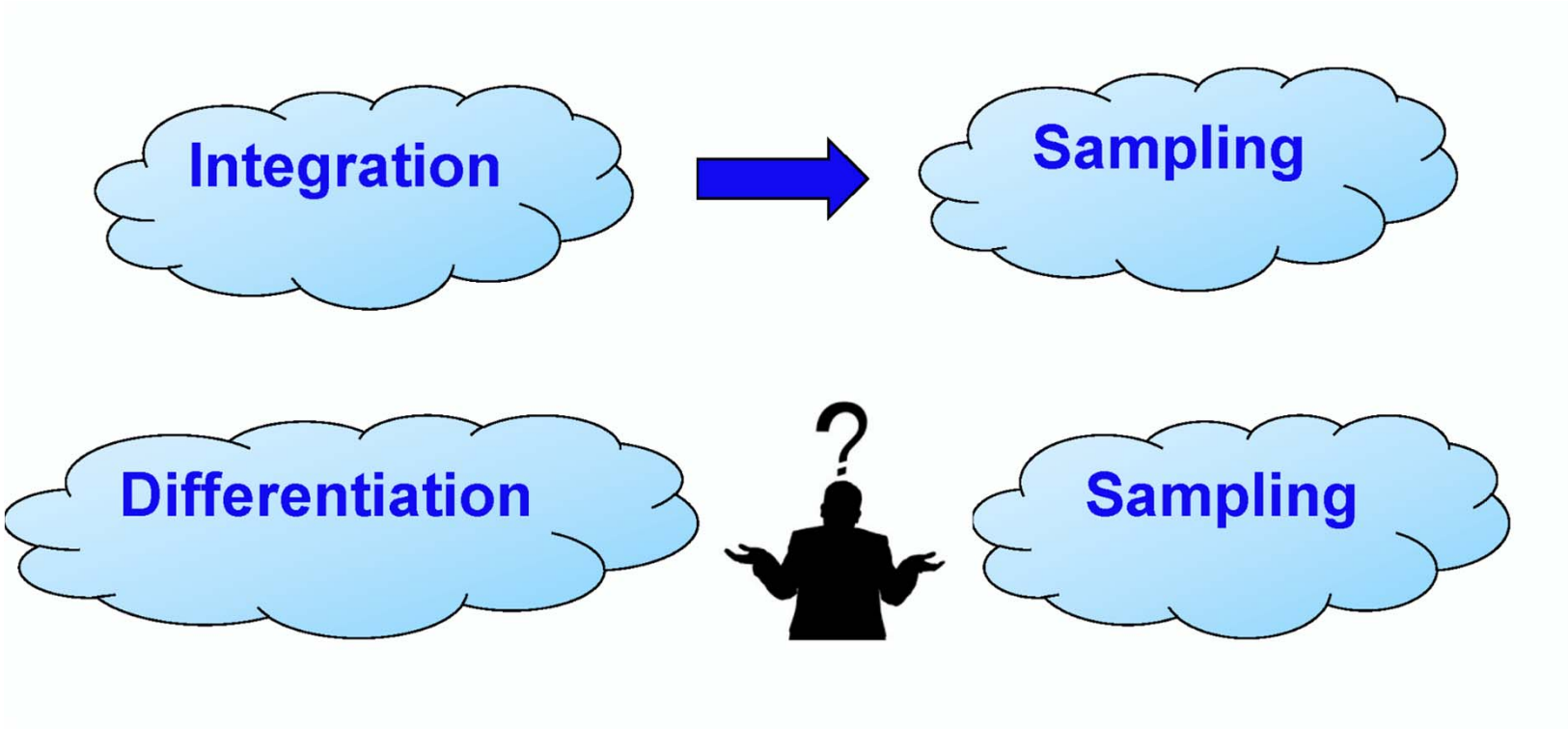
$$\sum_{k=0}^{P} a_k \psi_k(\vec{\xi}) = f\left(\sum_{j=0}^{t} \lambda_{j1} \psi_j(\xi_1), \ldots, \sum_{j=0}^{t} \lambda_{jd} \psi_j(\xi_d)\right)$$

Non Intrusive PC Expansion



- Responses are generated for different realizations of the uncertain inputs
- Software such as ABAQUS, NASTRAN/PATRAN, ANSYS can be used to get the response samples

Polynomial Chaos Expansion



PC Decomposition with Differentiation

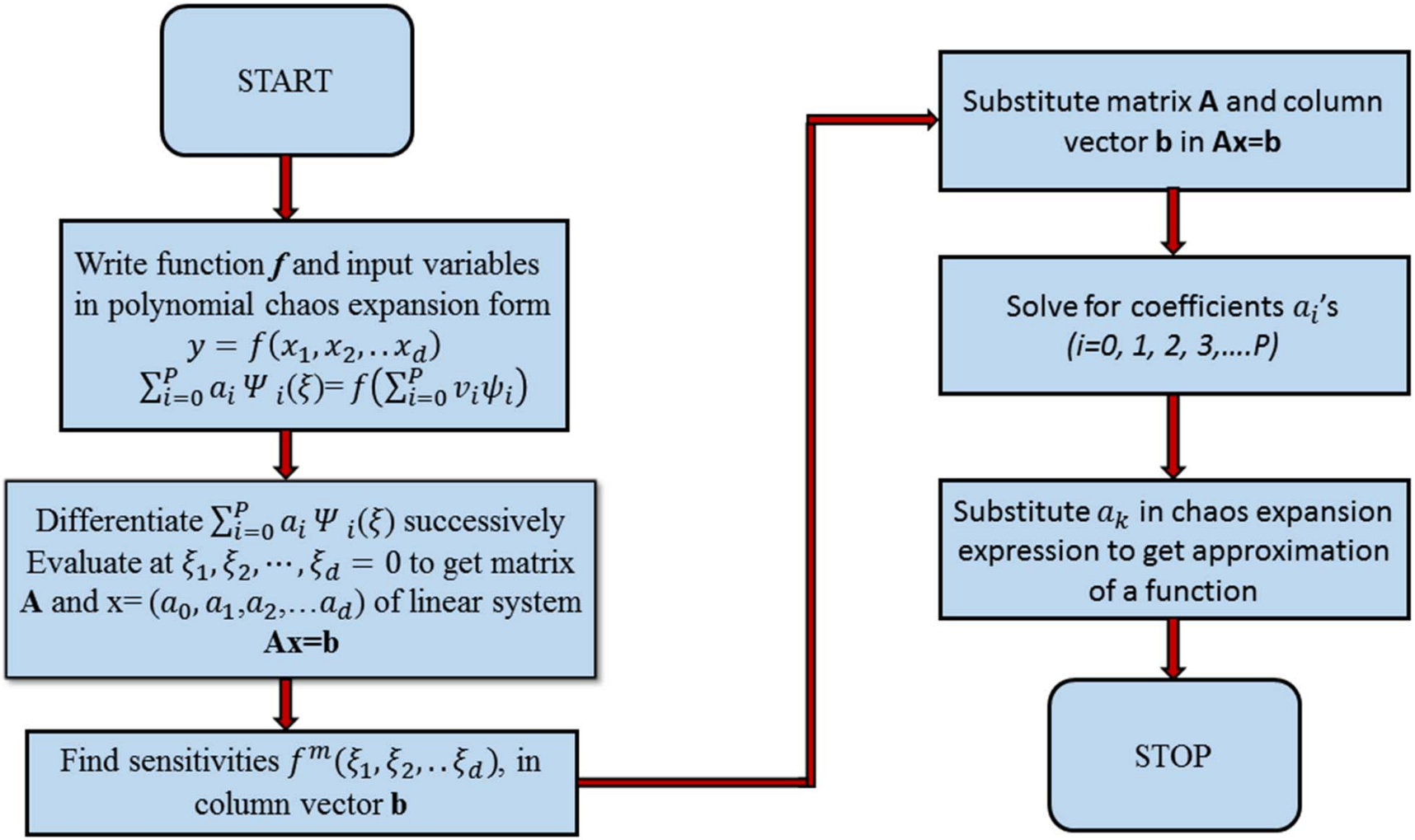
- Differentiate both sides of PC form of response with basis random variables, according to multi-indices
- Multi-indices: $\left(\binom{d}{n}\right) = \binom{d+n-1}{n}$

$$\frac{\partial^{m^{(k)}} \sum_{k=0}^{P} a_k \psi_k(\vec{\xi})}{\partial \xi_1^{m_1^{(k)}} \partial \xi_2^{m_2^{(k)}} \ldots \partial \xi_d^{m_d^{(k)}}} \Big|_{\xi_1, \xi_2, \ldots \xi_d = 0}$$

$$= \frac{\partial^{m^{(k)}} f\left(\sum_{j=0}^{t} \lambda_{j1} \psi_j(\xi_1), \ldots, \sum_{j=0}^{t} \lambda_{jd} \psi_j(\xi_d)\right)}{\partial \xi_1^{m_1^{(k)}} \partial \xi_2^{m_2^{(k)}} \ldots \partial \xi_d^{m_d^{(k)}}} \Big|_{\xi_1, \xi_2, \ldots \xi_d = 0}$$

- P+1 multi-indices gives linear system in the form: ***Ax=b***
- Evaluate at $\xi_1, \xi_2, \ldots \xi_d = 0$ or mean values of RV
- Obtain sensitivities using ModFFD and find a_k

Methodology of PCDD

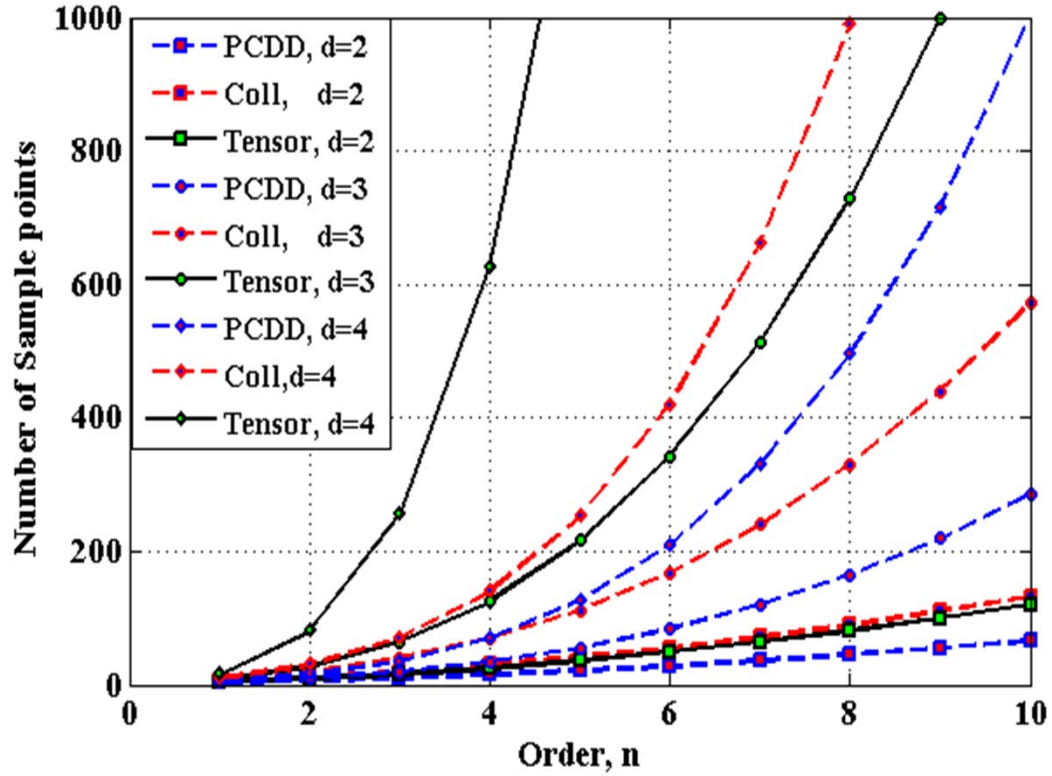


PC Decomposition with Differentiation

- Number of Samples for PCDD:

