Statistical Analysis of Periodic Structures and Frequency Selective Surfaces using the Polynomial Chaos Expansions

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***Abstract*—In many real world scenarios, there is always a difference between the performances of simulated and fabricated structures, often due to fabrication tolerances that introduce statistical variations in the physical parameters, e.g., the element size or the periodicity of a Frequency Selective Surface (FSS). In this communication, we address the problem of modeling periodic structures with statistical variations in their geometries, as is typically the case with Metamaterial devices designed for optical wavelengths, where the difficulties in their fabrication almost always introduce small variations in the dimensions of the elements that comprise the "periodic" array.**

***Index Terms*—Periodic Structures, Frequency Selective Surfaces (FSS), Polynomial Chaos Expansion, Latin Hypercube Sampling, Least–Angle Regression, Leave–One–Out Cross–Validation.**

I. Introduction

Recently, there has been considerable interest in the topics of Metamaterials (MTMs) and Frequency Selective Surfaces (FSSs) [1]–[4]. These FSS elements act as spatial filters whose passbands and stopbands depend on the geometrical parameters of its elements. Normally, the FSS structure is simulated during the design process and then fabricated to verify if indeed it has the predicted characteristics. It is not unusual to find that there is a considerable discrepancy between the simulated and measured results, even when there is only a minor difference between the designed and fabricated structures. This is especially true for Metamaterials used at optical wavelengths, where the difficulties in their fabrication almost always introduce small variations in the dimensions of the elements that comprise the "periodic" array. Typically, the effect of this type of variation in the unit cell parameters is studied by using the Monte Carlo (MC) methods. But if the variations are substantial, the MC method results in a highly computationally intensive problem.

In this work, we use the *polynomial chaos expansions* (PCEs) [5] in preference to the commonly used MC method, to develop a meta-model of the physical model of the FSS by using a polynomial expansion approach. In the following sections, we first describe the type of periodic element we are considering for this study. Next, we present the details of the method used to investigate the effects of the variations in the periodic elements. Finally, we include some numerical results to illustrate the application of the proposed method.

II. Periodic Structure with Uncertain Parameters

Periodic structures are typically modeled as infinite arrays of scatterers, and are commonly analyzed by imposing periodic boundary conditions to a unit cell to reduce the original problem to a manageable size and to reduce the computational burden. In this study, we use cross-dipole [6]–[7] as the FSS element (see Fig. 1).

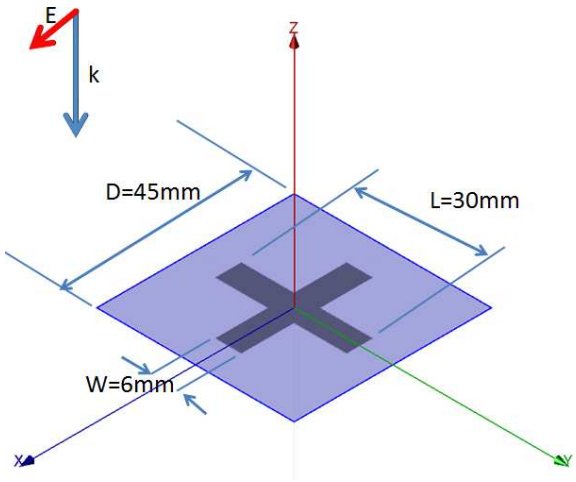


Fig. 1. The input parameters of cross-dipole FSS element

The cross-dipole has three parameters, namely (i) the periodicity $D_x = D_y = D$; (ii) length L; and (iii) width W, as shown in Fig. 1. We assume that these parameters follow normal distributions, and we compute the reflection coefficient for this structure for different values of D, L and W.

III. The Polynomial Chaos Expansions

The *PCEs* aim at modeling the response of a random output variable Y depending on input random parameters $\mathbf{X} = [x_1 \cdots x_m]$, linked by a physical model $Y = \mathcal{M}(\mathbf{X})$ [8], where the input parameters are supposed to be independent. Under these conditions we can use the PCE method to construct a meta-model of the physical model by using the following polynomial expansion:

$$Y = \sum_{\alpha \in \mathbb{N}^m} = a_\alpha \psi_\alpha(\mathbf{X}) \qquad (1)$$

Our purpose here is to substitute the physical model, which is computationally expensive to evaluate, by a meta-model that is much faster to work with. Once we have derived this meta-model, we can perform an MC method on this meta-model to study the propagation of the uncertainty of the input parameters in the physical model.

