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A FINITE ELEMENT METHOD-INFORMED NEURAL NETWORK FOR UNCERTAINTY QUANTIFICATION

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Abstract. Sampling approaches for uncertainty quantification for real-world engineering problems are associated with large computational time and cost. This cost comes from the expensive deterministic simulation. Usage of surrogate models is a common way to overcome this issue in engineering applications. A conventional Neural Network (NN) can be used for building such surrogates. However, these neural networks are built based on input-output pairs. It is not possible to verify that the predicted output satisfies underlying physics.

In this contribution, a physics-informed neural network based on a hybrid model of machine learning and classical Finite Element Method (FEM) is presented for forward propagation of uncertainty. The method uses FEM during both training and prediction stages. A surrogate model based on neural network for high dimensional problem is constructed by constraining the predictions of the neural network with the discretized partial differential equation of the system. During the training stage, the predicted solution from the FEM informed Neural Network(FEM-NN) is used to compute the residual using stiffness matrices and force vectors. This residual is used as a custom loss function from NN. This makes the whole training unsupervised as it does not require any output values. Hence, the need for expensive FEM solves is circumvented. The FEM-NN hybrid also gives an estimate of the accuracy of prediction by means of the calculated residual along with the prediction. The framework does not require mandatory expensive linear solves of the discretized equation instead substitutes the prediction from the neural network for computing the residual. This reduces the expensive training phase of the problem and can be applicable to real-world FEM simulations. The trained neural network is then sampled in a Monte Carlo (MC) manner to evaluate the statistics of the Quantities of Interest (QoI). The resulting FEM-NN hybrid is physics confirming and data-efficient. The efficacy of the framework is presented by a series of test case examples. The results are compared with classical MC results. The suitability of the method for the uncertainty quantification is studied and presented.

1 INTRODUCTION

There is an increasing demand for accurate predictions in computational mechanics while considering the uncertainties associated with the input parameters. A deterministic model alone is not sufficient for this purpose. A computational model with quantified uncertainties gives a clear insight into the behaviour of the structural system. The uncertainties of the inputs are propagated through the computational model to identify the uncertainties of the quantities of interest(QoI) [13]. Methods of uncertainty quantification can be classified into sampling-based approaches and non sampling-based approaches.

Sampling methods are widely used and are easy to implement. They do not require access to system matrices and hence are called non-intrusive methods. Classical Monte Carlo (MC) method is the commonly used sampling method [10]. MC method is based on random sampling from the input distribution and evaluating the computational model at each of these sampling points. The Quantities of interest are then collected to evaluate the probability measures of the quantities of interest. The convergence of the method depends on the number of model evaluations and can be very expensive, especially if the single model evaluation is computationally expensive. Hence, the applicability of MC based methods for real wold problems are challenging. The convergence of the MC estimate can be improved by various methods like the Latin hypercube sampling [8] and quasi Monte Carlo sampling [3] methods. Variance reduction techniques such as Multi level Monte Carlo (MLMC) [6] methods have also gained popularity in recent times.

Non sampling approach includes perturbation method, where a truncated multi-dimensional Taylor expansion for the output quantities of interest is used [2]. A class of methods called spectral method uses the uncertain parameter to be represented as an expansion called spectral expansion [5]. The input and output uncertain parameters are thus represented as series expansion called generalized Polynomial Chaos (gPC) and is used in various applications [14] [12] [7]. The advantages of a surrogate model is that it is easy to evaluate compared to the original computational model. Other surrogate methods include krigings and neural networks.