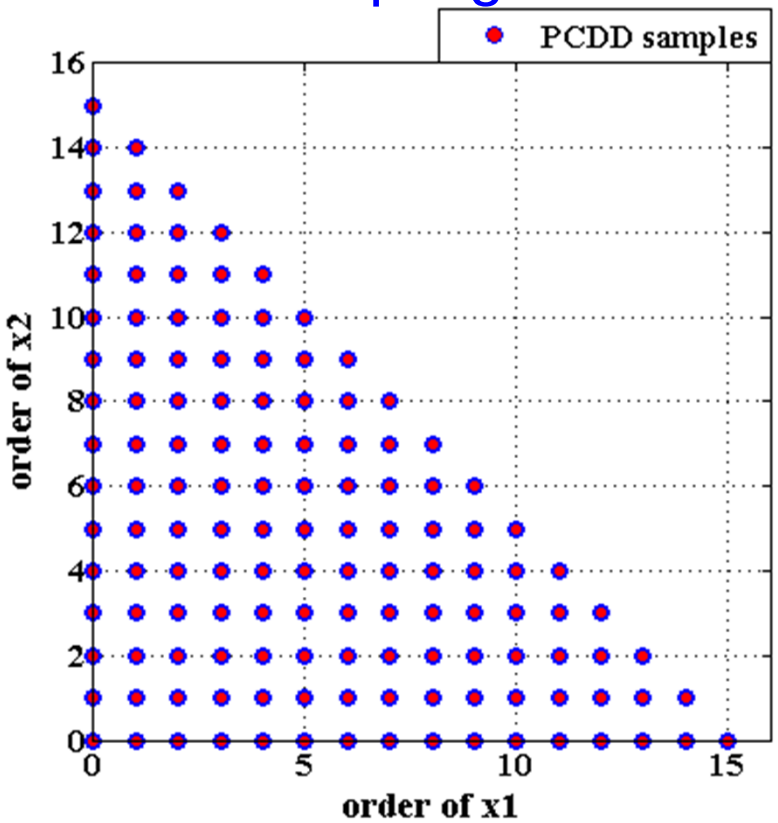
$$P+1=\binom{n+d}{n}=\frac{(n+d)!}{n!d!}$$

- For Quadrature, exponential increase with increase in dimension size➔ **"Curse of Dimensionality"**
- For Stochastic Collocation and PCDD faster rate of convergence



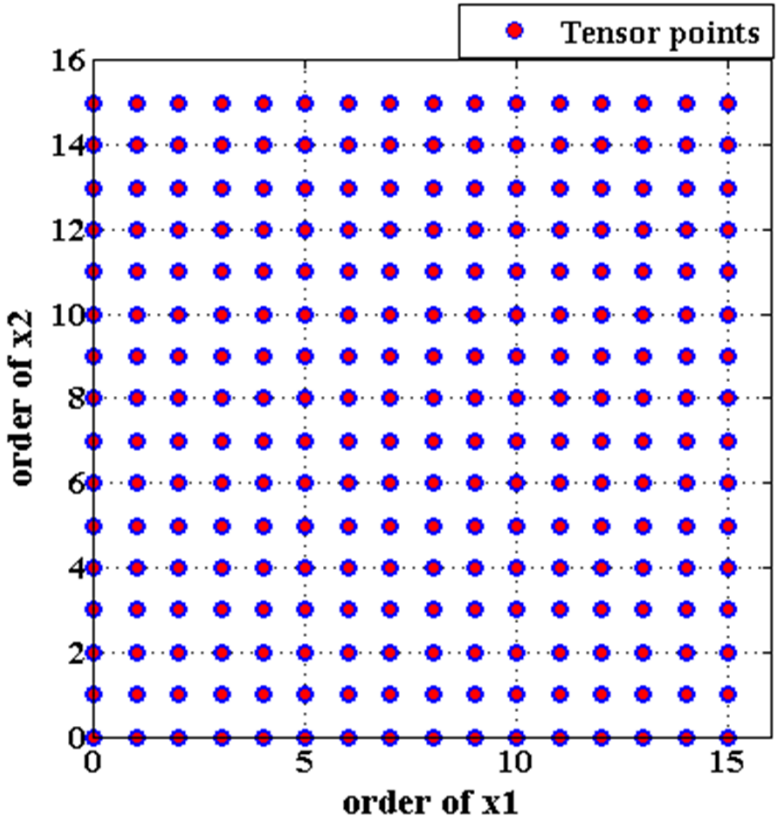
PC Decomposition with Differentiation

Small Sampling Domain



PCDD (*136*)

Large Sampling Domain



Tensor Points (*256*)

Comparison of Samples for *d=2* and *n=15*

Simple Example

$$Y = X^2$$

where X is Normally distributed random variable with mean and standard deviation as x_0 and x_1, respectively.

$$Y = y_0 + y_1\xi + y_2\left(\xi^2 - 1\right) \qquad X = x_0 + x_1\xi$$

Using differentiation technique,

$$\begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix} \begin{Bmatrix} y_0 \\ y_1 \\ y_2 \end{Bmatrix} = \begin{Bmatrix} {x_0}^2 \\ 2x_0x_1 \\ 2{x_1}^2 \end{Bmatrix}$$

- No approximation involved
- PC order of response should depend upon the relationship between input variables and response, not on the magnitude of uncertainty in input variables.
- As order of PC increases, the condition number of PC coefficient matrix increases

Variable Higher Order Sensitivities

- Higher Order Forward Finite Difference (ModFFD), uses Taylor Series expansion up to order *n*

$$f(x_1 + m_1^{(k)} h_1, \ldots, x_d + m_d^{(k)} h_d) = \sum_{j=0}^{P} \frac{f^{m^{(j)}}(x) \prod_{i=1}^{d} (m_i^{(k)} h_i)^{m_i^{(j)}}}{\prod_{i=1}^{d} m_i^{(j)}!} + O(h^{n+1})$$

- Multi-indices represent differentiation order, $|m^{(k)}|$

$$f^{\left(m_1^{(k)}, \ldots m_d^{(k)}\right)}(\vec{x}) = \frac{\partial^{m^{(k)}} f\left(\sum_{j=0}^{t} \lambda_{j1} \psi_j(\xi_1), \ldots, \sum_{j=0}^{t} \lambda_{jd} \psi_j(\xi_d)\right)}{\partial \xi_1^{m_1^{(k)}} \ldots \partial \xi_d^{m_d^{(k)}}} \Big|_{\xi_1, \ldots \xi_d = 0}$$

Methodology for ModFFD

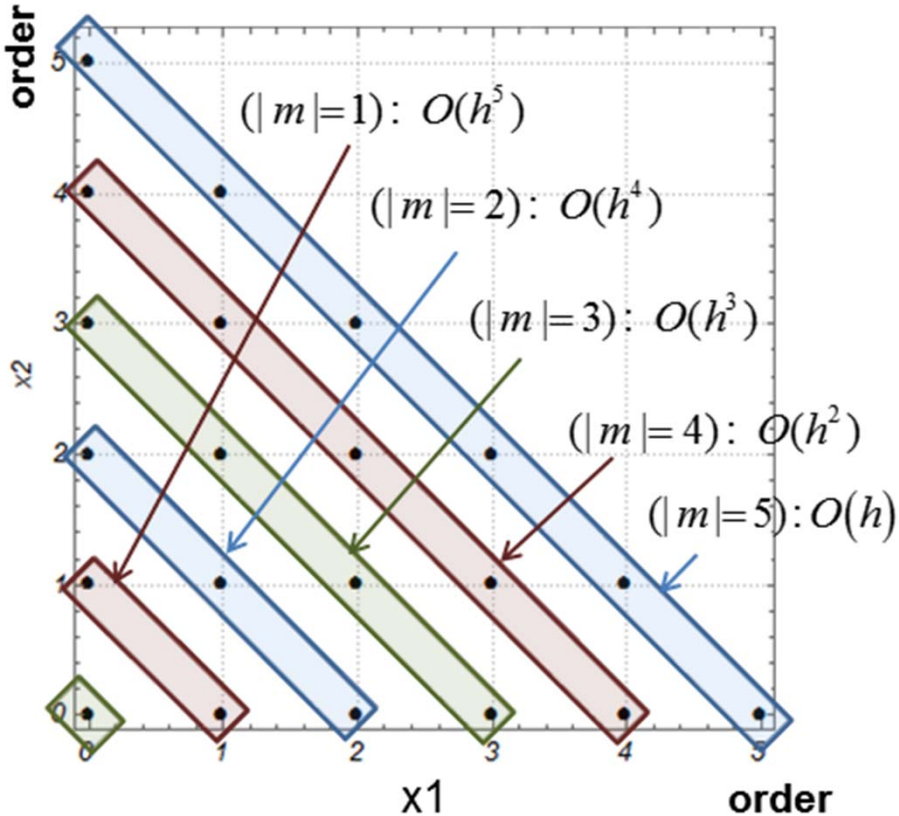
- Change step-sizes $(m_i^{(k)} h_i)$ using multi-indices to obtain ***P+1*** Taylor Series expansion equations and ***C*y=d***
- Unknown sensitivities are in vector, ***y***
- Obtain response values(samples), ***d*** for different realization of random input variables
- The $(P+1) \times (P+1)$ matrix, ***C*** contains components:

$$C(p,q) = \prod_{i=1}^{d} \frac{\left(\Delta h_i * m_i{}^{(p)}\right) \wedge \left(m_i{}^{(q)}\right)}{(m_i)^q!}$$

- Solve to get ***P+1*** sensitivities, $f^{(m)}$

Higher Order Finite Difference

- ModFFD has order of accuracy $\boldsymbol{O\left(h^{n-|m|+1}\right)}$ whereas FOFFD has $\boldsymbol{O(h)}$
- For small sum **|*m*|**, accuracy is high
- For large sum **|*m*|**, accuracy is similar to First Order Forward Finite Difference
- When chaos order increased, accuracy also increases



One-Dimensional Problem

$$y = e^{x}$$

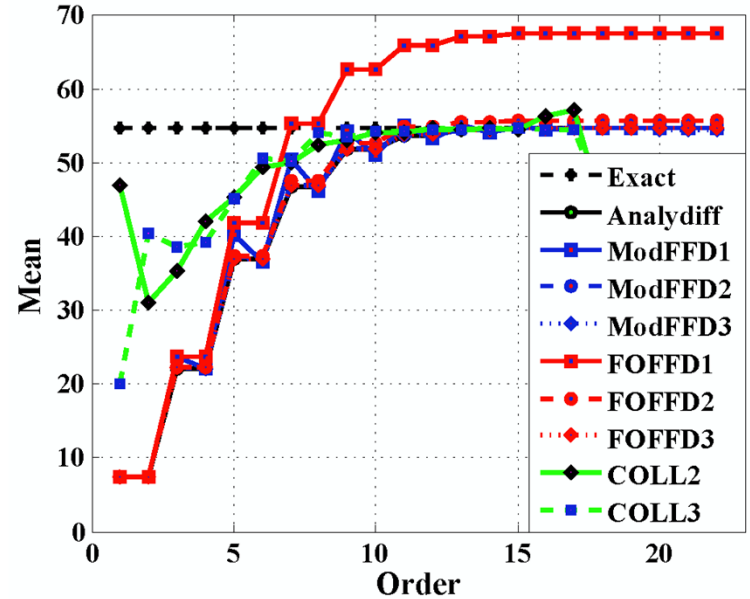
X is normally distributed RV with mean and standard deviation as 2.

