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MLS BASED SEQUENTIAL SRSM IN SPARSE GRID FRAMEWORK FOR EFFICIENT UNCERTAINTY QUANTIFICATION

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Abstract. *High fidelity models for uncertainty quantification of large structures in finite element framework are computationally exhaustive. Thus, there is a constant demand for efficient algorithm that uses optimal computational cost without compromising with the quality of the end results. With this in view, present study aims to develop a sequentially evolving stochastic response surface using Hermite family of orthogonal polynomials whose support points are generated in sparse grid framework. Using the values of the original model at these support points, unknown coefficients of the stochastic response surface are optimized by moving least square technique. It helps to reduce the number of original function evaluations to determine the coefficients as compared to other deterministic or random sampling techniques. Besides sparse grid scheme for support point generation, they are also populated sequentially as the optimization progresses in every iteration. The uniqueness of the proposed scheme is its adaptability by changing the order of the polynomials and the level of the sparse grid to minimize the overall computational cost. Multiple optima present in the original response can be identified by introducing additional penalty functions whenever they are required. Once the global response surface is ready, Monte-Carlo simulation or its advance version (e.g. Latin Hypercube Sampling) is adopted to generate the probability density functions for the output variables. Numerical studies are presented to prove the efficiency and accuracy of the proposed scheme as compared to other techniques available in the literature.*

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1 INTRODUCTION

Uncertainty is inevitable in physical systems where it naturally propagates affecting the performance. It can be broadly classified based on qualitative and quantitative sources [1]. These include randomness associated with analysis and formulation (i.e. epistemic uncertainty) and/or system parameters (i.e. aleatory uncertainty) [2]. For designers, quantifying and incorporating the amount of uncertainty based on the information w.r.t. parameters like input variables are vitally important. Hence, a demand for high fidelity approximate models to evaluate the uncertainty has been an active area of research. Especially, uncertainty in large structures modelled by finite element method requires better techniques as it is a computationally exhaustive exercise. Convergence of such approximate models is not always ensured which may lead to considerable error [1, 3]. To eradicate this error polynomial chaos expansion (PCE) and its variants [4, 5, 6] have been proposed using orthogonal polynomials. Thus, making the approximate model convergent in L^2 sense [4].

Although these methods yield accurate results with increase in order of the polynomial which often lead to large number of actual function calls. This problem is more critical with increase in number of random variables which is widely named as *curse of dimensionality*. Present study aims to develop a sequentially evolving stochastic response surface using orthogonal polynomials involving sparse support points.

2 PROBLEM STATEMENT

Apart from population based methods like Monte Carlo simulation (MCS), Latin hypercube sampling (LHS) etc. for uncertainty quantification, stochastic response surface method (SRSM) is widely used. It was proposed by Isukapalli [5] using PCE as a dimension reduction technique to simplify the complex relation of input-output variables which is mathematically expressed as

$$g(\xi) = \alpha_0 + \sum_{i_1=1}^{n} \alpha_{i_1}\Gamma_1(\xi_{i_1}) + \sum_{i_1=1}^{n}\sum_{i_2=1}^{i_1} \alpha_{i_1 i_2}\Gamma_2(\xi_{i_1}, \xi_{i_2}) + \dots + \sum_{i_1=1}^{n}\sum_{i_2=1}^{i_1}\cdots\sum_{i_o=1}^{i_{o-1}} \alpha_{i_1 i_2 \dots i_o}\Gamma_o(\xi_{i_1}, \xi_{i_2}, \dots, \xi_{i_o}) + \dots \tag{1}$$

where, $\xi_{i_1}, \xi_{i_2}, \dots, \xi_{i_o}$ are standard normal random variables. The function Γ_o is the orthogonal polynomial bases which can be developed using Hermite scheme [5]

$$\Gamma_o(\xi_{i_1}, \xi_{i_2}, \dots, \xi_{i_o}) = e^{\frac{1}{2}\xi^T\xi}(-1)^o \frac{\partial^o e^{-\frac{1}{2}\xi^T\xi}}{\partial\xi_{i_1}\partial\xi_{i_2}\dots\partial\xi_{i_o}}. \tag{2}$$