Neural networks can be used as a surrogate model and are created by considering the mapping between input-output pairs. The data generation for creating input-output pair is achieved by running multiple deterministic simulations and can be expensive like the sampling approaches. Also, the traditional NN based on input-output pair does not consider the underlying physics behind the problem. Recently Physics Informed Neural Network (PINN) [11] has been used to combine prior knowledge of the partial differential equation and the NN. A hybrid methodology which is data-efficient and physics conforming is introduced for numerical simulation by the authors [9]. Here, in this contribution we extend it to uncertainty quantification. The method is based on training the NN with a custom loss function from the FEM formulation of the underlying partial differential equation. The expensive linear solves are not required in this method as the training uses the custom FEM loss function. The method is physics conforming and data-efficient. The trained NN surrogate is used for UQ, by sampling from the surrogate in a Monte Carlo fashion. The details and applicability of the methodology for UQ is elaborated and critically evaluated here in this contribution. Section 2 explains the modelling details of the FEM informed NN surrogate for uncertainty quantification. section 3 includes the basics and implementation details of FEM-NN and the approach adopted for uncertainty quantification is also detailed in this section. The proposed method is applied to problems from structural engineering in Section 4. The results are presented and discussed in detail. The conclusions and outlook with advantages and challenges of FEM-NN for UQ is presented in Section 5.

2 MATHEMATICAL MODELLING

Any partial differential equation (PDE) for continuous solution field u with corresponding boundary condition on a given domain Ω is described by Eq. 1 . Numerical approximation of the same, in Galerkin-based finite element method, results in a system of linear equations as Eq. 2.

$$\mathcal{L}(u) = 0 \qquad\qquad \text{on } \Omega \tag{1}$$

$$K(u^h) \times u^h = F \tag{2}$$

where, $K(u^h)$ is the non-linear stiffness matrix, u^h is the discrete solution field, and F is the right hand side force vector. The system can be written in residual form as

$$r(u^h) = K(u^h)u^h - F \tag{3}$$

To obtain the solution u^h, a Newton-Raphson Method may be used. In case of a linear operator, it takes one iteration to converge. For a complex problem, with large number of elements the linear solve stage is the most computationally expensive step in the solution process.

2.1 Neural network surrogate construction and back propagation

A neural network is created as a mapping between input variables $\mathbf{x} = [x_1, x_2, ...x_m]$ from domain X to output variables $\mathbf{y} = [y_1, y_2, ...y_n]$ of domain Y. The input layer and output layer are connected by L number of hidden layers. Each layer is characterized by the trainable parameters - weights w_l and biases b_l. NN training is a minimization problem to find the trainable parameters that minimizes the discrepancy(called loss function) between the true value and the predicted value of the output. The loss δ minimization by updating the trainable parameters is called back propagation. In back propagation, the gradient of δ with respect to trainable parameters is calculated, and the trainable parameters are updated as,

$$w_l = w_l - \eta \frac{\partial \delta}{\partial w_l} \tag{4}$$

where,η is the learning rate. The derivatives in Eq. 4 are calculated using the chain rules.

$$\frac{\partial \delta}{\partial w_l} = \frac{\partial \delta}{\partial y} \frac{\partial y}{\partial w_l} \tag{5}$$

The first part of the Eq. 5 depends on the choice of the loss function. A common loss functions is the mean square error (MSE) $\delta_{MSE} = \frac{1}{m} \sum_{i=i}^{m} (y_i - y_i^t)^2$ where, y^t are the true values.

2.2 Finite element method informed neural network

In the FEM-NN hybrid algorithm proposed by [9] uses a custom loss function for the NN training. The euclidean norm of the residual vector r is used as the custom loss function. The residual r is computed using the prediction u from the neural network and system matrices from FEM. Custom loss

$$\delta_{FEM} = ||r||_2 \tag{6}$$

where r is given by Eq. 2. The custom loss is computed as,

$$\delta_{FEM} = ||r||_2 = \sqrt{\sum_{j=1}^{n} \sum_{i=1}^{n} (K_{j,i} u_i - F_j)^2} \tag{7}$$

In the back propagation the gradient of this custom loss function with respect to output is required to calculate the gradient of the loss function with respect to trainable parameters as in Eq. 5. The gradient of the custom loss function is obtained as

$$\frac{\partial \delta_{FEM}}{\partial y} = \frac{r^T K}{\delta} \tag{8}$$

where, r is the residual vector and K is the stiffness matrix. With this gradient of the custom loss function implemented, chain rule can be employed to compute the gradients required for back propagation. Second part of the Eq. 5 is readily available in all the neural network frameworks.