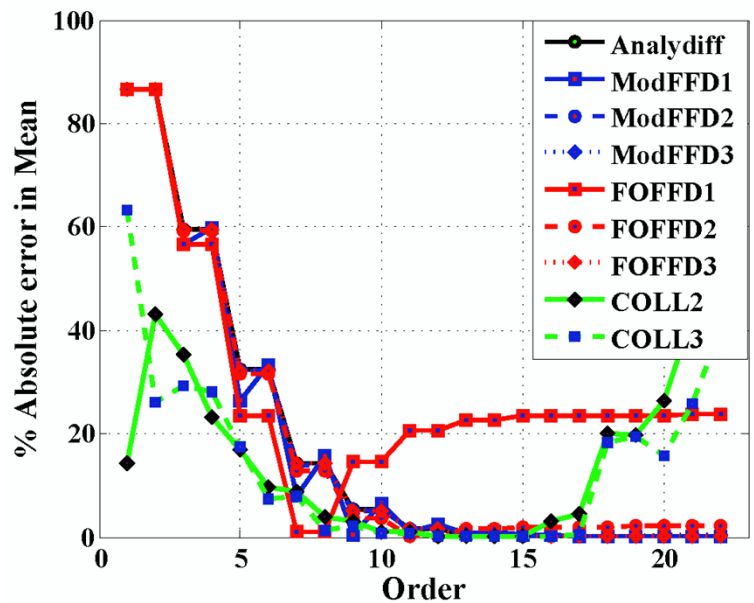
Hence, Y becomes Log-normal random variable

Exact values:

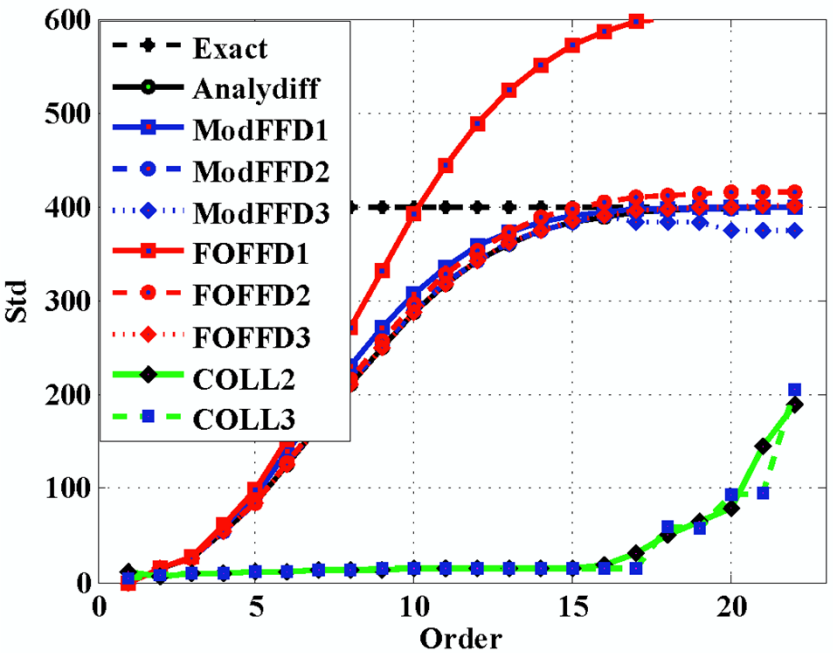
Mean	**54.59812**
Variance	*159773.8*
CoV	*7.3211*

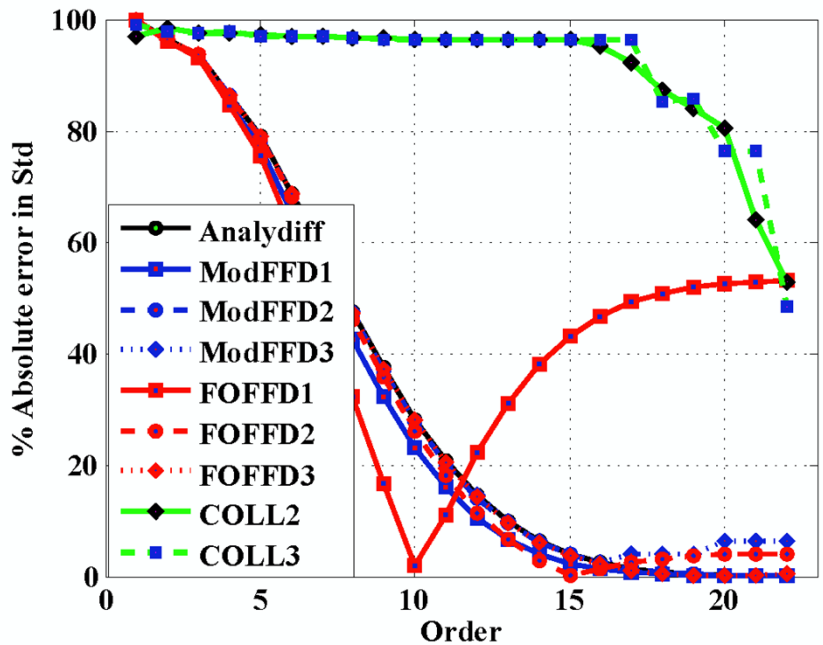
95% confidence bounds for variance with ***1e10*** samples: *[159769.4049, 159778.2621]*





One-Dimensional Problem





- Convergence obtained when chaos order, $n \geq 15$ in Mean and $n \geq 19$ in Std for PCDD
- ModFFD2 and FOFFD2 gave better results
- ModFFD2 has accuracy close to Analydiff
- However, Std obtained with Stochastic Collocation has large error and didn't converge until order n=22

Sensitivity Calculation

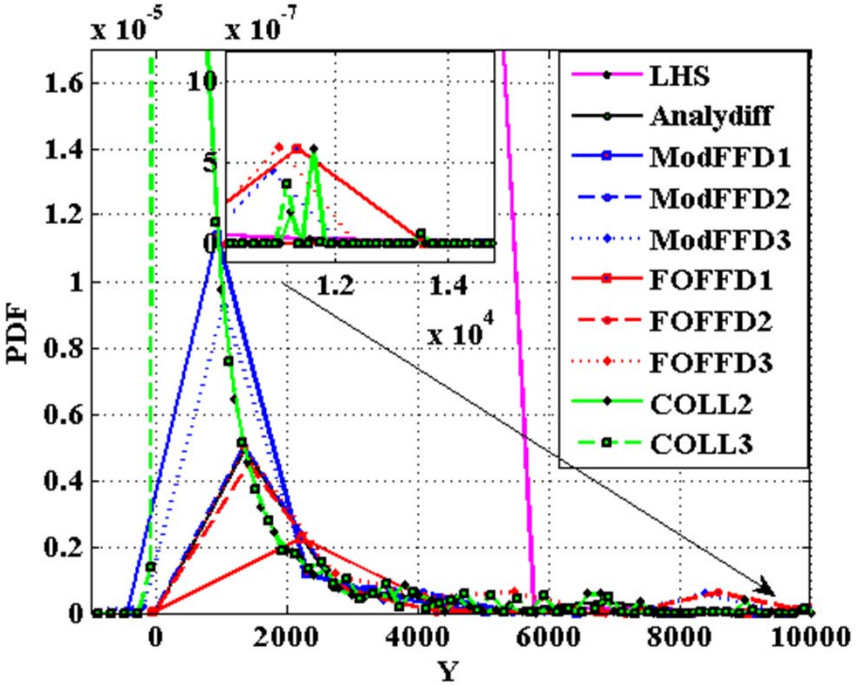
- Sensitivity values obtained for order *n=22*

k^{th} sensitivity	Sensitivities			% Absolute Error in Sensitivities	
	Analydiff	ModFFD2	FOFFD2	ModFFD2	FOFFD2
1	14.7781	14.7781	14.8552	0.0000	0.5016
2	29.5562	29.5562	29.8535	0.0000	1.0058
3	59.1124	59.1124	60.0066	0.0000	1.5125
20	3.8739e+06	3.8747e+06	4.2604e+06	0.0198	9.9745
21	7.7479e+06	7.7029e+06	8.5635e+06	0.5817	10.5263
22	1.5496e+07	1.7213e+07	1.7213e+07	11.0808	11.0808

Accuracy $O(h^{22})$ for 1st Order Sensitivity

Accuracy $O(h^{1})$ for 22nd Order Sensitivity

PDF for 1-D Problem



PDF for $y = e^x$

Chaos Order, *n*=22

Method	% Error of Mean	% Error of Std
Analydiff	*8.307e-4*	*0.131*
ModFFD2	*8.530e-4*	*0.118*
FoFFD2	*2.0311*	*8.302*
COLL, *np=2*	*41.005*	*52.652*

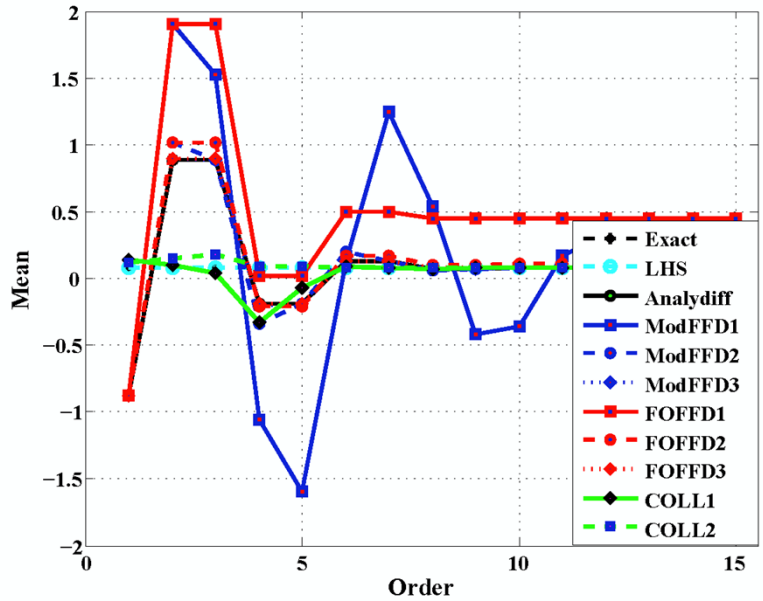
- ModFFD2 and FOFFD2 PDF plots are the best among ModFFD and FOFFD.
- Overall, ModFFD2 follows same pattern and is close to Analydiff
- No Convergence with Stochastic Point-Collocation

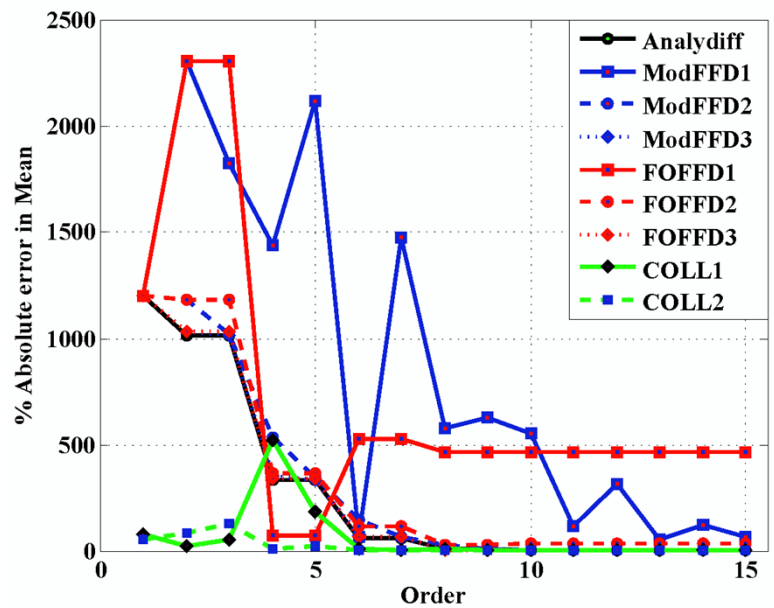
Two-Dimensional Problem

$$y = log(1 + x_1^2)*Sin(5*x_2)$$

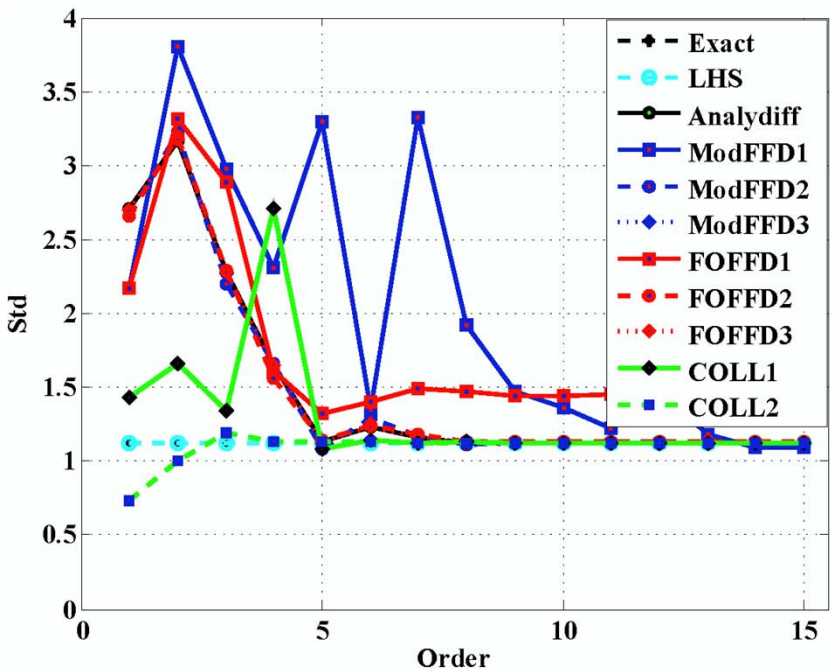
x_1 and x_2 are uniformly distributed with mean *2.0* and PDF1 and PDF2 height=*0.722*

