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Efficient yield estimation of multiband patch antennas by polynomial chaos-based Kriging

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Abstract

Yield estimation of antenna systems is important to check their robustness with respect to the uncertain sources. Since direct Monte Carlo sampling of accurate physics-based models can be computationally intensive, this work proposes the use of the polynomial chaos–Kriging (PC-Kriging) metamodeling method for fast yield estimation of multiband patch antennas. PC-Kriging integrates the polynomial chaos expansion (PCE) as the trend function of Kriging metamodel since the PCE is good at capturing the function tendency and Kriging is good at matching the observations at training points. The PC-Kriging method is demonstrated on two analytical cases and two multiband patch antenna cases and is compared with the PCE and Kriging metamodeling methods. In the analytical cases, PC-Kriging reduces the computational cost by over 40% compared with PCE and over 94% compared with Kriging. In the antenna cases, PC-Kriging reduces the computational cost by over 60% compared with Kriging and over 90% compared with PCE. In all cases, the savings are obtained without compromising the accuracy.

KEYWORDS

antenna yield estimation, Kriging, microstrip multiband patch antenna, Monte Carlo sampling, polynomial chaos expansions, polynomial chaos-based Kriging

1 | INTRODUCTION

Yield is the metric for checking the reliability of antenna system with respect to the uncertainties due to the manufacturing process.^{1,2} In particular, yield is the percentage of designs satisfying the design specifications. The process of yield estimation can be completed by running arbitrary number of high-fidelity simulation models,¹ such as full-wave electromagnetic (EM) model,³ using Monte Carlo sampling (MCS).⁴ The high-fidelity physics model evaluations are typically time-consuming, rendering the MCS-based yield estimation computationally impractical.

Metamodeling methods^{5,6} are widely used to alleviate the computational burden. There are generally two types of metamodels: data-fit metamodels⁷ and multifidelity metamodels.⁸ Data-fit metamodels utilize the high-fidelity physics-based simulation model evaluations as training points, while the multifidelity metamodels can make use of physics-based simulation models of varying degrees of accuracy. Multifidelity metamodels can be efficient when fast and good low-fidelity models are available. Data-fit metamodeling is more versatile because only one level of simulation model is needed.

Advanced data-fit metamodels have been successfully used for antenna system modeling and design at reduced computational costs. Rama Sanjeeva Reddy et al⁹ introduced the radial basis function neural network into design of

multiple function antenna arrays and obtained a success rate as high as 98%. Koziel et al¹⁰ constructed the fast data-fit Kriging metamodel as part of multiobjective design optimization of antennas handling arbitrary number of objective functions. Du and Roblin¹¹ introduced the polynomial chaos expansion (PCE) method for statistical metamodeling of the far field radiated by antennas undergoing random disturbances and validated the PCE model with a deformable canonical antenna.

This work introduces the use of the PC-Kriging metamodeling method¹² for the yield estimation of multiband patch antenna systems. PCE¹³ is well known for capturing the tendency of the objective function, whereas Kriging¹⁴ handles the observation values at training points well. The PC-Kriging method aims at integrating the advantages of both metamodeling methods expecting fewer training points required for constructing a reliable and fast model in lieu of the computationally expensive high-fidelity simulation model. The PC-Kriging method is demonstrated on the yield estimation of two multiband patch antenna cases, as well as two analytical test functions.

The remainder part of this paper is organized as follows. The next section provides the details of the yield estimation for antennas. The following section describes the metamodeling methods, including Kriging, PCE, and PC-Kriging, utilized in this work. Then, all metamodeling methods are demonstrated and compared with numerical examples. The paper ends with conclusion and suggestions of future work.

2 | ANTENNA YIELD ESTIMATION

Let $\mathbf{R}(\mathbf{x})$ denote the antenna responses of interest evaluated using an EM simulation model, eg, the reflection characteristic, and $\mathbf{x} \in \mathbb{R}^m$ the vector containing deterministic/uncertain design parameters. Let \mathbf{x}_0 represent the nominal design under ideal conditions. Let $d\mathbf{x}$ be the disturbance due to the manufacturing tolerances or uncertainties existing in the antenna system and can be sampled using pre-define empirical probabilistic distributions. Therefore, the actual designs taking the tolerances and uncertainties under consideration can be represented as $\mathbf{x}_0 + d\mathbf{x}$. Now, a counting function $H(\mathbf{x})$ is defined as follows.²

$$H(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{R}(\mathbf{x}) \text{ satisfies the design specifications} \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