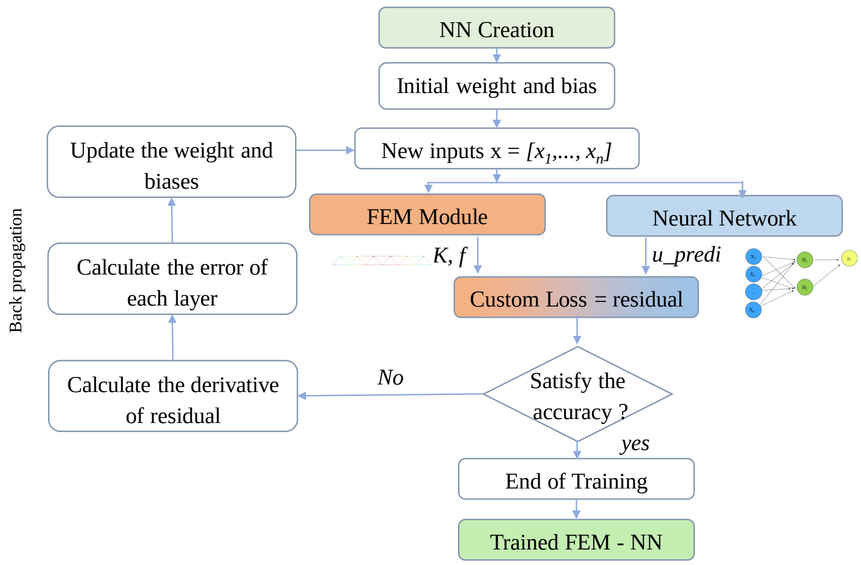

Figure 1: Details of the FEM-NN hybrid algorithm for training

2.3 Details of truss equation

For a linear elastic prismatic bar under axial force(T), the equilibrium of forces is given by,

$$AE\frac{du(x)}{dx} = T \tag{9}$$

Where, A, E are the cross sectional area and modulus of elasticity of the material. Taking the derivative of Eq.9 with respect to local coordinate x

$$\frac{d}{dx}\left[AE\frac{du(x)}{dx}\right] = 0 \tag{10}$$

2.4 Details of Euler Bernoulli beam

The Euler–Bernoulli equation describes a beam's deflection u under the applied load F_d:

$$\frac{\partial^2}{\partial z^2}\left[EI\frac{\partial^2 u(z)}{\partial z^2}\right] = F_d(z) \tag{11}$$

where, $u(z)$ describes the deflection of the beam at position z under load $F_d(z)$.

3 FEM informed Neural Network methodology

Figure 1 depicts the adopted workflow for the training of FEM-NN hybrid. The created NN with user defined structure is initialized with initial wights and biases. In the training phase each of the new inputs are fed into both the FEM module and the Neural Network. The method needs access to the system