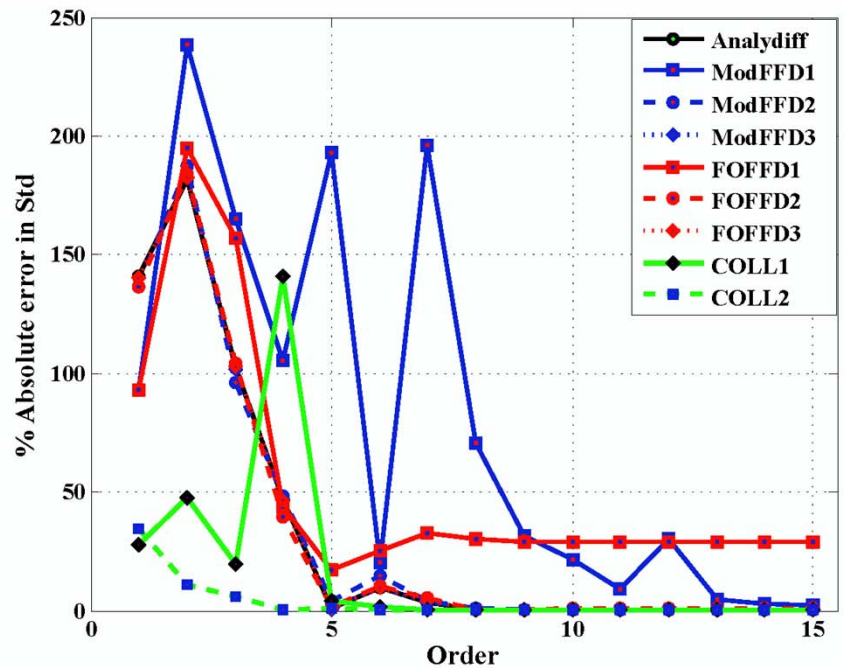
$f(x_1, x_2)$	Mean	Std
$Exact$	*0.0791*	*1.1241*
MC	*0.0778*	*1.1260*
$95\%\ CI\ of\ MC$	*[0.0708, 0.0852]*	*[1.1229, 1.1289]*





Two-Dimensional Problem

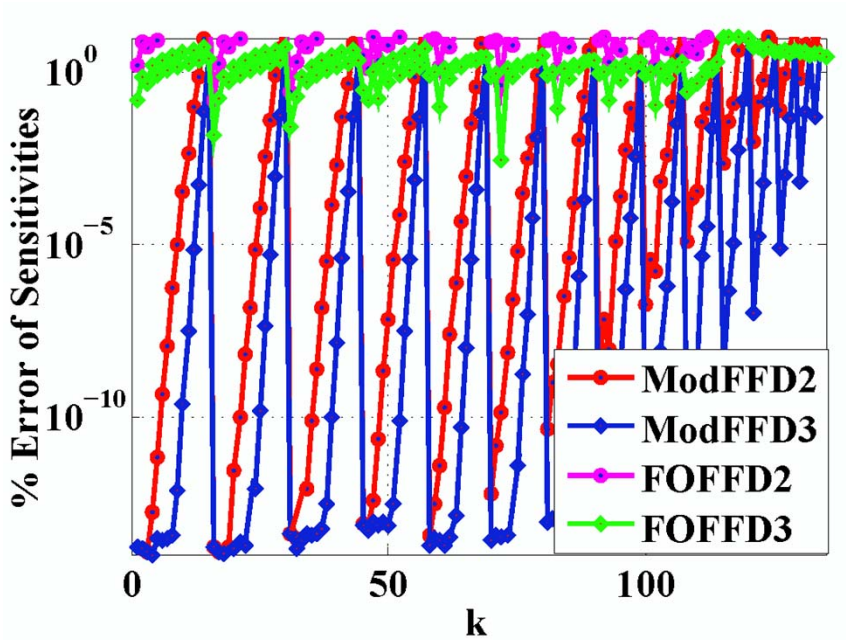




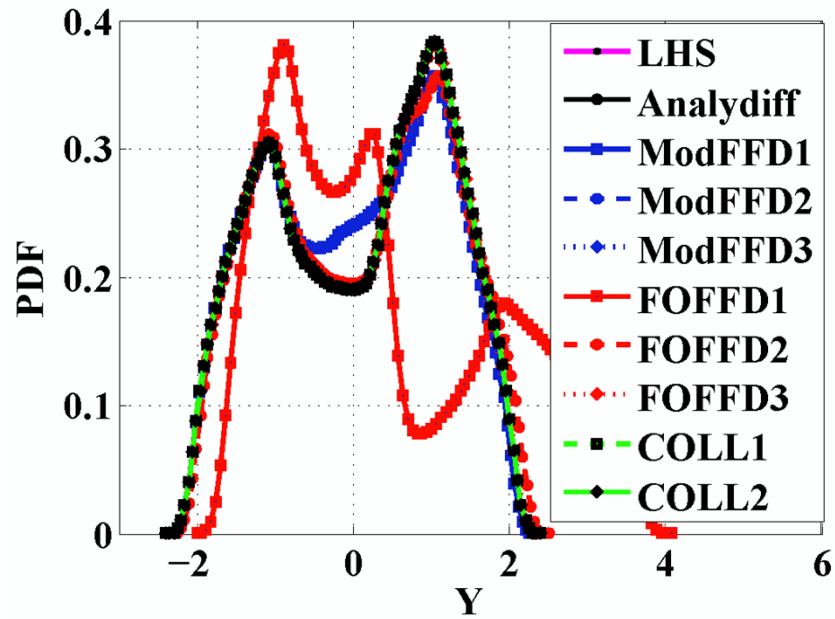
- ModFFD1 with large step-size converged at very high order and FOFFD1 has large error
- Onwards order ***10***, error almost zero for Analydiff, ModFFD2, ModFFD3, FOFFD3
- Stochastic Collocation and ModFFD2 have equivalent performance

Two-Dimensional Problem

For ***d=2*** and ***n=15*** → ***136 terms***



Sensitivities



PDF

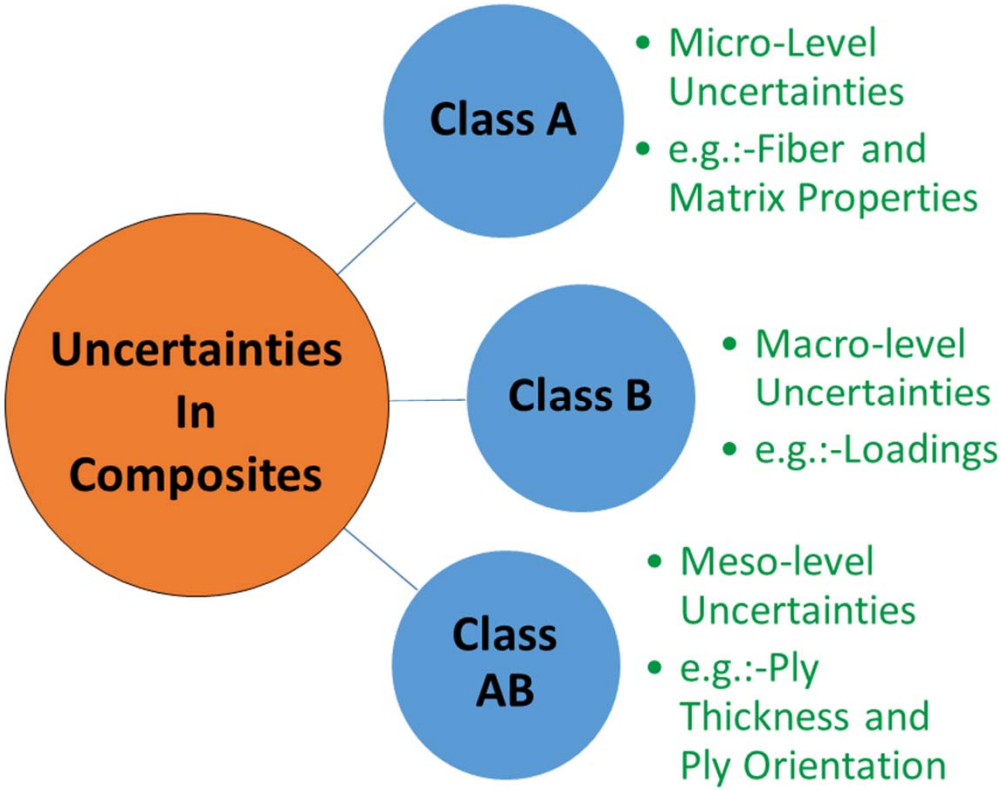
- ModFFD has mostly negligible error
- Few sensitivities of ModFFD with order ***n=15***, have error ≥ ***5%***, similar to FOFFD

- PDF plots of the Analydiff, ModFFD2, and Colloc2 are similar to LHS simulations

Composite Laminate Problems

- Uncertainties exist at different level of Composite
- Accumulates as we go higher level
- Affects overall performance and reliability
- Uncertainty type: - I). Epistemic, due to inherent randomness in input parameters and II). Aleatory, due to uncertainties in mathematical models
- Prevalent methods for UQ in Composites: Sampling techniques and Perturbation approaches
- Spectral approaches with higher accuracy are being used more recently

Uncertainties in Composites



Epistemic Uncertainties in Composites

- Class AB captures uncertainties at different scales, so modeling generally preferred at meso-scale

Macroscale Modelling

- Uncertainties considered at ply-level
- Two cases studied: **I)** Uncertain material properties ***(4 RV)*** **II)** Uncertain material and geometric properties ***(20 RV)***
- Deterministic model is Eight layered, simply-supported plate under uniform pressure on top surface (***11,000 Pa***)
- MSC.NASTRAN used as ***black box*** to generate response for samples
- PCDD Samples are generated using step-sizes:

$$\frac{\Delta x_i}{x_{i,mean}} \approx 10^{-2}$$

- LHS simulation, PCDD, and Stochastic Point-Collocation (COLL) used to obtain stochastic responses,