These functions are dictated by the order o to limit the number of unknown coefficients $\mathbf{b} = \{\alpha_0\, \alpha_1\, \dots\, \alpha_{nn\dots n}\}^T$. Thus, the Eq. 1 can be simplified to

$$\tilde{g}(\xi) = \sum_{i=0}^{o} \Xi_i(\xi)\mathbf{b}_i = \Xi(\xi)\mathbf{b} \tag{3}$$

Gauss quadrature points (a.k.a. collocation points) [5] are generated using roots of the Hermite polynomial bases for evaluating the original $g(\,.\,)$ at certain locations (further referred as support points). These points help in evaluating the unknowns in the above equation as

$$\mathbf{b} = (\Xi^{\mathrm{T}}\Xi)^{-1}\Xi^{\mathrm{T}}\mathbf{g} \tag{4}$$

In the above equation, **g** is the vector of original $g(\,.\,)$ values. To solve it, the equation must not be underdetermined system which means number of support points n_e must be equal to or greater than number of coefficients **b** (i.e. n_b). For collocation scheme, the number of points rises exponentially (i.e. $n_e = (o+1)^n$) which leads to the curse of dimensionality and sabotages the benefits of this surrogate model. The present study focuses on addressing this issue with an efficient method.

3 PROPOSED METHOD: SEQUENTIAL SRSM

The proposed method uses advanced regression based PCE coupled with sparse grid support points in an iterative framework for sequential development of stochastic response surface to determine uncertainty.

3.1 Moving Least Square Technique

To incorporate both global and local approximation for a better response surface of nonlinear function, the unknown coefficients are determine by minimizing weighted mean square error. This weight function w varies with the Euclidean distance of the concerned point and support point and thus, it is widely called as moving least square (MLS) technique. The weighted squared error can be given as [7]

$$\delta(\xi) = \sum_{i=1}^{p} w(\xi - \xi_i)\{\tilde{g}(\xi_i) - g(\xi_i)\}^2. \tag{5}$$

Minimizing the above equation with respect to unknown coefficients gives

$$\mathbf{b} = (\Xi^{\mathrm{T}}\mathbf{W}\Xi)^{-1}(\Xi^{\mathrm{T}}\mathbf{W})\mathbf{g}. \tag{6}$$

where, weight matrix $\mathbf{W} = diag[w(\xi - \xi_1)\, w(\xi - \xi_2)\, \ldots\, w(\xi - \xi_{n_b})]$. The weight function w is defined as regularized weight which is given by [7]

$$w(\xi - \xi_i) = \begin{cases} \dfrac{\left\{1+\left(\lambda\frac{\|\xi-\xi_i\|}{\hat{d}}\right)^2\right\}^{-\frac{1+\lambda}{2}} - (1+\lambda^2)^{-\frac{1+\lambda}{2}}}{1-(1+\lambda^2)^{-\frac{1+\lambda}{2}}} & \text{if } \|\xi - \xi_i\| \le \hat{d} \\ 0 & \text{if } \|\xi - \xi_i\| > \hat{d} \end{cases} \tag{7}$$

In the above equation, $\hat{d}$ is the influence radius and λ is adopted as 10^{-5} for better accuracy, as proposed by Most and Bucher [7].