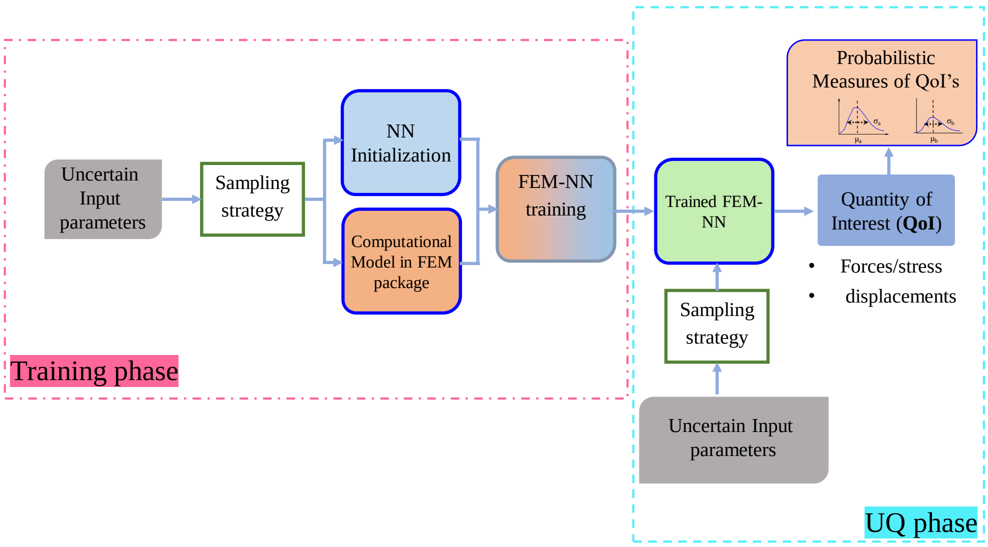

Figure 2: FEM-NN hybrid algorithm for uncertainty quantification with various stages

matrices and is hence intrusive. The custom loss function is calculated from Eq. 7 using the system matrices from the FEM module and the prediction from the NN. The loss function is compared with the convergence criteria and the training is done until the convergence is met. In case the convergence is not met the loss is back propagated with the calculated gradient as in Eq. 5. The weights and biases are updated as in Eq. 4. It can be seen that during training the solution from FEM module is not required. The expensive linear solves are not required in the hybrid FEM-NN methodology. The NN training also incorporates the FEM module and hence the physics during training.

3.1 FEM - NN Hybrid methodology for uncertainty quantification

The trained model from the previous step can be used for uncertainty quantification as shown in Figure 2. During the UQ phase the trained NN is used as surrogate and sampling is done from the input distributions. The QoI are evaluated for the inputs from the trained NN. Sampling from the NN is fast and is inexpensive. During the prediction phase, an estimate of accuracy in the prediction is also obtained in terms of the residual. The ensemble of QoI are then analysed to obtain the statistical quantities and probability measures of the QoI.

4 NUMERICAL STUDY

Two numerical examples are elaborated in this section to show the effectiveness of the proposed algorithm for uncertainty quantification.

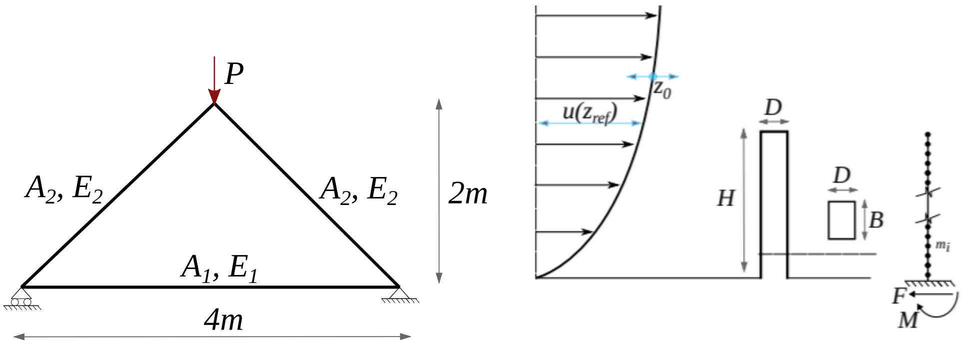

Figure 3: Numerical examples considered a)three bar truss b)building structure under wind

4.1 Three bar truss with uncertain loads and material parameters

A three bar linear truss with uncertain loads and material properties is considered as shown in Figure 3 a. The node location is considered deterministic. The problem is modelled in open source FEM solver called Kratos [4]. The uncertain input parameters are tabulated in Table 1. The input uncertain parameters include both the system parameters and the loading parameters.