Macroscale Modelling

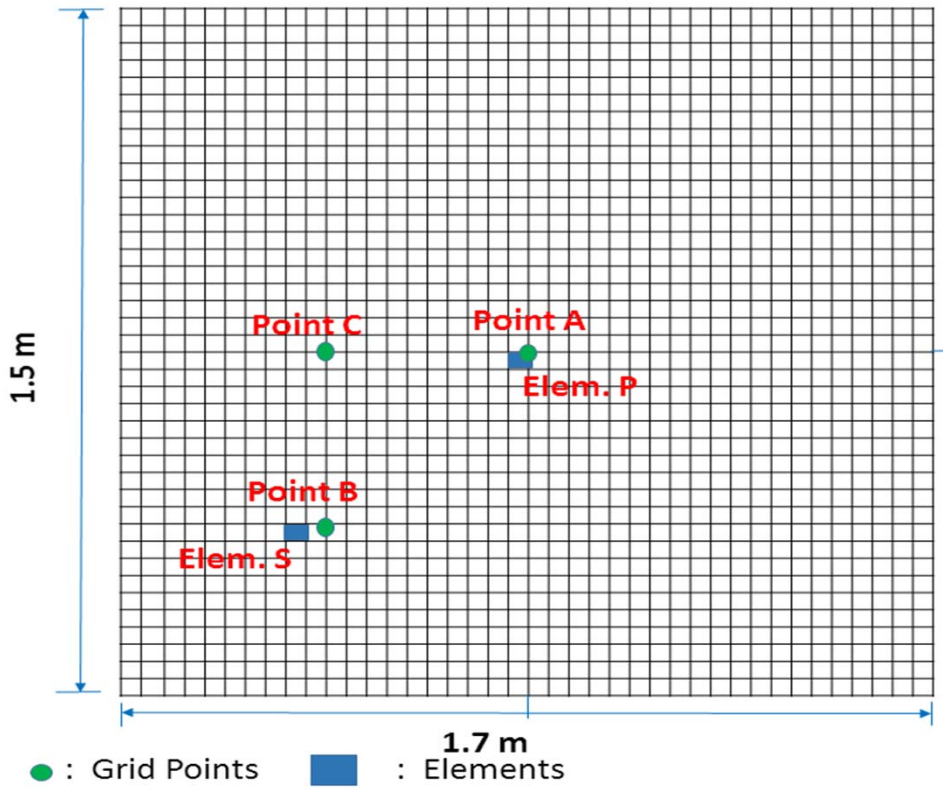
Material and Geometric Properties of CFRP laminate

Random

Type	Random Variables	Mean	Std
Material Properties	$E_{11}\ (GPa)$	142.215	7.366
	$E_{22}\ (GPa)$	8.555	0.343
	ν_{12}	0.251	0.091
	$G_{12}\ (GPa)$	4.376	0.216
Geometric Properties	$t_i\ (mm),\ i = 1,2,\ldots,8$	4.7	0.5
	$\theta_1,\ \theta_3,\ \theta_6,\ \theta_8\ (\mathrm{deg})$	0	10
	$\theta_2,\ \theta_4,\ \theta_5,\ \theta_7\ (\mathrm{deg})$	90	10
Plate Dimensions	Length (a=1.7 m), & Width (b=1.5 m)		

- All input random variables have ***Gaussian Distribution***
- Assume Mean values of Geometric properties for ***4 RV*** problem

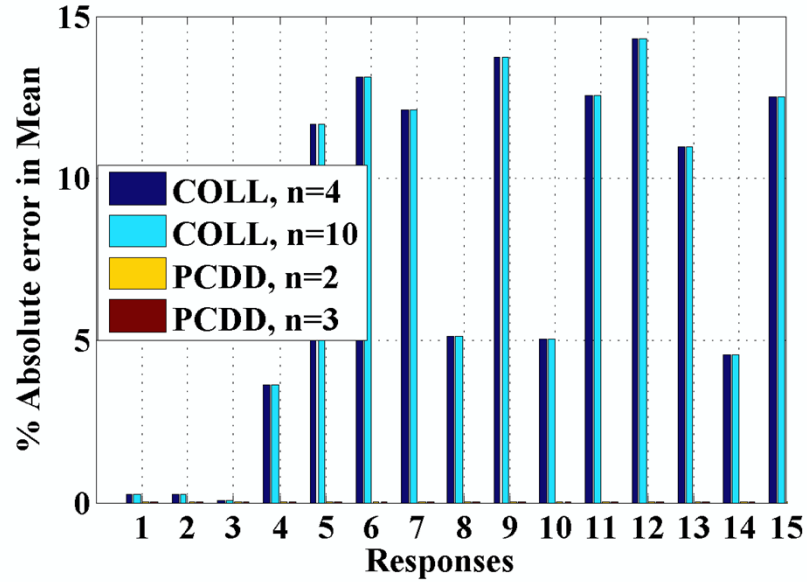
Mesh of a Composite Laminate

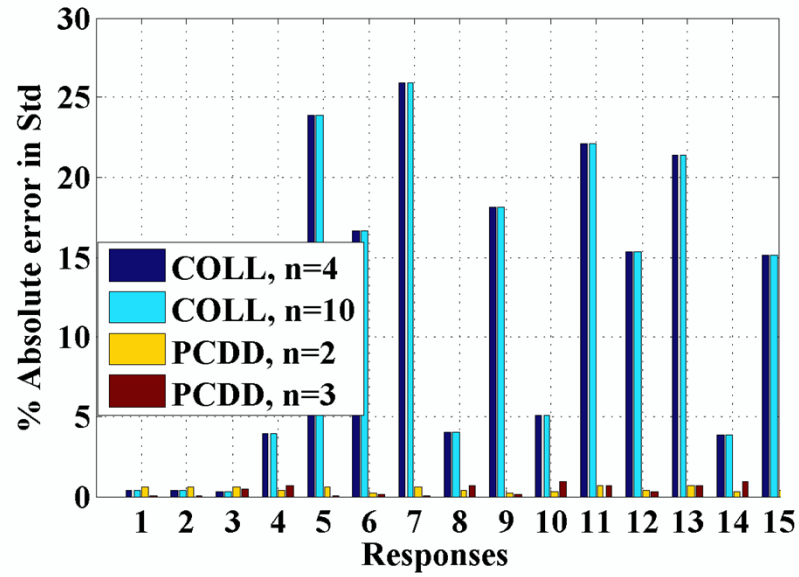


$\mathbf{40 \times 40}$
$\boldsymbol{QUAD4\ 2D}$
elements

- Transverse displacements calculated at Grid Points A, B, and C $(y_i, i = 1, 2, 3)$
- In-plane stresses calculated for top and bottom layer of Element P and Element S $(y_i, i = 4, \ldots, 15)$

Macroscale Modeling: Problem 1





- Effective Material Properties $(E_1, E_2, \nu_{12}, G_{12})$ as Uncertain inputs
- For all the ***15*** responses, PCDD has negligible error in Mean and less error in Std
- Stochastic Point-Collocation did not yield accurate results even with chaos order ***10 (using 2,002 LHS samples)***

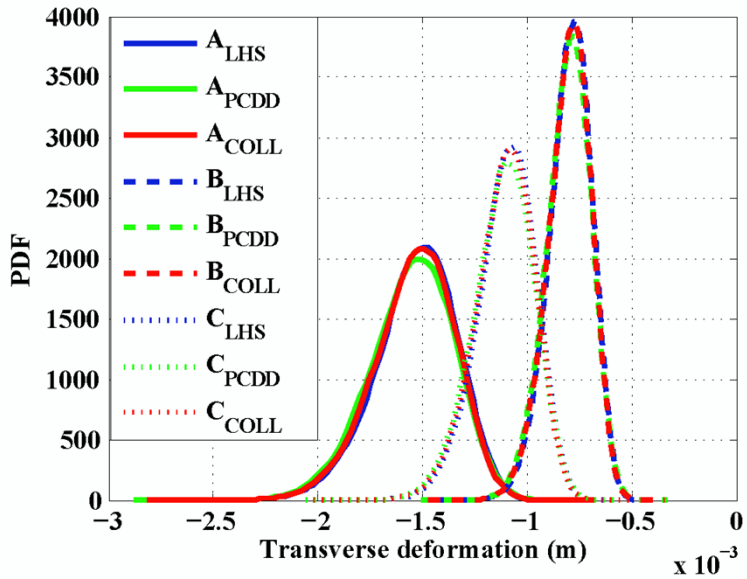
Macroscale Modeling: Problem 2

- Effective Material Properties ($E_1, E_2, \nu_{12}, G_{12}$) and Geometric Properties (θ_i and t_i) are uncertain➔ ***20 random inputs***

Response	LHS simulations		PCDD, *n=2*		COLL, *n=3*	
	Mean	*Std*	*Mean*	*Std*	*Mean*	*Std*
w_A	*-1.533*	*0.195*	*-1.551*	*0.201*	*-1.540*	*0.196*
w_B	*-0.796*	*0.102*	*-0.804*	*0.105*	*-0.800*	*0.1033*
w_C	*-1.101*	*0.139*	*-1.114*	*0.144*	*-1.109*	*0.140*
$\sigma_{max}\|_{,S_t}$	*-0.555*	*0.158*	*-0.544*	*0.159*	*-0.577*	*0.159*
$\sigma_{min}\|_{,S_t}$	*-6.458*	*1.770*	*-6.394*	*1.763*	*-5.755*	*1.719*
$\tau_{max}\|_{,S_t}$	*2.951*	*0.941*	*2.924*	*0.932*	*2.589*	*0.915*
$n_{samples}$ for best results	***50,000***		***231***		***3,542***	

