Data-Driven Arbitrary Polynomial Chaos for Uncertainty Quantification in Filters

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Abstract **─** A non-intrusive arbitrary polynomial chaos (aPC) method is applied to a problem of a band-stop filter with geometrical imperfections. The construction of aPC scheme only requires evaluating a finite number of moments, and does not involve assigning analytical probability density functions for the uncertain parameters of a stochastic model. Therefore, aPC is well suited for applications where the uncertain parameters are represented by raw data samples, as with the case of experimental measurements. The numerical examples show that the aPC approach is accurate even with a limited number of input samples.

Index Terms **─** Data-driven arbitrary polynomial chaos, generalized polynomial chaos, Monte Carlo sampling, uncertainty quantification.

I. INTRODUCTION

Methods of uncertainty quantification (UQ) have been widely used with computational electromagnetics (CEM) to address real-world problems that have probabilistic interpretation. Classically, the well-known Monte Carlo (MC) method is used to estimate the influence of the uncertain parameters on the output metrics of a stochastic model [1-3]. However, the MC method is a sampling method that requires large number of realizations to obtain accurate results. Therefore, in many cases applying the MC method is challenging, especially when incorporated with full-wave solvers. Alternatively, the generalized polynomial chaos (gPC) method [4,5] overcomes this drawback for a modest number of input parameters. In the gPC approach, the probability density function (PDF) of the output is interpolated by orthogonal polynomials defined uniquely for a given probability distribution. In [4], recursive relations of polynomial bases are provided for various types of parametric distributions.

Recently, Oladyshkin and Nowak [6] introduced a moment-based polynomial chaos approach referred to as arbitrary polynomial chaos (aPC). The construction of the polynomial bases in aPC does not require an exact knowledge of the input distributions and depends solely on the input moments. This allows aPC to be used with a broad range of applications, including applications with known input distributions (as in gPC), and with data-driven applications where only limited data samples are available (usually through measurements). Another advantage of aPC, is that since the input data are processed directly in the algorithm through the input moments, undesirable errors related to distribution fitting are avoided.

The objective of this paper is to introduce the non-intrusive aPC method [6] in uncertainty analysis of CEM applications. A band-stop filter based on an electromagnetic band gap (EBG) cell is considered as a model problem. The case studies address geometrical imperfections induced during the manufacturing process. This includes imperfections in the size and the corners of the EBG cell. To emphasize the data-driven concept, part of the work considers the treatment of limited input data sets.

II. MODEL PROBLEM

The notch filter considered in this paper consists of microstrip line suspended over a mushroom-type electromagnetic band gap (MSEBG) cell. The filter configuration is shown in Fig. 1. All the metals including the strip, the EBG cell, and the ground are assumed as perfect conductors. The filter is assumed to be placed in freespace. This is modelled by applying radiation boundary conditions (RBC) on a transparent box that encapsulates the computational domain. The size of the box is chosen such that its faces are located no less than a quarter-wave length from the filter, except at the two ends of the strip line, where waveports are placed to excite the structure. The resonance frequency (f_r) and the bandwidth (BW) are determined by computing the transmission coefficient (S_{12}). This is achieved here via 3D full-wave solver HFSS [9]. For a filter operating at $f_r = 94$GHz and BW $= 7.62$GHz, the input parameters (see Fig. 1 (b)) are set as: $w = 0.21$mm, $\varepsilon_1 = \varepsilon_2 = 3.78$, $h_1 = h_2 = 1$mm, $r = 0.075$mm, and $t =$

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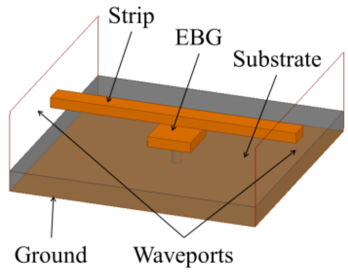
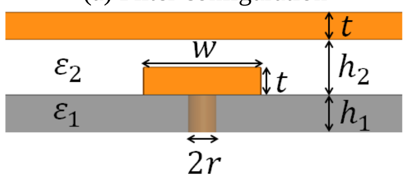
0.05mm. Figure 2 shows the transmission coefficient of the filter with respect to frequency. BW is defined where S_{12} falls below -20dB.