3.2 Sparse Grid

Computational cost is usually associated with number of function evaluations required by approximate methods. In order to reduce this cost, sparse grid scheme is used to generate small product grids. These smaller grids are derived from the full grid as used in collocation scheme. Smolyak's algorithm is used for generating such points by forming tensor product of smaller grids as [8]

$$\mathscr{S}_q = \sum_{|i|_1 \le q+n-1} (\Delta_{i_1} \otimes \Delta_{i_2} \otimes \cdots \otimes \Delta_{i_n})\mathbf{g} \tag{8}$$

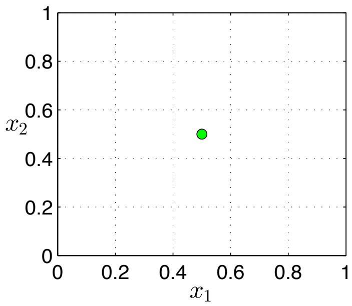
where, $\Delta_i = V_{m_i} - V_{m_{i-1}}$, for $i \geq 1$ and $i \in \mathbb{N}^n$. One of the widely accepted scheme is Clenshaw-Curtis [9] which generates equidistant nodes. The number of points in each direction are determined by [10]

$$m_i = \begin{cases} 1 & \text{for } i = 1 \\ 2^{i-1} + 1 & \text{for } i > 1 \end{cases} \tag{9}$$

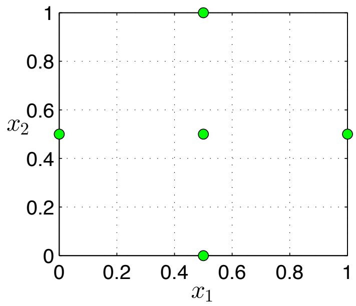
and the respective coordinates of these points are evaluated using

$$x_i^j = \begin{cases} \frac{j-1}{m_i - 1} & \text{for } j = 1, 2, \ldots, m_i \text{ and } m_i > 1 \\ \frac{1}{2} & \text{for } j = 1 \text{ and } m_i = 1 \end{cases} \tag{10}$$

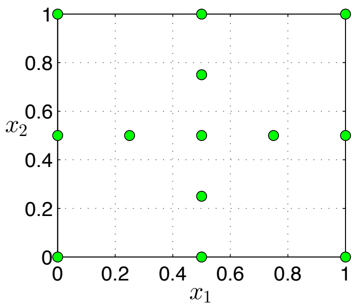
Fig. 1 shows the support points generated using limited tensor products [10] where $x_i^j \in [0, 1]$.



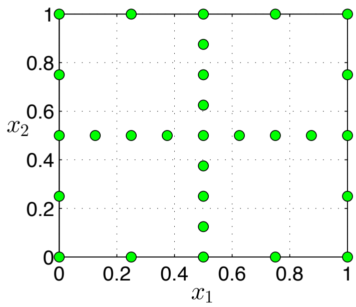
(a) $q = 0, n = 2$



(b) $q = 1, n = 2$



(c) $q = 2, n = 2$



(d) $q = 3, n = 2$

Figure 1: Sparse grid generated using Clenshaw-Curtis scheme

It can be noticed that the number of points and its coordinates in each direction is dictated by m_i which is further influenced by level of sparse grid q. This leads to hierarchically generation of sparse grid with less points than the full grid collocation scheme. In case of large number of variables n the difference between the schemes significantly increases. However, number of points exponentially grows with the level q which might generate more points than the collocation scheme, thus a judicial use is required.

3.3 Proposed Sequential Strategy

For developing the sequential strategy, maxima and minima are determined using the constructed response surface as

$$\begin{array}{ll} \max_{\xi} & \tilde{g}(\xi) \\ \text{s. t.} & \xi \in \Omega_{\xi} \end{array} \tag{11}$$

$$\begin{array}{ll} \min_{\xi} & \tilde{g}(\xi) \\ \text{s. t.} & \xi \in \Omega_{\xi} \end{array} \tag{12}$$

respectively. Optimization process often encounters more than one maxima and/or minima over the iterations. To identify these points or regions weight function is included for penalty. It modifies the stochastic response surface by a continuous and differentiable function as

$$\tilde{g}_m(\xi) = \tilde{g}(\xi) + \sum_{k=1}^{n_m} \breve{g}_k(\xi). \tag{13}$$