Units: w (***mm***) and stresses (***MPa)***

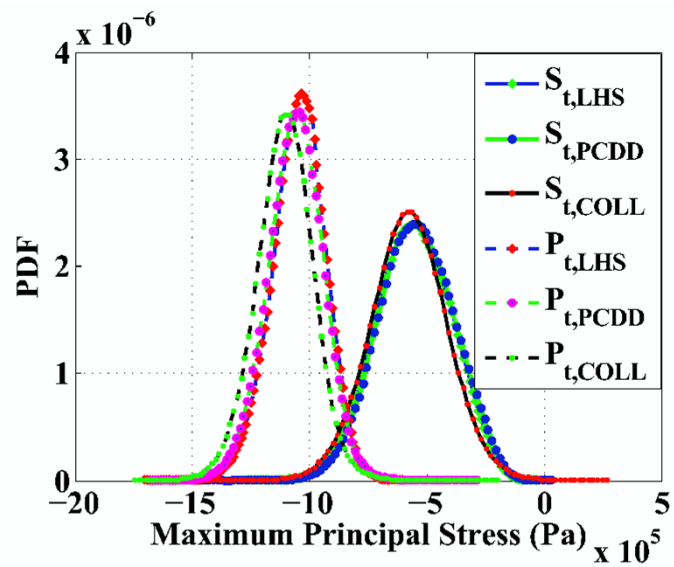
Macroscale Modeling: Problem 2

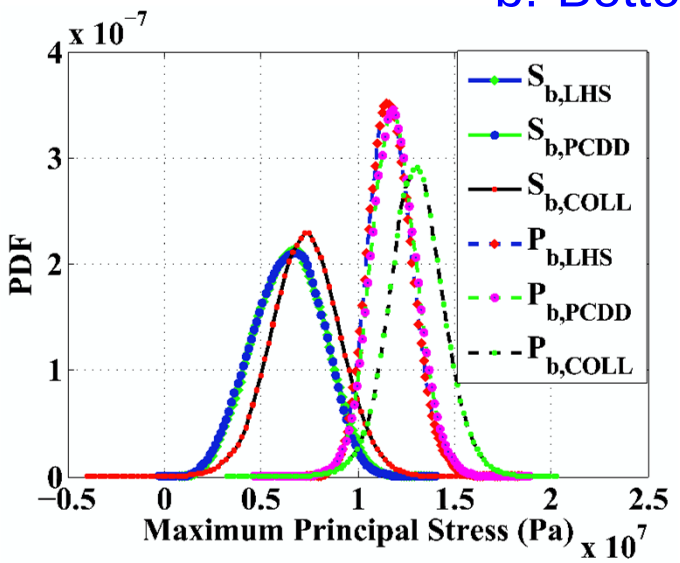


Subscripts for Stresses

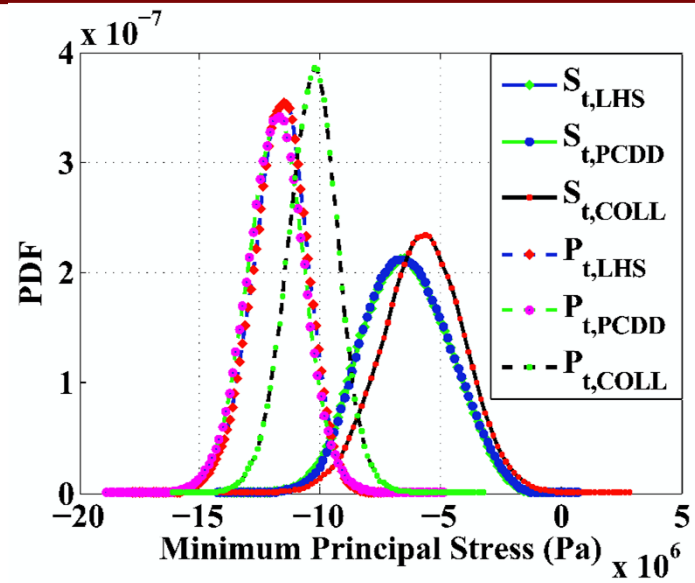
t:- Top Layer

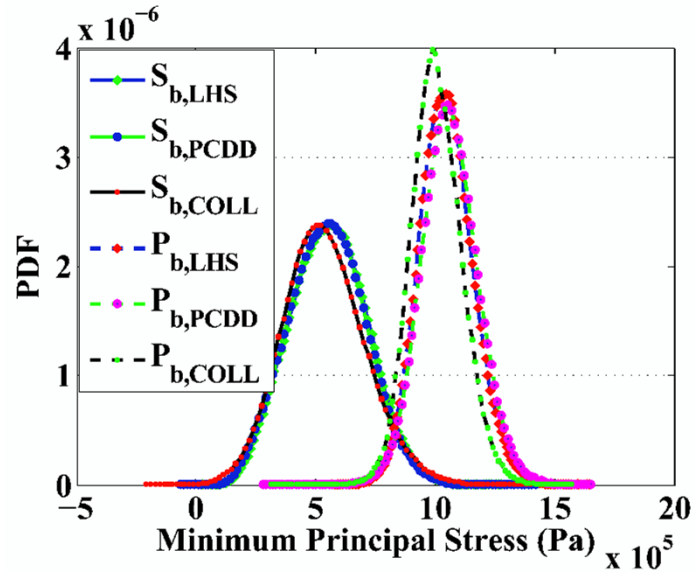
b:-Bottom Layer

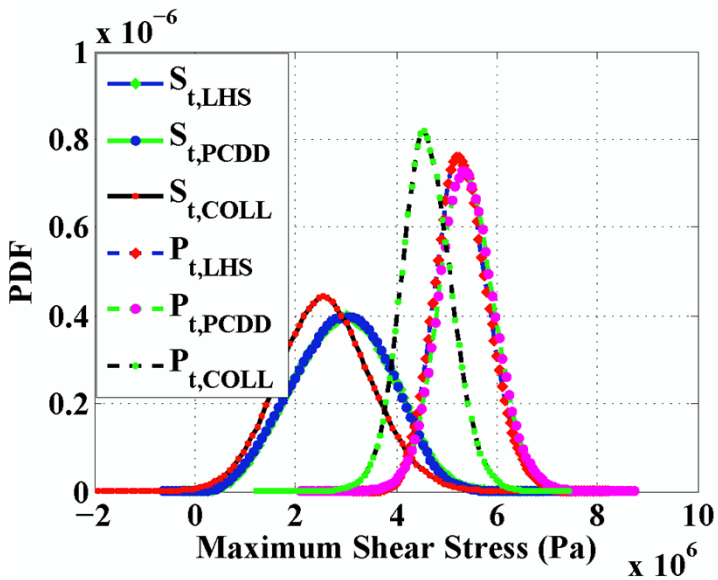


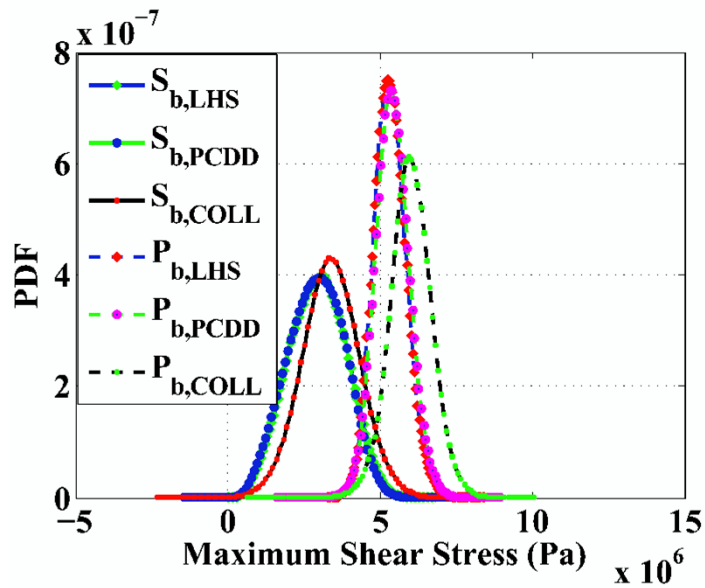


Macroscale Modeling: Problem 2

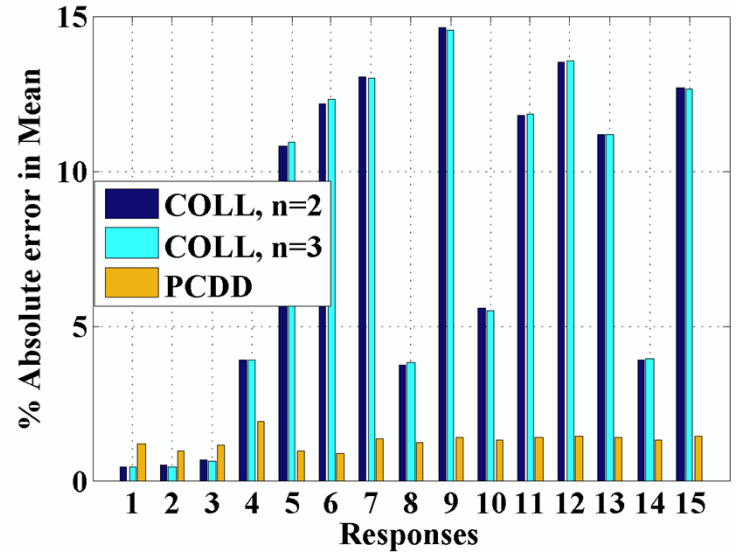


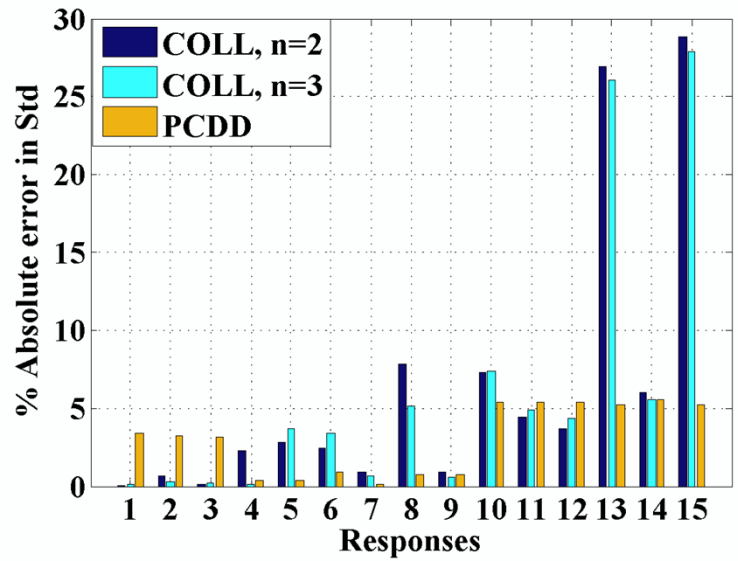






Macroscale Modeling: Problem 2





- For PCDD, responses y_i, ***i=4-9*** required ***n=2*** (***231*** samples) while remaining responses required ***n=3*** (***1,771*** samples)
- Transverse displacements with COLL are more accurate than PCDD whereas in-plane stresses with PCDD have less error in both Mean and Std
- With COLL less accurate solution obtained for stresses even with ***n=3*** (***3,542*** *samples*) and higher error with ***n=4*** (***21,252*** samples)

Macroscale Modeling: Problem 2

- For transverse displacements and stresses, less than ***2%*** error in mean
- Displacements have max. error of almost ***3%*** and stresses have max. error of ***5%*** in standard deviation
- With Stochastic Collocation only the transverse displacements are accurate
- Using ***231*** samples, provided similar results to ***50,000*** LHS simulations and more accurate than Stochastic Collocation

Multiscale Modeling

- Uncertainties considered starting from constituents (fiber and matrix) level that results in uncertain Material properties and uncertain responses
- Geometric Uncertainties also considered
- UQ for multiscale can be performed in two ways:
  i. First obtain stochastic model for Material properties using PCDD with uncertain constituents inputs, then obtain stochastic responses
  ii. Directly obtain stochastic model for responses without finding stochastic model for Material properties
- First method is preferred in Multiscale analysis for use with commercial software, like ***MSC.NASTRAN***

Multiscale Modeling: Microscale

- Uncertainties in fiber and matrix properties considered ($E_{11}^{f}, E_{22}^{f}, E^{m}, V_{f}, \upsilon_{12}^{f}, \upsilon^{m}, G_{12}^{f}$)
- Random inputs are represented using PC expansion, for instance,

$$E_{11}^{f} = \sum_{j=0}^{t1} \lambda_{j1} \psi_{j}\left(\xi_{1}\right)$$

- Existing micromechanics models can be used

  e.g.:- Voight, Reuss, Halpin Tsai, Method of Cells
- Highly accurate Halpin Tsai model used
- Instead of micromechanics model, FEM can be used, but computationally expensive

Multiscale Modeling: Microscale

- Effective Material Properties of a Lamina considered as random, $E_1, E_2, \nu_{12}, G_{12}$
- **Longitudinal Modulus of Elasticity, (E_1)**

$$E_1 = E_{11}^f V_f + E^m (1 - V_f); \quad \text{and} \quad E_1(\xi_1, \xi_3, \xi_4) = \sum_{k=0}^{P1} E_{1k} \psi_k(\xi_1, \xi_3, \xi_4)$$

- **Transverse Modulus of Elasticity, (E_2)**

$$E_2 = E_m \left(\frac{1 + \xi \eta V_f}{1 - \eta V_f} \right); \quad \text{where} \quad \eta = \frac{\left(\frac{E_{2f}}{E_m} \right) - 1}{\left(\frac{E_{2f}}{E_m} \right) + \xi}$$

ξ :- curve fitting parameter dependent on fiber packing arrangement

where $\xi = 2$ (for E_2, while using circular fibers)

$$E_2(\xi_2, \xi_3, \xi_4) = \sum_{k=0}^{P2} E_{2k} \psi_k(\xi_2, \xi_3, \xi_4)$$

Multiscale Modeling: Microscale

Major Poisson's Ratio, (ν_{12})

$$\upsilon_{12} = \upsilon_{12}^{f} V_f + \upsilon^{m}(1 - V_f); \quad \text{and} \quad \upsilon_{12}(\xi_4, \xi_5, \xi_6) = \sum_{k=0}^{P3} \upsilon_{12k} \psi_k(\xi_4, \xi_5, \xi_6)$$