Then, the yield at the nominal design introduced above, ie, the percentage of satisfying designs out of the total designs, is found as follows.²

$$Y(\mathbf{x}^0) = \frac{\sum_{j=1}^N H(\mathbf{x}^0 + d\mathbf{x}^j)}{N}, \quad (2)$$

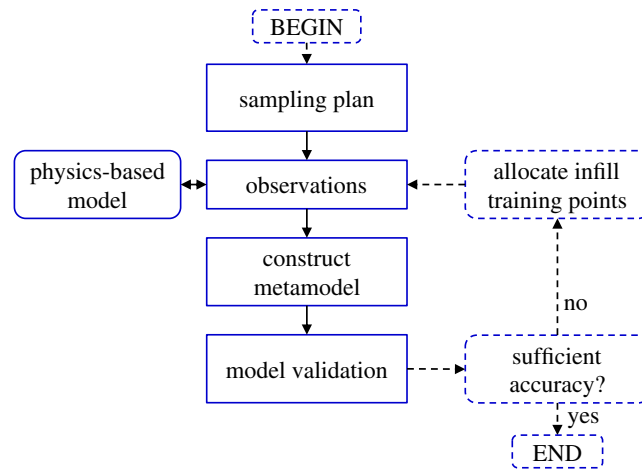
where $d\mathbf{x}^j$, $j = 1, 2, \dots, N$ are the disturbances with pre-assigned empirical probabilistic distributions as introduced above. Estimating the yield using (2) can be computationally impractical if the model evaluation $\mathbf{R}(\mathbf{x})$ is time-consuming.

3 | METAMODELING METHODS

In this work, the PC-Kriging¹² metamodeling method is introduced to antenna yield estimation to alleviate the computational burden. This section describes the overall metamodeling process and the specific methods utilized in this work. Specifically, Kriging,¹⁴ PCE,¹⁵ and PC-Kriging¹² are described. Metrics used for model validation are defined.

3.1 | Process flow

The metamodeling^{5,16} process is shown in Figure 1. The construction process starts with generating a sampling using Latin hypercube sampling (LHS)¹⁷ for the training data set, on which the physics-based model is run to

FIGURE 1 A flowchart of the metamodeling process

obtain the observations. With the training data set and the associated observations, the metamodel is constructed. The metamodel is then validated using a set of testing data generated by MCS¹⁸ by comparing the root-mean-square error (RMSE) (described in Section 3.6) with a user-defined accuracy threshold, which is set to 1% of the standard deviation of the testing observations in this work. If the RMSE is not small enough, an arbitrary number of training points are added to the initial sampling plan, and the iteration is continued until sufficient accuracy is reached.

3.2 | Sampling plan

Monte Carlo sampling¹⁹ and LHS²⁰ are the sampling tools used in this work, and a description of each follows. MCS¹⁹ is a commonly used technique of random sampling probability distributions, and the generated sampled values can be randomly from anywhere within variability space. The process of MCS starts with random numbers within the range of [0, 1] with replacement. The generated random numbers are used as the probabilities of associated cumulative density functions of the variability parameters, and the corresponding values are obtained using quantile functions. MCS is used in this work for the testing data set. LHS²⁰ aims at randomly sampling the given probability distributions of the variability parameters more effectively than MCS. This goal is achieved by stratifying the probability distributions into equal intervals on the cumulative scale [0, 1] and then complete random sampling within each interval, which avoids clustering the generated numbers. Then, the generated numbers are used as the probabilities of associated cumulative density functions as the aforementioned process. And the last one step is to find the corresponding values using quantile functions. The training data set is generated using LHS in this work.