In the above equation, n_m is the total number of multiple optimas and $\breve{g}_j(\xi)$ represents penalty function which is expressed as [11]

$$\breve{g}_k(\xi) = \begin{cases} \frac{\vartheta|\xi^{*,i}|_2|\nabla\tilde{g}(\xi^{*,i})|_2}{[(\gamma|\xi^{*,i}|_2)^2-(\vartheta|\xi^{*,i}|_2)^2]^2}(r_k^2 - |\xi - \xi^{*,i}|_2^2)^2 & \text{if } |\xi - \xi^{*,i}|_2 \leq r_k \\ 0 & \text{if } |\xi - \xi^{*,i}|_2 > r_k \end{cases} \tag{14}$$

As suggested by Der Kiureghian and Dakessian [11] the constant parameters ϑ and γ are considered to be 0.75 and 1.10, respectively, and influence radius of penalty function $r_k = \gamma|\xi^{*,i}|_2$. The convergence criteria for the optimization with penalty function is given by

$$\cos^{-1}\left[\frac{\xi^{*,k+1}.\xi^{*,k}}{|\xi^{*,k+1}|_2|\xi^{*,k}|_2}\right] \leq \theta_m \tag{15}$$

$$|\xi^{*,k+1} - \xi^{*,k}|_2 \leq |\xi^{*,k}|_2. \tag{16}$$

which is required to identify new optimal point. The convergence angle θ_m between foot of the penalty weight function and optimal point is assumed to be 66° for $\gamma = 1.10$. For more information one can refer to [11].

4 NUMERICAL ANALYSIS

For brevity, in this section two applications of the proposed method is discussed. One is of a benchmark problem with non-algebraic terms resulting in multiple maxima-minima points whereas the second problem demonstrates the proposed method for a real structure with correlated non-normal random variables.

4.1 Example 1: Franke's Function

The first problem is a non-algebraic function which is mathematically expressed as

$$\begin{aligned} g(\mathbf{x}) = & \tfrac{3}{4}e^{\left\{-\frac{1}{4}(9x_1-2)^2-\frac{1}{4}(9x_2-2)^2\right\}} + \tfrac{3}{4}e^{\left\{-\frac{1}{49}(9x_1-2)^2-\frac{1}{10}(9x_2-2)^2\right\}} \\ & + \tfrac{1}{2}e^{\left\{-\frac{1}{4}(9x_1-7)^2-\frac{1}{4}(9x_2-3)^2\right\}} - \tfrac{1}{4}e^{\left\{-(9x_1-4)^2-(9x_2-7)^2\right\}} \end{aligned} \tag{17}$$

and is widely used for testing surrogate models. The parameters x_1 and x_2 are independent normal random variables with mean 0.400 and standard deviation 0.100. Complexity in the problem is due to multiple optima points. The proposed method is applied which first determines the global maxima as in Fig. 2 (c) which is further penalized for finding any other maxima. The next maxima is evaluated as shown in Fig. 2 (h). Following the similar procedure and on searching the next maxima converges to the first maxima as shown in Fig. 2 (i). Since all the possible maximums are located, now the proposed method optimizes the response surface for