The UQ problem is solved using the proposed FEM-NN hybrid method. The QoI is the vertical displacement at the application of the load. The probability density function (PDF) and cumulative Density function (CDF) of the QoI are shown in Figure 4. The PDF follows a Gaussian distribution. The results are compared with that of MC with 10,000 samples. The number of samples from the FEM-NN hybrid surrogate is also kept as 10,000 to have similar sampling error. The reference solution is obtained by doing a MC with 100,000 samples. It can be observed from the figure that the reference and FEM-NN hybrid are in close agreement showing the applicability of the method.

The first four moments of the QoI are tabulated in Table 2. The FEM-NN hybrid results are compared

Table 1: Input uncertain parameters for the 3 bar truss problem

Uncertain inputs	distribution	mean	standard deviation
$A_1(m^2)$	Gaussian	2.0×10^{-3}	2.0×10^{-4}
$A_2(m^2)$	Gaussian	1.0×10^{-3}	1.0×10^{-4}
$E_1(Pa)$	Gaussian	2.1×10^{11}	2.1×10^{10}
$E_2(Pa)$	Gaussian	2.1×10^{11}	2.1×10^{10}
$P(N)$	Gaussian	5.0×10^{5}	5.0×10^{4}

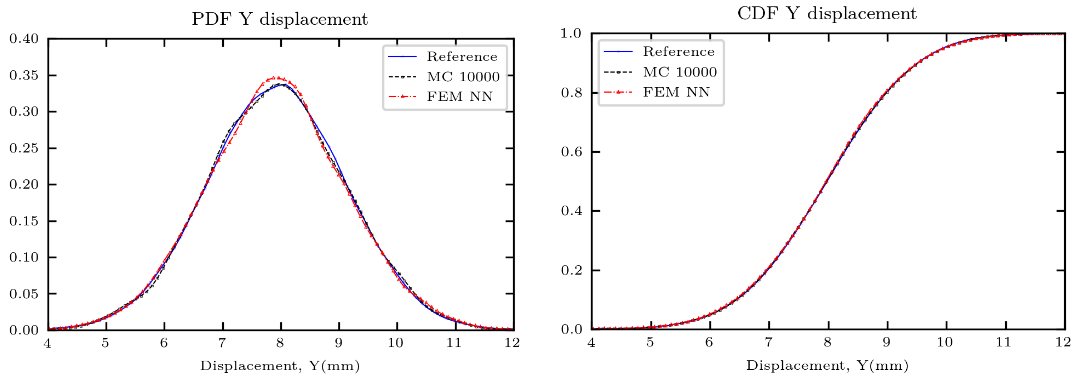

Figure 4: Comparison of FEM-NN with MC for 3 bar truss problem

with that of the reference and MC simulation results. The error in the mean value is 0.16%. This indicate the efficacy of the method in predicting the stochastic results. The higher moments are also captured with accuracy by FEM-NN. It should be noted that the MC 10,000 required 10,000 model evaluations and linear solves. However, the FEM-NN required 0 linear solves during training because of the incorporation of the custom loss function.

Table 2: Comparison of results for the 3 bar truss problem

	Mean	Standard deviation	Skewness	Kurtosis
Reference	7.92896	1.19067	-0.015154	0.01921
MC 10,000	7.92842	1.18379	-0.007303	0.02333
FEM-NN	7.91661	1.18622	-0.013229	0.02655

4.2 Response of building structure under uncertain wind loads

A building structure under uncertain wind loads is considered in this example. The CAARC [1] building geometry is used for the study. The uncertainties comes from the wind loading. A weibull distribution is assumed for the mean wind speed and the uncertainty in the terrain category is captured via uncertain roughness length. The wind velocity profile along the height is hence uncertain. A static analysis is done with the loads at each height computed as