In (1), the ψ_α are multivariate orthogonal polynomials, which constitute a set of basis functions in the corresponding probabilistic space. Initially built for Gaussian input parameters, the PCE theory has been extended to other types of input probability density functions (PDFs) as the so-called *generalized PCE* theory [9]; for instance, Legendre polynomials can be used as a basis for uniform input PDFs spanning the range [-1,1].

The a_α coefficients in (1) are the unknowns that are yet to be computed. In the family of non-intrusive resolution methods, we choose the regression approach here. The principle is to truncate the expansion to set up a regression problem as described in [10], and to use the ordinary least-square method to compute the coefficients. The choice of this method is mainly motivated by its ease of resolution and its efficiency from the computational cost point of view [10].

However, since we have no information on the impact of the truncation on the quality of the model, this regression approach requires an iterative experimental procedure that uses the estimated accuracy of the obtained meta-model. For example, for a given design of experiments with a given number of simulation points, if the quality of the obtained meta-model is not sufficient, the design of the experiment should be improved with new simulation points in order to have a more accurate model. In this study, we will use the *latin hypercube sampling* (LHS) technique [11] to create the experimental designs that we employ. To add new simulation points to these designs, we will use the *nested LHS* technique [8].

There are several different types of techniques that we might employ for the truncation of this polynomial expansion presented in (1). Classically, in the regression technique, one uses the full-PC truncation, in which one retains the polynomials $\{\psi_\alpha, 0 \leq |\alpha| \leq p\}$ for a chosen degree p. Thus, the number P of polynomials that are retained in the full-PC truncation depends on the degree p, and therefore depends on the number of points in the experimental design, because of conditioning problems of the information matrix arising in the least square estimation. For this given degree p, the number of polynomials kept in the full PC truncation [10], is equal to:

$$P = \begin{pmatrix} M+p \\ p \end{pmatrix} \tag{2}$$

We observe that the number of polynomials increases with the dimensionality M of the input parameters and with the degree p. Thus, if we want a high degree p, we would need to compute a large number of simulation points in the experimental design. In view of this, we choose to employ an optimized truncation based on the *least-angle regression* (LARS) [13] algorithm use to select iteratively among a candidate set of polynomials the most influencing ones onto the output variable that would be kept in the truncation. The so-called LARS truncation is described in detail in [12].

To assess the quality of the meta-model, the ideal case is to determine the generalization error. For each $\mathbf{X}$, the error can be expressed as

$$Err = \mathbb{E}\left[\left(\mathcal{M}(\mathbf{X}) - \hat{\mathcal{M}}(\mathbf{X})\right)^2\right] \tag{3}$$

where $\mathcal{M}(\mathbf{X})$ is the physical model, $\hat{\mathcal{M}}(\mathbf{X})$ is the obtained PCE meta-model and $\mathbb{E}$ is the expectation operator. But, if we only know $\mathcal{M}(\mathbf{X})$ for a few points (those of the LHS experimental design), we can at best estimate this generalization error. A well-known way to estimate this error is the *leave-one-out cross-validation* (LOOCV) [14]. The principle is to take one point $\boldsymbol{x}^{(i)}$ out of the experimental design, to compute the metamodel $\hat{\mathcal{M}}^{(-i)}$ on the remaining points, and to calculate the prediction error at $\boldsymbol{x}^{(i)}$ as follows:

$$\Delta^{(i)} = \mathcal{M}\left(\boldsymbol{x}^{(i)}\right) - \hat{\mathcal{M}}^{(-i)}\left(\boldsymbol{x}^{(i)}\right) \tag{4}$$

By computing $\Delta^{(i)}$ for all $\boldsymbol{x}^{(i)}$ in the experimental design, we can derive the following estimate of the generalization error:

$$Err_{LOO} = \frac{1}{N}\sum_{i=1}^{N} {\Delta^{(i)}}^2 \tag{5}$$

The LOO error is slightly more optimistic than the actual generalization error, but it yields much better error estimate than if we consider a simple empirical mean-squared error. From this LOO error, we can extract a deterministic coefficient Q^2 (which is the equivalent to the well-known R^2 coefficient):

$$Q^2 = 1 - \frac{Err_{LOO}}{\hat{\mathbb{V}}(Y)} \tag{6}$$

where $\hat{\mathbb{V}}(Y)$ is the estimated variance of the output Y. The closer is the estimate of the coefficient Q^2, the better is the quality of the meta-model, and we will use this coefficient as a measure of the quality of the meta-model in this study. It has been shown in [15] that the LOOCV method generally performs well in terms of generalization error bias.