Shear Modulus of Elasticity, (G_{12})

$$G_{12} = G_m \left(\frac{1 + \xi \eta V_f}{1 - \eta V_f} \right); \quad \text{and} \quad \eta = \frac{\left(\frac{G_f}{G_m} \right) - 1}{\left(\frac{G_f}{G_m} \right) + \xi}$$

where $\xi = 1$. Matrix is isotropic, $G_m = \dfrac{E_m}{2(1 + \upsilon_m)}$

Hence,

$$G_{12}(\xi_3, \xi_4, \xi_6, \xi_7) = \sum_{k=0}^{P4} G_k \psi_k(\xi_3, \xi_4, \xi_6, \xi_7)$$

Multiscale Modeling: Macroscale

- Performance behavior of Composite depends on stochastic effective material properties and geometric properties
- Stochastic response can be represented as:-

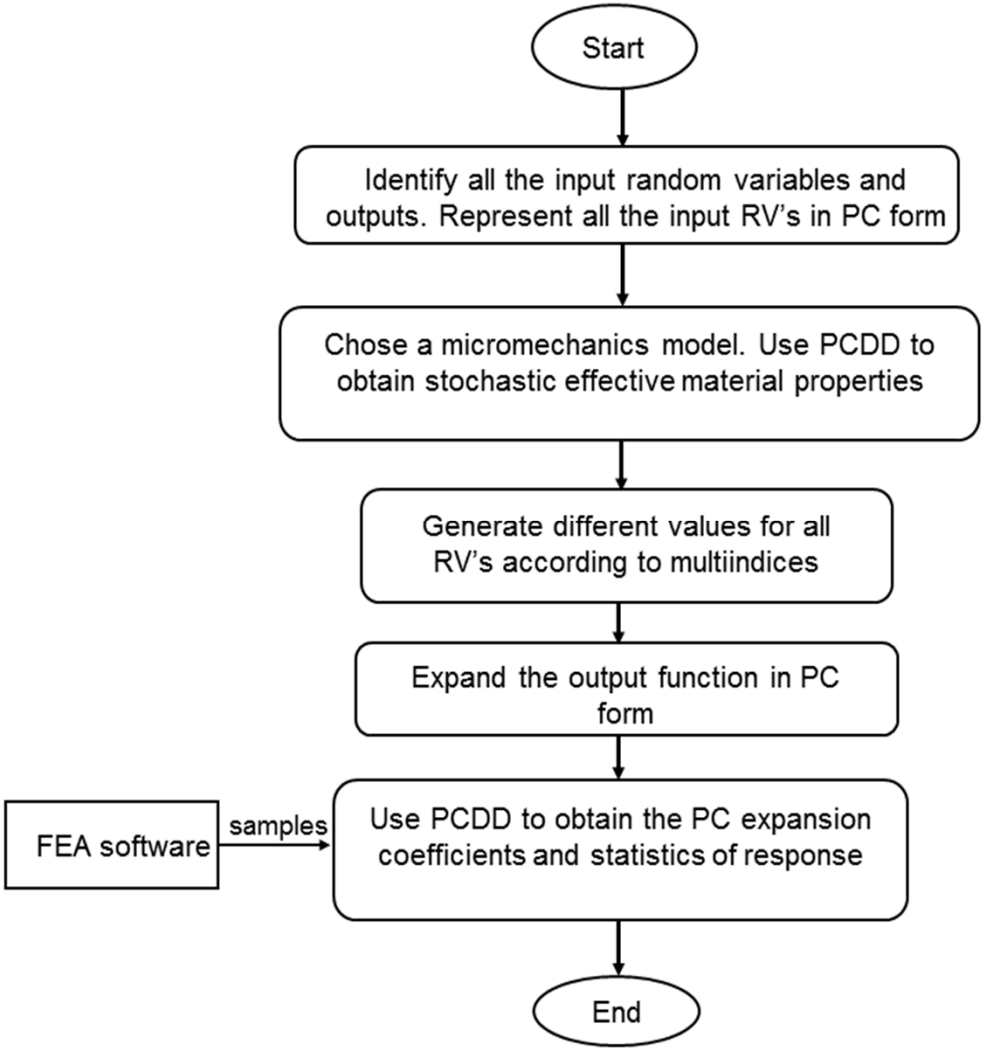
$$f = f\left(E_{11}^{f}, E_{22}^{f}, E^{m}, V_{f}, \upsilon_{12}^{f}, \ \upsilon^{m}, G_{12}^{f}, t_1, \ldots, t_8, \theta_1, \ldots, \theta_8\right)$$
$$= f\left(\xi_1, \xi_2, \ldots, \xi_7, \xi_8, \ldots, \xi_{15}, \xi_{16}, \ldots, \xi_{23}\right)$$

- The constitutive equation using CLPT is:-

$$\left\{\frac{N\left(\vec{\xi}\right)}{M\left(\vec{\xi}\right)}\right\} = \left[\frac{A\left(\vec{\xi}\right) \quad | \quad B\left(\vec{\xi}\right)}{B\left(\vec{\xi}\right) \quad | \quad D\left(\vec{\xi}\right)}\right]\left\{\frac{\varepsilon^{0}\left(\vec{\xi}\right)}{\kappa\left(\vec{\xi}\right)}\right\}$$

- However, PCDD uses deterministic codes (here ***MSC.NASTRAN***) as black box and requires no modification of constitutive equations

Multiscale Modeling



Multi-scale Modeling Framework of CFRP Composite Laminate

Multiscale Modeling

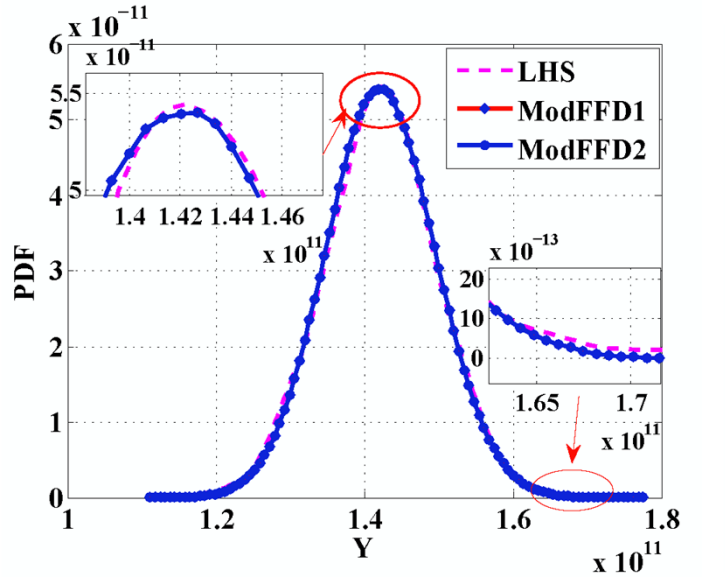
- Eight layered, simply-supported edges under uniform pressure on top surface (***11,000 Pa***)
- **MSC.NASTRAN** used with $\mathbf{20 \times 20}\ \boldsymbol{QUAD4\ 2D}$ elements
- All ***23*** input random variables have ***Gaussian Distribution***

Type	Random Variables	Mean	Std
Constituents Material Properties	$E_{11}^{f}\ (MPa)$	$2.137*10^5$	$1.034*10^5$
	$E_{22}^{f}\ (MPa)$	$1.380*10^5$	690.000
	$E^{m}\ (MPa)$	0.200	0.010
	ν_{12}^{f}	0.251	0.091
	ν^{m}	0.350	0.017
	V_f	0.660	0.013
	$G_{12}^{f}\ (MPa)$	$1.380*10^4$	690.000
Geometric Properties	$t_i\ (mm),\ i = 1,2,\ldots,8$	4.7	0.5
	$\theta_1,\ \theta_3,\ \theta_6,\ \theta_8$ (deg)	0	10
	$\theta_2,\ \theta_4,\ \theta_5,\ \theta_7$ (deg)	90	10
Plate Dimensions	Length (a=1.7 m), & Width (b=1.5 m)		

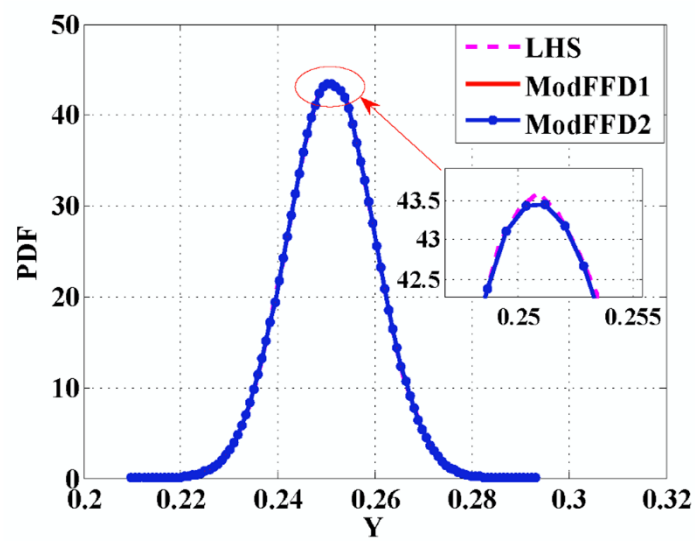
- Constituents material properties and geometric properties are random

Multiscale Modeling: Results

- Four Stochastic Material Properties model
- ModFFD1, ModFFD2, and ModFFD3 represents the PCDD using ModFFD with step-sizes ***(h=1e-1, h=1e-2, h=1e-3). Compared with 1e+06 LHS simulations***



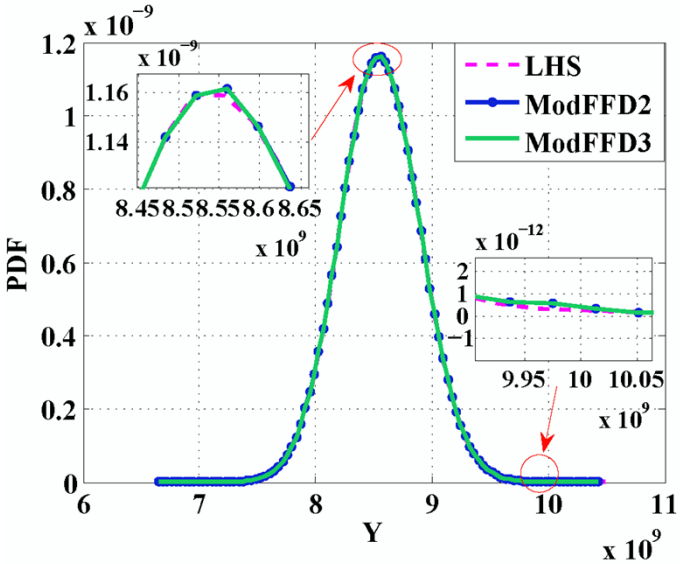
E_1



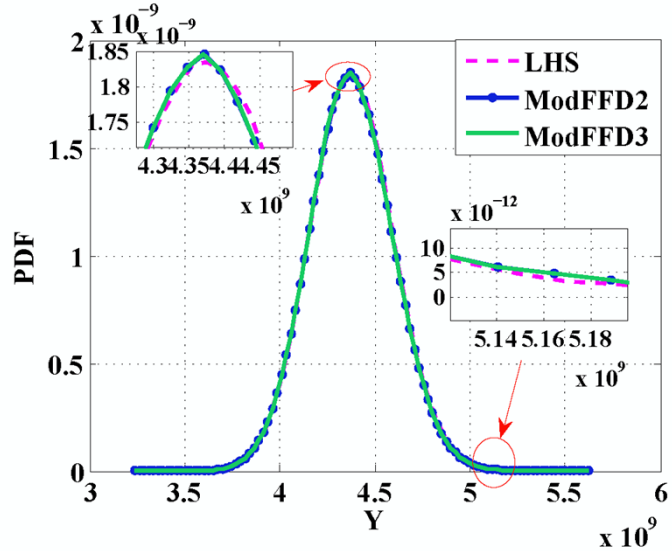
ν_{12}

- **Convergence with Order *2* and *10* Samples**
- **Convergence with Order *2* and *10* Samples**