3.3 | Kriging

Kriging^{14,21} models the training data set as a Gaussian process using

$$M^{KR} = \mathbf{f}^T(\mathbf{X})\boldsymbol{\beta} + \sigma^2 Z(\mathbf{X}), \quad (3)$$

where $\mathbf{X} \in \mathbb{R}^m$ is the vector of m -dimensional system variability parameters, $\mathbf{f}^T(\mathbf{X}) = [f_0(\mathbf{X}), \dots, f_{p-1}(\mathbf{X})] \in \mathbb{R}^p$ is the vector of p -dimension regression basis functions, both ordinary basis function $\mathbf{f}_T = [1, 1, 1, \dots, 1]$ and linear basis function $\mathbf{f} = [1, X_1, X_2, \dots, X_m]^T$ are investigated in this work, $\boldsymbol{\beta} = [\beta_0(\mathbf{X}), \dots, \beta_{p-1}(\mathbf{X})] \in \mathbb{R}^p$ denotes the vector of corresponding coefficients to be determined, $\mathbf{f}^T(\mathbf{X})\boldsymbol{\beta}$ is called the trend function, σ^2 is the constant variance of the Gaussian process, and $Z(\mathbf{X})$ represents the local deviation from the trend function and is modeled as a stationary Gaussian process with zero mean and unit variance.

A Gaussian exponential spatial correlation function is used in this work and is defined as follows.²¹

$$R(\mathbf{X}_{\text{tr}}, \mathbf{X}'_{\text{tr}}) = \exp \left[- \sum_{k=1}^m h_k |X_{\text{tr},k} - X'_{\text{tr},k}|^2 \right], \quad (4)$$

where \mathbf{X}_{tr} and \mathbf{X}'_{tr} are two random vectors of variability parameters within training data set and $\mathbf{h} = [h_1, h_2, \dots, h_m]^T$ denotes the vector of unknown hyperparameters to be tuned.

The Kriging predictor for any untried \mathbf{X} is written as follows.²¹

$$M^{KR}(\mathbf{X}) = \mathbf{f}^T \boldsymbol{\beta} + \boldsymbol{\beta}^T \mathbf{R}^{-1} (\mathbf{Y}_{\text{tr}} - \mathbf{F}\boldsymbol{\beta}), \quad (5)$$

where \mathbf{Y}_{tr} is the observations of training database, $F_{ij} = f_j(x_i)$, where $i = 1, 2, \dots, N_{\text{tr}}$, $j = 1, 2, \dots, N_{\text{tr}} + 1$, N_{tr} is the total number of training data, \mathbf{r} is the vector of cross correlation between the point to be predicted (\mathbf{X}) and each training point, here $r_i = R(\mathbf{X}, \mathbf{X}_{\text{tr},i}; \boldsymbol{\beta})$, \mathbf{R} is the correlation matrix among the training points with $R_{ik} = R(X_{\text{tr},i}, X_{\text{tr},k}; \boldsymbol{\beta})$, where $i, k = 1, 2, \dots, N_{\text{tr}}$, and $\boldsymbol{\beta}$ and σ^2 are given by

$$\hat{\boldsymbol{\beta}} = (\mathbf{F}^T \mathbf{R}^{-1} \mathbf{F})^{-1} \mathbf{F}^T \mathbf{R}^{-1} \mathbf{Y}_{\text{tr}}, \quad (6)$$

and

$$\hat{\sigma}^2 = 1/N_{\text{tr}} (\mathbf{Y}_{\text{tr}} - \mathbf{F}\hat{\boldsymbol{\beta}})^T \mathbf{R}^{-1} (\mathbf{Y}_{\text{tr}} - \mathbf{F}\hat{\boldsymbol{\beta}}). \quad (7)$$

The maximum likelihood estimation on \mathbf{h} is found by solving

$$\hat{\mathbf{h}} = \underset{\mathbf{h}}{\text{argmin}} \left(\frac{1}{2} \log(\det(\mathbf{R})) + \frac{N_{\text{tr}}}{2} \log(2\pi\sigma^2) + N_{\text{tr}}/2 \right). \quad (8)$$

3.4 | Polynomial chaos expansions

Polynomial chaos expansion¹⁵ has the generalized formulation

$$M(\mathbf{X}) = \sum_{i=1}^{\infty} \alpha_i \Phi_i(\mathbf{X}), \quad (9)$$

where $\mathbf{X} \in \mathbb{R}^m$ is a vector with random independent components, described by a probability density function of \mathbf{X} , $M(\mathbf{X})$ is a map of \mathbf{X} , i is the index of i th polynomial term, Φ_i is multivariate polynomial basis, and α_i is the corresponding coefficient of the basis function. Legendre and Hermite basis¹³ will be used for uniform and normal distribution, respectively.