Table 3: Input parameters for the building structure under wind loads

inputs	distribution	Values
Height (H)	-	180m
Width (W)	-	45m
Length (D)	-	30m
Frequency (f)	-	0.2Hz
Density	-	160 kg/m^3
Damping ratio	-	0.05
Mean wind velocity	Weibull	Mean = 20 m/s, shape parameters = 2
Roughness length	Uniform	[0.1, 0.7]

$$F_d(z) = \frac{\rho V(z)^2 A C_d}{2} \tag{12}$$

where, ρ is the air density, $V(z)$ is the velocity at height z, A is the reference area and c_d is the coefficient of drag for the cross section. The structure is modelled as an Euler-Bernoulli beam as shown in Figure 3 b. The governing equation is described in Eq. 11. The input parameters are tabulated in Table 3.

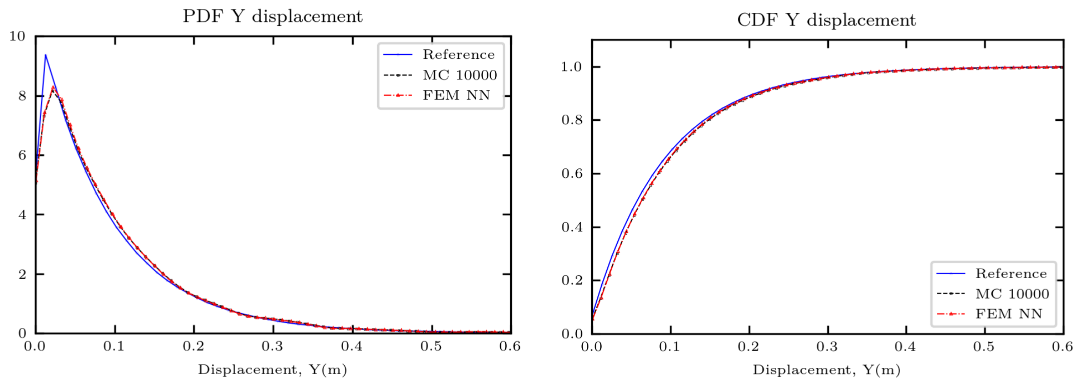

Figure 5: Comparison of FEM-NN with MC for the structure under wind loads problem

The UQ analysis is carried out with the proposed FEM-NN hybrid method and MC with 10,000 and reference solution with 100,000 samples. The QoI is the horizontal displacement at the top of the building. The probability density function (PDF) and cumulative Density function (CDF) of the QoI are shown in Figure 5. The results obtained are in good agreement with that of reference solution. To quantify the results, the first four moments are tabulated in Table 4. The error in the mean is less than 0.01% showing close agreement with the results. Other higher order moments are captured accurately by the method. The deviation in the kurtosis from reference value may be attributed to the sampling error as the values of MC 10000 and FEM-NN are comparable

Table 4: Results for the building structure under wind loads

	Mean	Standard deviation	Skewness	Kurtosis
Reference	0.092774	0.094128	2.08002	6.61567
MC 10,000	0.093232	0.095423	2.20634	8.17860
FEM-NN	0.092765	0.094416	2.22340	8.32967

5 CONCLUSIONS AND OUTLOOK

The proposed FEM-NN hybrid is used for uncertainty quantification. The method serves as an efficient surrogate for uncertainty quantification. The FEM-NN are in close agreement with MC simulation results. The main advantage of the method lies in the fact that expensive linear solves are avoided in the training phase. When compared to traditional Neural network, the FEM-NN hybrid is intrusive and required no linear solves during training. The FEM-NN hybrid can give a description of the accuracy in terms of the computed residuals. The conventional NN can be trained for a collection of QoI and hence the network can be small. However, the FEM-NN hybrid need to be trained for all the nodal quantities. For real-world problem with high number of elements this is challenging, as this will result in a huge network to train. The FEM-NN hybrid results in a complete stochastic picture. Hence, if a new QoI is required or more analysis is desired, it is possible to do so in FEM-NN hybrid without additional training. Even though the method is promising for uncertainty quantification applications, more research is required in addressing the challenges associated with problems of increased complexity. The method is promising and improvements in FEM and NN domains will enrich the efficiency and reduce the short comings.