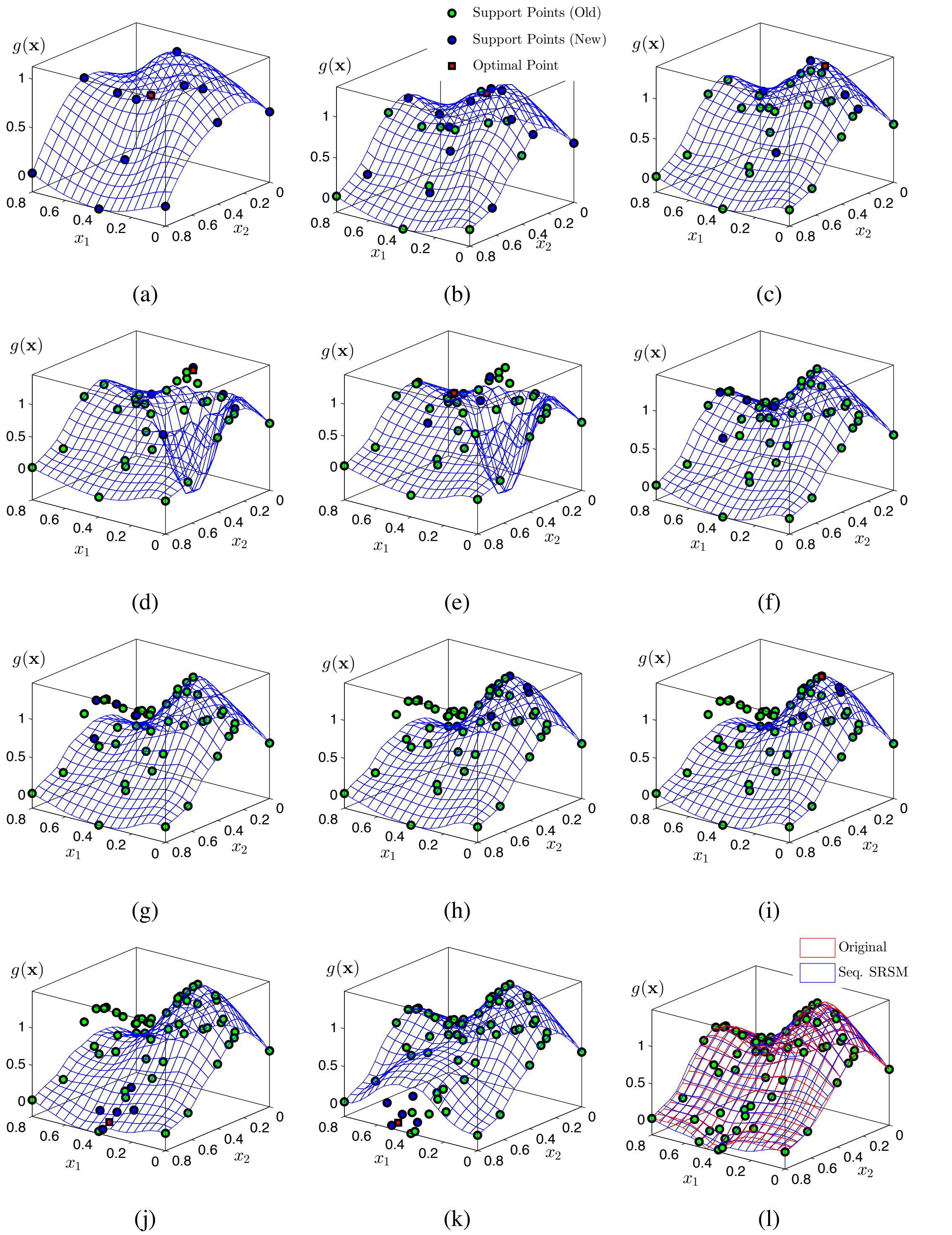


Figure 2: Comparison of (a) *pdf* and (b) CDF of a random variable following Weibull distribution evaluated from different methods

minima. Similar strategy is followed which results in the sequential stochastic response surface as presented in Fig. 2 (l). Once the response surface is constructed, MCS are conducted over it. The results of uncertainty quantification are presented in Fig. 3 and Table 1. The proposed method yields results close to direct MCS on the Franke's function with less number of function