Multiscale Modeling: Results



E_2



G_{12}

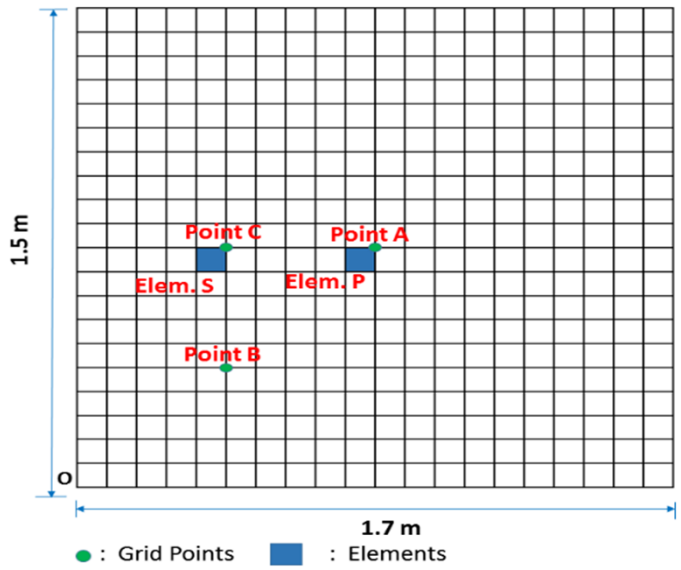
- **Convergence with Order *4* and *35* Samples**
- **Convergence with Order *5* and *56* Samples**

Method	E_1 (GPa)		E_2 (GPa)		ν_{12}		G_{12} (GPa)	
	Mean	Std	Mean	Std	Mean	Std	Mean	Std
PCDD	142.215	7.366	8.555	0.343	0.251	9.11e-3	4.736	0.216
LHS	142.215	7.356	8.555	0.343	0.251	9.11e-3	4.380	0.217
% Error	3.73e-4	1.60e-1	6.40e-5	3.48e-2	2.86e-5	4.15e-2	8.50e-2	5.67e-2

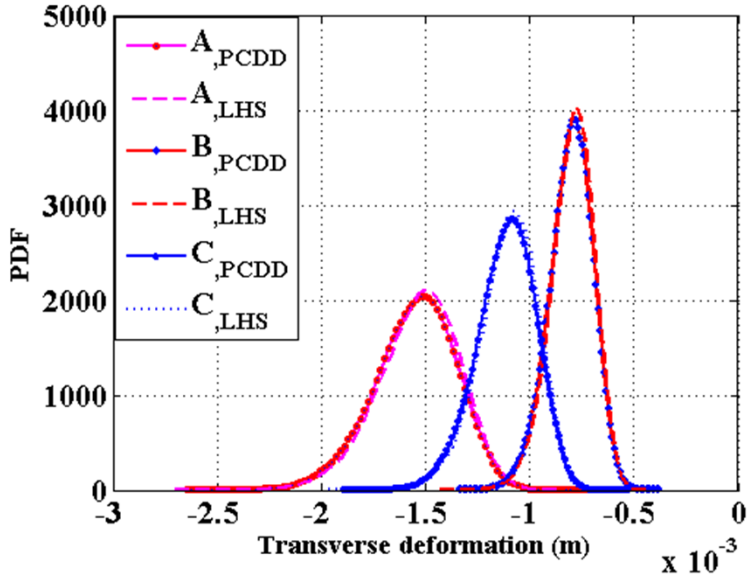
Highly Accurate

Multiscale Modeling: Results

- Stochastic Effective material properties along with Uncertain Geometric Properties considered
- Transverse displacements at grid points
- In-plane stresses of the elements calculated at top and bottom layer

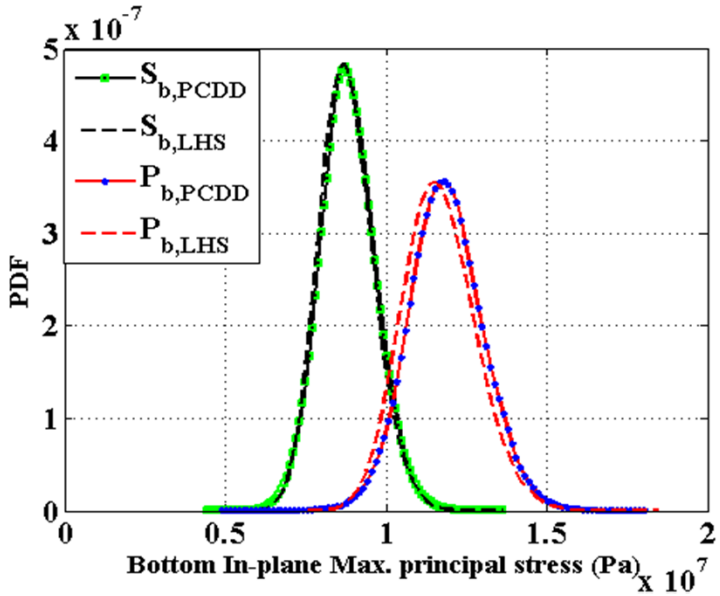


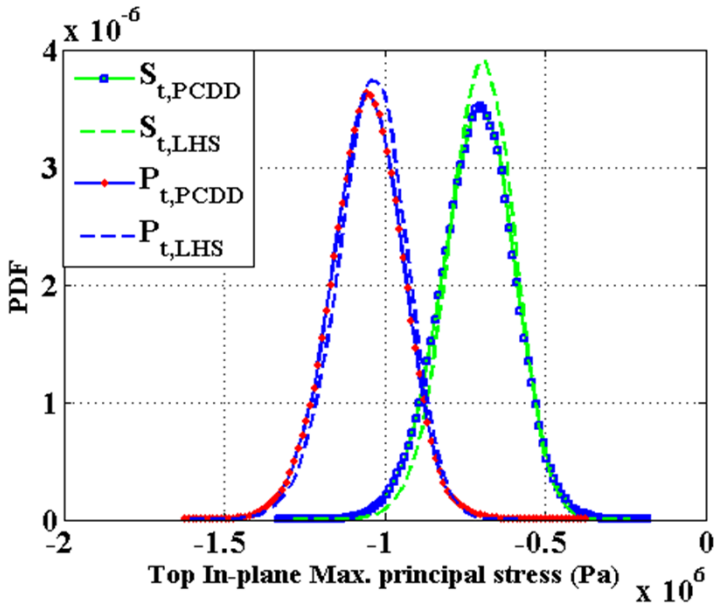
20×20 $QUAD4$ $2D$ elements

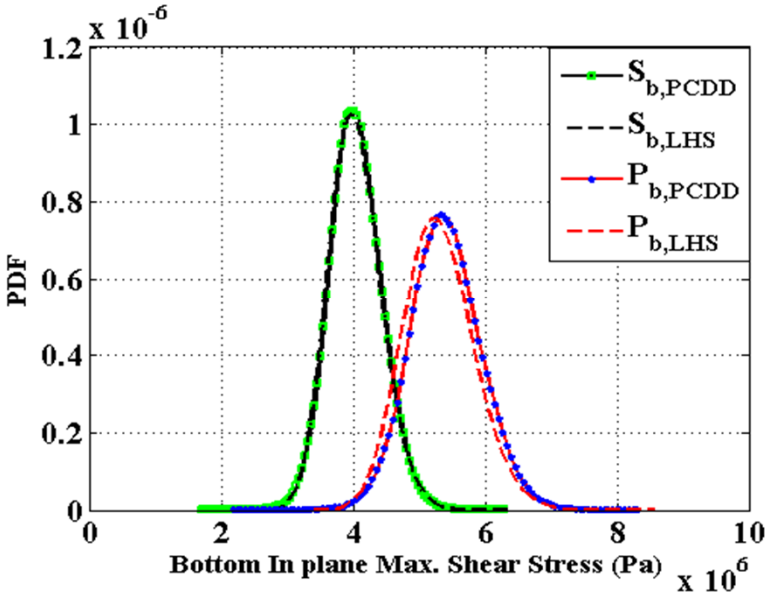


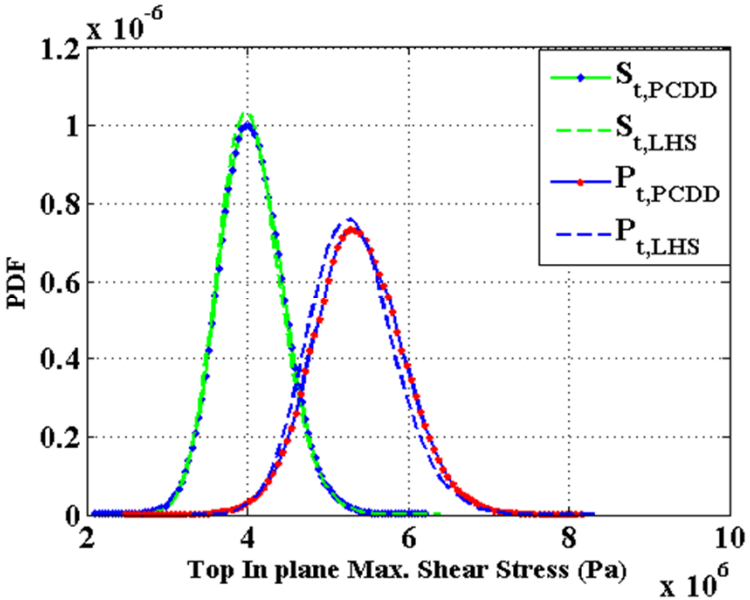
- **The PDFs match well**

Multiscale Modeling: Results









Multiscale Modeling: Results

- PCDD with PC order two required *300* samples

300 PCDD samples Vs *50,000* LHS simulations

Response	PCDD		LHS simulations	
	Mean	*Std*	*Mean*	*Std*
w_A	*-1.555*	*0.200*	*-1.534*	*0.196*
w_B	*-0.803*	*0.105*	*-0.796*	*0.103*
w_C	*-1.114*	*0.142*	*-1.102*	*0.140*
$\sigma_{max}\|_{,S_b}$	*8.822*	*0.859*	*8.770*	*0.842*
$\tau_{max}\|_{,S_b}$	*4.044*	*0.395*	*4.034*	*0.393*
$\sigma_{max}\|_{,P_b}$	*11.869*	*1.155*	*11.648*	*1.131*
$\tau_{max}\|_{,P_b}$	*4.044*	*0.395*	*4.034*	*0.393*

Units: w **(*mm*)** and stresses (***MPa)***

Multiscale Modeling: Results

- PDFs of PCDD and LHS simulations are in close agreement for all responses
- Using only ***300*** PCDD samples provided similar accuracy to ***50,000*** LHS simulations
- Higher accuracies observed in mean as compared to standard deviation
- Transverse displacements has higher accuracies than in-plane stresses
- Transverse displacements have max. error of ***1.2%*** and ***2.1%*** in Mean and Std, respectively
- In-planes stresses have error of ***0.26%~3.65%*** and ***0.45%~5.09%*** in Mean and Std

Conclusion and Future Work

- PCDD is a new Non-Intrusive technique for UQ
- ModFFD is a higher accuracy method for Sensitivity Calculation and is used in PCDD
- The number of samples required is very less *(equal to number of polynomials)* than existing non-intrusive methods
- Very high accuracy results obtained for analytical problems
- Results of CFRP composite laminate problems with uncertainties at different scales demonstrated satisfactory results with huge computational savings
- For response with higher order of magnitudes, PCDD converged faster and accurately than Stochastic Point-Collocation
- PCDD and Stochastic Point-Collocation have similar accuracy in some cases

Conclusion and Future Work

- Improve the Computational Efficiency even further
- Improve the accuracy by increasing the number of Samples
- Dimension Adaptive PC, Sparse PC, and Adaptive Sampling
- Implementation of PCDD in Robust Optimization

Thank You !!!