References

[1] A. L. Braun and A. M. Awruch. Aerodynamic and aeroelastic analyses on the caarc standard tall building model using numerical simulation. *Computers & Structures*, 87(9-10):564–581, 2009.

[2] D. G. Cacuci and R. Fang. Sensitivity and uncertainty analysis of counter-flow mechanical draft cooling towers—i: Adjoint sensitivity analysis. *Nuclear Technology*, 198(2):85–131, 2017. doi: 10.1080/00295450.2017.1294429. URL https://doi.org/10.1080/00295450.2017.1294429.

[3] R. E. Caflisch. Monte carlo and quasi-monte carlo methods. *Acta Numerica*, 7:1–49, 1998. doi: 10.1017/S0962492900002804.

[4] P. Dadvand, R. Rossi, and E. Oñate. An object-oriented environment for developing finite element codes for multi-disciplinary applications. *Archives of Computational Methods in Engineering*, 17 (3):253–297, 2010. ISSN 11343060. doi: 10.1007/s11831-010-9045-2.

[5] R. G. Ghanem and P. D. Spanos. *Stochastic Finite Elements: A Spectral Approach*. Springer-Verlag, Berlin, Heidelberg, 1991. ISBN 0387974563.

[6] M. B. Giles. Multilevel Monte Carlo methods. (2015):259–328, 2017. doi: 10.1017/S096249291500001X.

[7] A. Kodakkal, S. K. Saha, K. Sepahvand, V. A. Matsagar, F. Duddeck, and S. Marburg. Uncertainties in dynamic response of buildings with non-linear base-isolators. *Engineering Structures*, 197:109423, 2019. ISSN 0141-0296. doi: https://doi.org/10.1016/j.engstruct.2019.109423. URL

https://www.sciencedirect.com/science/article/pii/S0141029618343359.

[8] W.-L. Loh. On latin hypercube sampling. *Ann. Statist.*, 24(5):2058–2080, 10 1996. doi: 10.1214/aos/1069362310. URL https://doi.org/10.1214/aos/1069362310.

[9] R. E. Meethal, B. Obst, M. Khalil, A. Ghantasala, A. Kodakkal, K.-U. Bletzinger, and R. Wüchner. Finite element method-enhanced neural network and hybrid model for simulation. *under submission*, 2021.

[10] N. Metropolis and S. Ulam. The monte carlo method. *Journal of the American Statistical Association*, 44(247):335–341, 1949. doi: 10.1080/01621459.1949.10483310. URL https://www.tandfonline.com/doi/abs/10.1080/01621459.1949.10483310. PMID: 18139350.

[11] M. Raissi, P. Perdikaris, and G. E. Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, 378:686–707, 2019.

[12] K. Sepahvand, M. Scheffler, and S. Marburg. Uncertainty quantification in natural frequencies and radiated acoustic power of composite plates: Analytical and experimental investigation. *Applied Acoustics*, 87:23–29, 2015. ISSN 0003-682X. doi: https://doi.org/10.1016/j.apacoust.2014.06.008. URL https://www.sciencedirect.com/science/article/pii/S0003682X14001595.

[13] R. C. Smith. *Uncertainty Quantification: Theory, Implementation, and Applications*. Society for Industrial and Applied Mathematics, USA, 2013. ISBN 161197321X.

[14] G. Stefanou. The stochastic finite element method: Past, present and future. *Computer Methods in Applied Mechanics and Engineering*, 198(9):1031–1051, 2009. ISSN 0045-7825. doi: https://doi.org/10.1016/j.cma.2008.11.007. URL https://www.sciencedirect.com/science/article/pii/S0045782508004118.