In practice, the total number of sample points needed does not have to be infinite; instead, a truncated form of the PCE is used and is described as

$$M(\mathbf{X}) \approx M^{PC}(\mathbf{X}) = \sum_{i=1}^P \alpha_i \Phi_i(\mathbf{X}), \quad (10)$$

where $M^{PC}(\mathbf{X})$ is the truncated PCE model and P is the total number of required sample points, given by

$$P = \frac{(p+n)!}{p!n!}, \quad (11)$$

where p is the required order of the PCE and n is the total number of random variables.

The observations of the training data set are constructed as summation of PCE predictions at the same design points and the corresponding residuals as

$$M(\mathbf{X}) \approx M^{PC}(\mathbf{X}) + \epsilon_{PC} = \sum_{i=1}^P \alpha_i \Phi_i(\mathbf{X}) + \epsilon_{PC} \equiv \boldsymbol{\alpha}^T \boldsymbol{\Phi}(\mathbf{X}) + \epsilon_{PC}, \quad (12)$$

where ϵ_{PC} is the residual between $M(\mathbf{X})$ and $M^{PC}(\mathbf{X})$, which is to be minimized by least-squares methods. The coefficients $\boldsymbol{\alpha}$ can be determined by solving the least-squares minimization problem

$$\hat{\boldsymbol{\alpha}} = \operatorname{argmin}_{\boldsymbol{\alpha}} \mathbb{E}[\boldsymbol{\alpha}^T \boldsymbol{\Phi}(\mathbf{X}) - M(\mathbf{X})]. \quad (13)$$

The ordinary least-squares (OLS) method¹³ is an analytical solution to problem (13) with

$$\hat{\boldsymbol{\alpha}} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{Y}_{\text{tr}}, \quad (14)$$

where \mathbf{Y}_{tr} is vector of model responses, $A_{i,j} = \Phi_i(x^j)$, $j = 1, \dots, n$, $i = 1, \dots, P$. Another way of determining the coefficients is by the least-angle regression (LARS),²² which is an advanced regression method for solving (13) after adding an L_1 norm term of the unknown coefficients scaled by a penalty factor (λ) to favor low-rank solution²³ as

$$\hat{\boldsymbol{\alpha}} = \operatorname{argmin}_{\boldsymbol{\alpha}} \mathbb{E}[\boldsymbol{\alpha}^T \boldsymbol{\Phi}(\mathbf{X}) - M(\mathbf{X})] + \lambda \|\boldsymbol{\alpha}\|_1. \quad (15)$$

The two main steps in the LARS method are initialization and iteration.¹³ The initialization step sets all PCE coefficients $\boldsymbol{\alpha}$ as $\mathbf{0}$ making the residual of each observation the observation itself and defines a candidate set containing all orthogonal PCE bases and an empty active set. The iteration step finds a PCE basis Φ_i , which is the most correlated with current residual, and puts it into the active set; then, the optimal value of the least squares is determined and moves the associated coefficient α_i towards the optimal value until another basis Φ_j is found to have the same correlation with current residual. The previous step is iterated until the size of active set reaches the required number of samples or the total number of observations.

Conventional PCE follows the standard form truncation scheme (10). The sparsity-of-effect principle²⁴ claims that the interaction terms do not have much effect on the PCE prediction. Following this idea, the hyperbolic truncation scheme,¹³ which is also known as the q -norm method, is applied for sparse PCE construction. The hyperbolic truncation technique is expressed as

$$A^{M,p,q} = \left\{ \boldsymbol{\alpha} \in A^{M,p} : \sum_{i=1}^N \left(\frac{\alpha_i}{p} \right)^q \leq 1 \right\}. \quad (16)$$

If $q = 1$, the hyperbolic truncation is the same as standard truncation scheme. For $q < 1$, the hyperbolic truncation can reduce the interactive terms further based on standard truncation schemes.

3.5 | Polynomial chaos-based Kriging

PC-Kriging^{12,25} is a state-of-the-art metamodeling approach, which combines the well-established techniques Kriging and PCE. The descriptions in Sections 3.3 and 3.4 show that the ways of constructing Kriging and PCE make these two metamodeling techniques be regression type and interpolation type, respectively. Because of these characteristics, Kriging captures the local variations well, while PCE captures the global behavior. PC-Kriging aims at combining the advantages of Kriging and PCE for a more efficient metamodeling technique.