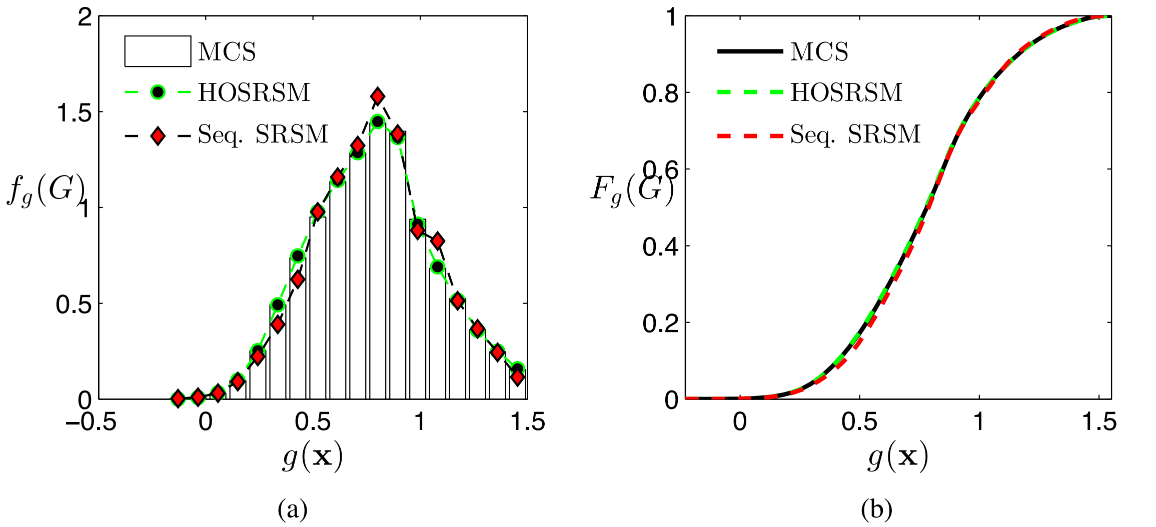


Figure 3: Comparison of (a) *pdf* and (b) CDF of Franke's function using Sequential SRSM

Method	Function Calls	Mean	Standard Deviation	Maximum
MCS	100000	0.7796	0.2828	1.5007
HOSRSM	108	0.7783	0.2848	2.6217
Seq. SRSM	66	0.7881	0.2741	1.4977

Table 1: Results for Franke's function using Sequential SRSM

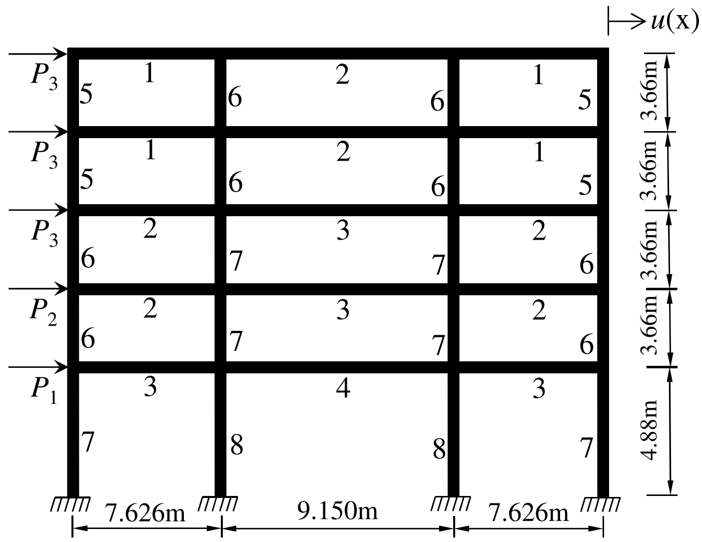


Figure 4: Portal frame with loading

evaluations than higher order SRSM (HOSRSM) [12]. This demonstrates the efficiency of the proposed method.

Element number	Area	Moment of inertia	Young's modulus
1	A_5	I_5	E_1
2	A_6	I_6	E_1
3	A_7	I_7	E_1
4	A_8	I_8	E_1
5	A_1	I_1	E_2
6	A_2	I_2	E_2
7	A_3	I_3	E_2
8	A_4	I_4	E_2