Here the LOOCV is used not only to estimate the accuracy of the generated meta-model, but also to determine the number of LARS polynomials kept in the truncation that provides the best possible accuracy. The entire procedure of PCE construction is summarized as follows:

- Build an initial LHS design of experiments of a given number of points.
- Perform the LARS algorithm to select iteratively the most influencing polynomials among a candidate set of polynomials.
- For each possible number of LARS polynomials kept in the truncation, build the corresponding LARS-PC meta-model and assess its accuracy with the LOOCV.
- Retain the number of LARS polynomials with the highest Q^2 value.
- If the final accuracy of the meta-model is not satisfactory, i.e., if the corresponding Q^2 value is not sufficiently high, add new simulation points in the design of experiment using NLHS technique.
- Restart the entire procedure from the second step until the obtained accuracy is satisfactory.

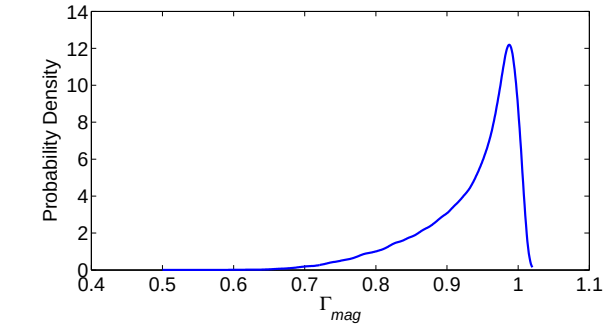
IV. Results

In this study, we are interested in two different output variables, namely the Magnitude (Γ_{mag}) and the Phase (Γ_{phase}) of the Reflection Coefficient. We use three input parameters (see Fig. 1) that follow the normal distribution, and their properties are shown in Table I.

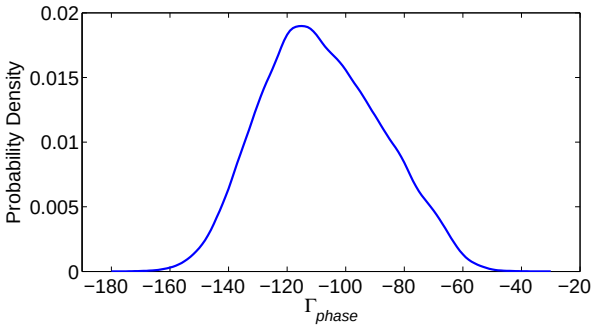
TABLE I
Input Parameters

	D	L	W
Mean	45mm	30mm	6mm
Standard Deviation	2.25mm	1.5mm	0.3mm

We have constructed a LHS design in which the simulation points iteratively increase from 100 by following the nested LHS technique [8]. For each sample of points, a best LARS-PC meta-model was built together with its Q^2 coefficient. Then if the Q^2 coefficient is not sufficiently high, we enrich the LHS design with new sample points until the quality of the best meta-model is sufficiently satisfactory. We have studied both Γ_{mag} and Γ_{phase}, and have obtained Q^2 values



(a)



(b)

Fig. 2. Probability Density as functions of (a) Magnitude of Reflection Coefficient and (b) Phase of Reflection Coefficient

of 0.9921 and 0.9937, respectively, for Γ_{mag} and Γ_{phase} with 400 simulation points. By taking the square root of the corresponding Err_{LOO} (6), we have an estimation of the general root-mean-square error (RMSE) of our models. Then, the RMSE is estimated to be 6.31×10^{-5} and 3.17, respectively, for Γ_{mag} and Γ_{phase}. With these two computationally easy-to-compute LARS-PC meta-models, we can now perform a classic MC method and deduce the distribution of our output variables. The resulting estimated distributions are plotted in Fig. 2.

In Fig. 2(a), we can see that the Γ_{mag} values become slightly above 1, which is clearly non-physical. This behavior can be attributed to the sweeping window of the function used to compute the distribution. Indeed, since there is a high density of the value for 1, and theoretically none above 1, the sweeping window realizes a mean distribution in this area, which explains the crossing. This type of crossing can also be the result of the inaccuracy of the computed LARS-PC model. In fact, even if we have a very good fit on average, the error of the model can become more important in this region, in which there is a high density and where the output variable seems to have an asymptotic behavior. This is due to the fact that the polynomial chaos can have some difficulties to fit in an area where the output is locally constant. In spite of this, our model has very good performance in term of fitting, and we should simply keep in mind that values greater than 1 are non-physical.

V. Conclusion

In this communication, we have utilized a newly introduced technique [5] for modeling periodic structures with statistically varying input parameters. The proposed technique yields accurate results for the reflection characteristics with fewer simulation runs than those needed in a crude Monte Carlo simulation.

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