The PC-Kriging metamodel is defined as the Kriging model,²¹ whose trend function is used as a constructed PCE metamodel on the same set of training data set. PC-Kriging has the generalized formula as follows:

$$M(\mathbf{X}) \approx M^{\text{PC-Kriging}}(\mathbf{X}) = \sum_{i=1}^P \alpha_i \Phi_i(\mathbf{X}) + \sigma^2 Z(\mathbf{X}), \quad (17)$$

where $M^{\text{PC-Kriging}}$ is the approximation using PC-Kriging, the first term of right-hand side is the truncated-form PCE, which is used as the trend function within the universal Kriging formula, and σ and $Z(\mathbf{X})$ denote the constant standard deviation and the zero mean and unit variance stationary Gaussian process, respectively, as described in Section 3.3.

The construction of PC-Kriging consists of the following main steps:

1. Construct PCE orthogonal bases corresponding with the distributions of random inputs.
2. Reduce the total number of bases by applying hyperbolic truncation scheme.
3. Solve for PCE coefficients using LARS method to construct PCE metamodel.
4. Insert the constructed PCE model as trend function of the universal Kriging.
5. Calculate the unknown coefficients within the Kriging model in step 2 using maximum likelihood method as shown in Section 3.3.

3.6 | Model validation

The metamodels are validated against the physics-based model observations using the RMSE, which is defined as

$$RMSE = \sqrt{\sum_{i=1}^{N_t} (\hat{Y}_i - Y_i)^2 / N_t}, \quad (18)$$

where N_t is the total number of testing data and \hat{Y}_i and Y_i are the metamodel estimation and observation of the i th testing point, respectively. In this work, 1% of the standard deviation of testing points ($1\% \sigma_{\text{testing}}$) is used as an accuracy threshold of the RMSE value of the metamodel. Specifically, if the RMSE is smaller than $1\% \sigma_{\text{testing}}$, the metamodel is sufficiently accurate for further implementation. Otherwise, resampling a larger training data set is required following (11) for a higher order PCE.

4 | NUMERICAL EXAMPLES

The PC-Kriging method is applied on two analytical test functions, the Ishigami function and the short column function, and two physics-based antenna yield estimation cases. For the purpose of demonstration, the computational cost of each metamodel is based on the total number of training points required to reach the prescribed accuracy level.

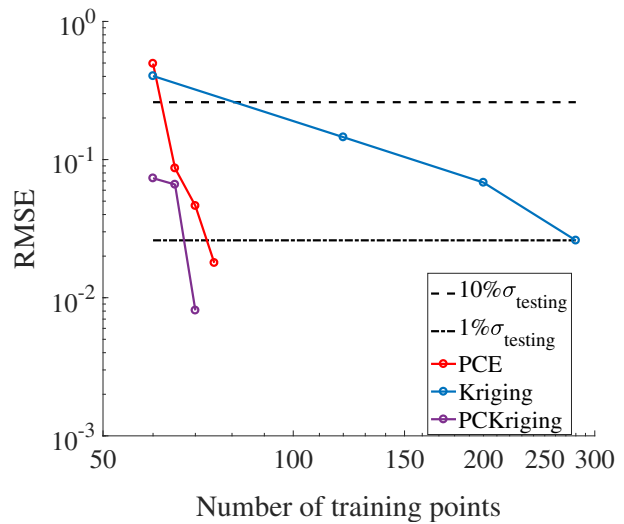
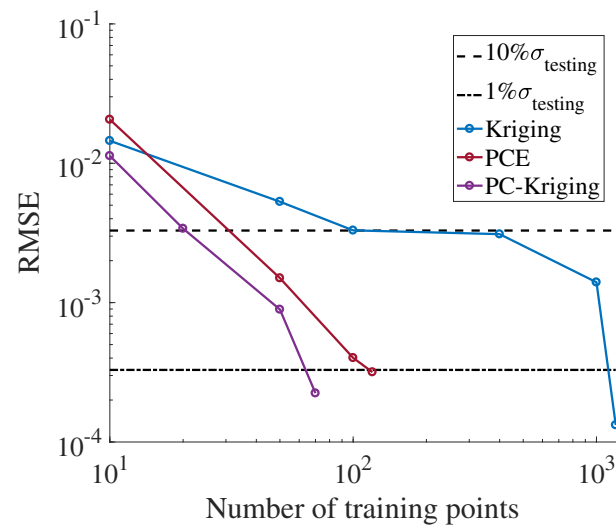
4.1 | Ishigami function

The Ishigami function²⁶ exhibits strong nonlinearity and nonmonotonicity and is commonly used for validating uncertainty analysis methods. This work uses the version developed by Sobol' and Levitan,²⁷ which is defined as

$$f(\mathbf{X}) = \sin(X_1) + 7\sin^2(X_2) + 0.1X_3^4\sin(X_1), \quad (19)$$

where all three uncertain parameters X_1 , X_2 , and X_3 follow a uniform distribution $\mathcal{U}(-\pi, \pi)$.