Table 2: Properties of the portal frame elements

Random variables	Units	Mean	Standard deviation	Distribution
E_1	kN/m^2	$2.174 \times 10^{+7}$	$1.915 \times 10^{+6}$	Lognormal
E_2	kN/m^2	$2.380 \times 10^{+7}$	$1.915 \times 10^{+6}$	Lognormal
P_1	kN	71.175	28.470	Gumbel
P_2	kN	88.970	35.590	Gumbel
P_3	kN	133.454	40.040	Gumbel
A_1	m^2	0.313	0.056	Lognormal
A_2	m^2	0.372	0.074	Lognormal
A_3	m^2	0.506	0.093	Lognormal
A_4	m^2	0.558	0.112	Lognormal
A_5	m^2	0.253	0.093	Lognormal
A_6	m^2	0.291	0.102	Lognormal
A_7	m^2	0.373	0.121	Lognormal
A_8	m^2	0.419	0.139	Lognormal
I_1	m^4	8.134×10^{-3}	1.038×10^{-3}	Lognormal
I_2	m^4	1.151×10^{-2}	1.298×10^{-3}	Lognormal
I_3	m^4	2.137×10^{-2}	2.596×10^{-3}	Lognormal
I_4	m^4	2.596×10^{-2}	3.029×10^{-3}	Lognormal
I_5	m^4	1.082×10^{-2}	2.596×10^{-3}	Lognormal
I_6	m^4	1.410×10^{-2}	3.461×10^{-3}	Lognormal
I_7	m^4	2.328×10^{-2}	5.625×10^{-3}	Lognormal
I_8	m^4	2.596×10^{-2}	6.490×10^{-3}	Lognormal

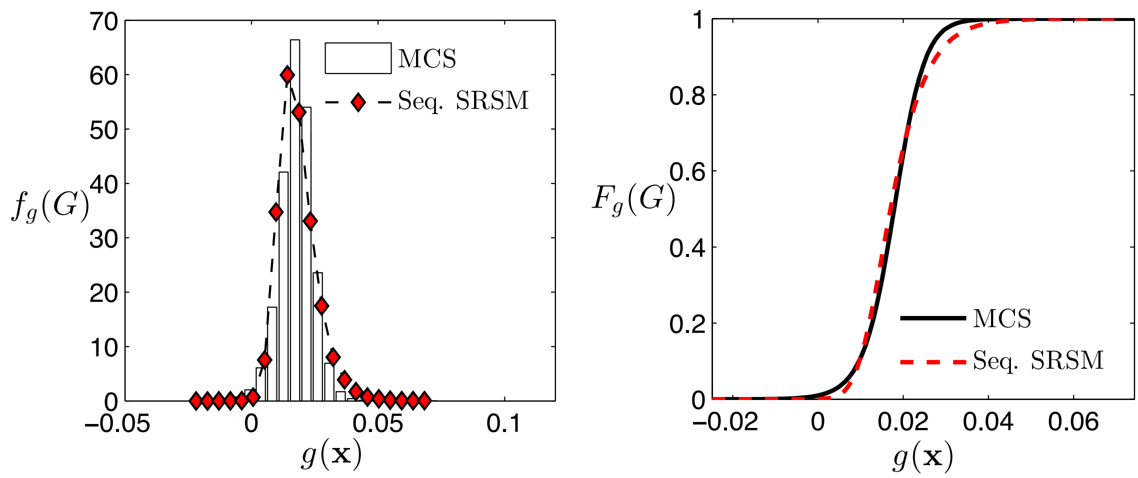
Table 3: Properties and distribution of random variables in Example 2

4.2 Example 2: Portal Frame

In this section, uncertainty caused in horizontal displacement $u(\mathbf{x})$ of the top floor of portal frame due to random variables is evaluated. The details of the multi-storey multi-bay portal frame is shown in Fig. 4 and Table 2. Properties of the random variables is presented in Table

3. These random variables are correlated as

$$\rho = \begin{matrix} E_1 \\ E_2 \\ P_1 \\ P_2 \\ P_3 \\ A_1 \\ A_2 \\ \vdots \\ I_8 \end{matrix} \begin{bmatrix} 1 & & & & & & & & \\ 0.90 & 1 & & & & & & & \\ 0 & 0 & 1 & & & & & & \\ 0 & 0 & 0.95 & 1 & & & & & \\ 0 & 0 & 0.95 & 0.95 & 1 & & & & \\ 0 & 0 & 0 & 0 & 0 & 1 & & & \\ 0 & 0 & 0 & 0 & 0 & 0.13 & 1 & & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \\ 0 & 0 & 0 & 0 & 0 & 0.13 & \cdots & 0.13 & 1 \end{bmatrix} \tag{18}$$