The RMSE values, based on 1000 MCS testing points, versus the number of LHS training points are given in Figure 2. The results show that PC-Kriging requires only 70 training points, while Kriging and PCE require 300 and 75 samples, respectively. It can be seen that PC-Kriging has the steepest convergence rate and performs better than Kriging and PCE metamodels at the same number of training points.

FIGURE 2 Metamodel construction of the Ishigami function**FIGURE 3** Metamodel construction of the short column function

4.2 | Short column function

The short column function models a structural column with uncertainties due to the material properties. The function is given as

$$f(\mathbf{X}) = 1 - \frac{4X_2}{bh^2X_1} - \frac{X_3^2}{b^2h^2X_1^2} \quad (20)$$

where b is the width of the cross section and equals 5 mm, h is the depth of the cross section and equals 15 mm, X_1 , X_2 , and X_3 are the uncertain parameters in this case, and $X_1 \sim \mathcal{LN}(5, 0.5)$ MPa is the yield stress (\mathcal{LN} represents a lognormal distribution), $X_2 \sim \mathcal{N}(2000, 400)$ MNm is the bending moment (\mathcal{N} represents a normal distribution), and $X_3 \sim \mathcal{N}(500, 100)$ N is the axial force.

Figure 3 shows that all metamodeling approaches can reduce the RMSE when increasing the total number of training points. The Kriging, PCE, and PC-Kriging metamodels, however, need different number of samples to reach the 1% testing accuracy. In particular, Kriging needs around 1200 training points, and PCE around 120 training points, whereas PC-Kriging requires only around 70 training points. Thus, PC-Kriging needs around 42% fewer samples than PCE and around 94% fewer than Kriging. In this case, the PC-Kriging metamodel at each number of training points utilizes a 14th degree of the PCE as the trend function.

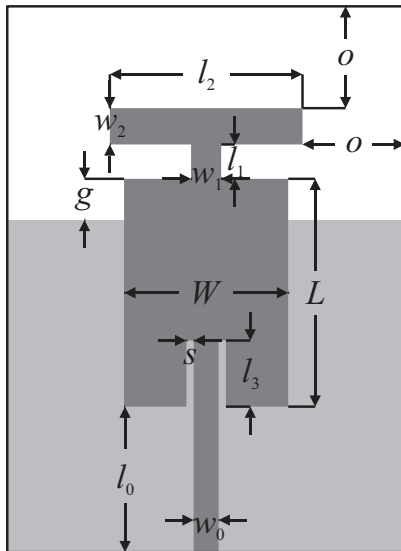


FIGURE 4 Geometry of the dual-band patch antenna. Ground plane shown with light gray shade

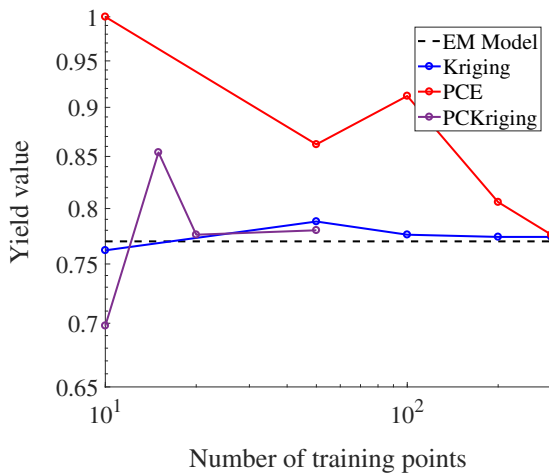


FIGURE 5 Case I convergence of yield estimation as a function of the number of sampling points

4.3 | Multiband patch antenna

The geometry of the microstrip dual-band patch antenna utilized in this work is given in Figure 4. The antenna is implemented on a 0.762-mm-thick Taconic RF-35 dielectric substrate ($\epsilon_r = 3.5$). The independent geometry parameters are $\mathbf{x} = [L \ l_1 \ l_2 \ l_3 \ l_4 \ W \ w_1 \ w_2 \ g]^T$. The EM model \mathbf{R} is implemented in CST.² The nominal design, corresponding to the antenna resonances allocated at the frequencies 2.4 and 5.8 GHz, is $\mathbf{x}_0 = [14.18 \ 3.47 \ 12.44 \ 5.06 \ 15.56 \ 0.65 \ 8.29 \ 5.60]^T$ (all dimensions in mm).

The antenna yield is estimated for the following specs: $|S_{11}| \leq -10$ dB for both 2.4 and 5.8 GHz. It is assumed that Gaussian distribution of the geometry deviation vector $d\mathbf{x}$ has a zero mean and a standard deviation of 0.05 mm (case I) and 0.08 mm (case II).

The parametric study on the convergence of the yield value versus the number of training points is shown in Figures 5 and 6. The PCE, Kriging, and PC-Kriging metamodeling approaches are compared with the direct MCS of the EM model involving 500 model evaluations. In case I, the direct MCS and the metamodeling approaches give a comparable yield estimate. In case II, however, the direct MCS method gives a slightly lower yield value (0.490) than the metamodeling methods (0.528–0.580), indicating that further samples are needed with the direct MCS approach.

In case I ($\sigma = 0.05$ mm), the number of model evaluations needed by PCE and Kriging to reach yield estimations comparable with the direct MCS approach is 300 and 100, respectively, whereas the PC-Kriging requires only 20 training points (cf Table 1). Thus, in case I, the PC-Kriging needs over 93% fewer samples than PCE and 80%

FIGURE 6 Case II convergence of yield estimation as a function of the number of sampling points

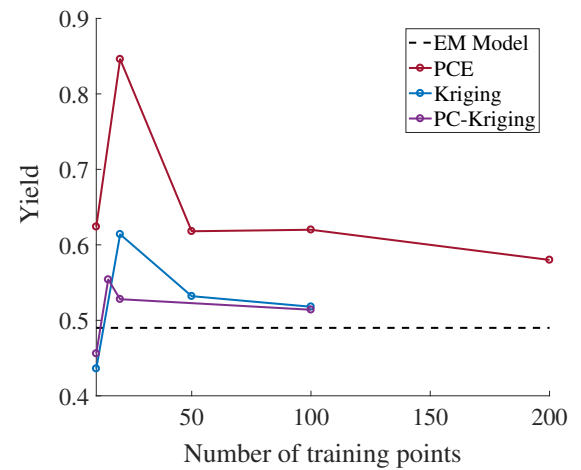


TABLE 1 Computational cost of the yield estimation

Case	Parameter Deviations σ , mm	Method	Estimated Yield	Model Evaluations
I	0.05	MCS on EM model	0.770	500
		PCE	0.776	300
		Kriging	0.776	100
		PC-Kriging	0.776	20
II	0.08	MCS on EM model	0.490	500
		PCE	0.580	200
		Kriging	0.532	50
		PC-Kriging	0.528	20

Abbreviations: EM, electromagnetic; MCS, Monte Carlo sampling; PC, polynomial chaos; PCE, PC expansion.

fewer samples than Kriging. In case II ($\sigma = 0.08$ mm), PC-Kriging still needs 20 model evaluations, but PCE required 200, and Kriging required 50. Therefore, in case II, PC-Kriging needs 90% fewer samples than PCE and 60% fewer than Kriging.

5 | CONCLUSION

The polynomial chaos-based Kriging (PC-Kriging) metamodeling method has been applied to the yield estimation of antennas. The PC-Kriging is constructed as a combination of PCE and Kriging. The former is utilized as a trend function for the latter. The approach was demonstrated on the Ishigami analytical function, the short column analytical function, and the yield estimation of a dual-band microstrip patch antennas. The numerical results indicate that PC-Kriging offers considerable reduction of the computational cost when compared with both PCE and Kriging. Future work will be focused on the characterization of the approach for antenna yield estimation, specifically in terms of its scalability with respect to the parameter space dimension as well as statistical moments of the input probability distribution. Future work will also consider the statistically based design of antennas using PC-Kriging.

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