(a) (b)

Figure 5: Comparison of (a) *pdf* and (b) CDF of multi-storey portal frame using Sequential SRSM

Method	Function Calls	Mean	Standard Deviation	Maximum
MCS	100000	0.0177	0.0073	0.0736
Seq. SRSM	1269	0.0176	0.0075	0.0748

Table 4: Results for multi-storey portal frame using Sequential SRSM

To perform the static analysis, finite element method is performed using software package like ANSYS 13.0. Similar to previous example, MCS is used as benchmark with sample size 10^5 and sequential SRSM is solved to determine uncertainty. The results of uncertainty quantification are presented in Fig. 5 and Table 4. The proposed method yields results close to direct MCS on the portal frame with very less number of function evaluations. This proves the efficiency of the proposed method for determining uncertainty quantification in real structures with non-normal correlated random variables.

5 CONCLUSIONS

Present study demonstrates an efficient uncertainty quantification method using sequential SRSM. It employs MLS based PCE with Hermite polynomial basis which is formed sequentially with support points generated by Clenshaw-Curtis sparse grid scheme. It produces equidistant points in each progressive iterations based on the optimization of maxima and minima. The method also proposes flexibility in the choice of sparse grid level and polynomial order in each iteration to minimize computational burden with adequate accuracy. Multiple optimal points are determined in this method using penalty function. Numerical study considering benchmark and real problems elucidates the accuracy and efficiency of the proposed sequential SRSM.

REFERENCES

[1] A. Haldar, S. Mahadevan, *Reliability assessment using stochastic finite element analysis*. John Wiley & Sons, Inc., 2000.

[2] A. Der Kiureghian, O. Ditlevsen, Aleatory or epistemic? Does it matter? *Structural Safety*,**31** (2), 105–112, 2009.

[3] S. Kameshwar, A. K. Rathi and A. Chakraborty, A Modified Gradient Based Reliability Analysis for Nonlinear Nonalgebraic Limit States Using Polynomial Chaos Expansion. *Proceedings of* 4^{th} *International Congress on Computational Mechanics and Simulation*, Hyderabad, India, December 10–12, 2012.

[4] R. G. Ghanem and P. D. Spanos, Stochastic Finite Elements: A Spectral Approach. Springer-Verlag New York, USA, 1991.

[5] S. S. Isukapalli, Uncertainty analysis of transport-transformation models *Ph.D. dissertation*,Rutgers, The State University of New Jersey, 1999.

[6] D. Xiu and G. E. Karniadakis, Modeling uncertainty in flow simulations via generalized polynomial chaos. *Journal of Computational Physics*, **187** (1), 137–167, 2003.

[7] T. Most and C. Bucher, A Moving Least Squares weighting function for the Element-free Galerkin Method which almost fulfills essential boundary conditions. *Structural Engineering and Mechanics*, **21** (3), 315–332, 2005.

[8] O. L. Maitre and O. M. Knio, Spectral Methods for Uncertainty Quantification. Springer Netherlands, 2010.

[9] C. W. Clenshaw and A. R. Curtis, A Method for Numerical Integration on an Automatic Computer. *Numerische Mathematik*, **2** (1), 197–205, 1960.

[10] A. Klimke and B. Wohlmuth, Computing Expensive Multivariate Functions of Fuzzy Numbers using Sparse Grids. *Fuzzy Sets and Systems*, **154** (3), 432–453, 2005.

[11] A. Der Kiureghian and T. Dakessian, Multiple design points in first and second-order reliability. *Structural Safety*, **20** (1), 37–49, 1998.

[12] H. P. Gavin and S. C. Yau, High-order limit state functions in the response surface method for structural reliability analysis. *Structural Safety*, **30** (2), 162–179, 2008.