(a) Filter configuration



(b) Input parameters

Fig. 1. Notch filter.

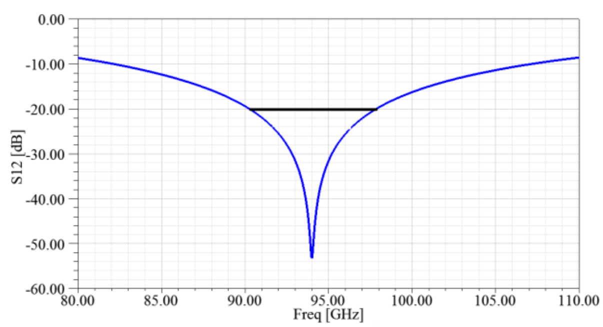


Fig. 2. S_{12} parameter.

III. STATISTICAL FRAMEWORK

A. Non-intrusive polynomial chaos

Consider a vector of independent random variables $\boldsymbol{x} = \{x_1, x_2, \dots, x_N\}$, defined on a sample space Ω, with a joint probability density function (PDF) $f_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{i=1}^{N} f_{X_i}(x_i)$. N is the dimension of $\boldsymbol{x}$ and f_{X_i} is the marginal PDF of x_i. The kth moment of x_i is defined as:

$$\mu_{k,i} = \int_{\Omega_i} x_i^k \, f_{X_i}(x_i) \partial x. \quad (1)$$

However, in some problems f_{X_i} is not known and only M number of x_i samples is available. In this case the moments are given by:

$$\mu_{k,i} = \frac{1}{M} \sum_{j=1}^{M} x_{i,j}^k. \quad (2)$$

Let $y = g(\boldsymbol{x})$ be the model under consideration. x_i represents an input under uncertainty such as the geometrical sizes and the electrical parameters of the filter, while y represents an output of interest, i.e., the resonance frequency or the bandwidth. y can be approximated by the expansion:

$$y(\boldsymbol{x}) = y(x_1, x_2, \dots, x_N) = \sum_{i=0}^{\mathrm{P_{out}}} \alpha_i \Phi_i\,(x_1, x_2, \dots, x_N), \quad (3)$$

where α_i are unknown coefficients, and $\mathrm{P_{out}}$ refers to the number of terms included in the expansion. Φ_i forms a set of multidimensional orthogonal polynomials with respect to $f_{\boldsymbol{X}}(\boldsymbol{x})$:

$$\langle \Phi_i, \Phi_j \rangle = \int_{\Omega} \Phi_i(\boldsymbol{x}) \Phi_j(\boldsymbol{x}) f_{\boldsymbol{X}}(\boldsymbol{x}) \partial \boldsymbol{x} = \left\| {\Phi_i}^2 \right\| \delta_{i,j}. \quad (4)$$

Based on the orthogonality condition in Eq. (4), the coefficients α_i can be determined by the spectral projection method:

$$\alpha_i = \frac{\langle y, \Phi_i \rangle}{\left\| {\Phi_i}^2 \right\|}. \quad (5)$$

The expression in (5) is usually handled by Gaussian quadrature. However, with data-driven applications the locations of the Gaussian weights would vary with different realizations of input sample sets. This can be challenging, especially when full-wave solvers are used to evaluate the system response at these points. In a more convenient method, α_i can be determined from $\mathrm{P_{out}} + 1$ fixed collocation points as:

$$\begin{bmatrix} \Phi_0(\mathbf{x}_0) & \Phi_1(\mathbf{x}_0) & \cdots & \Phi_{\mathrm{P_{out}}}(\mathbf{x}_0) \\ \Phi_0(\mathbf{x}_1) & \Phi_1(\mathbf{x}_1) & \cdots & \Phi_{\mathrm{P_{out}}}(\mathbf{x}_1) \\ \vdots & \vdots & \ddots & \vdots \\ \Phi_0(\mathbf{x}_{\mathrm{P_{out}}}) & \Phi_1(\mathbf{x}_{\mathrm{P_{out}}}) & \cdots & \Phi_{\mathrm{P_{out}}}(\mathbf{x}_{\mathrm{P_{out}}}) \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_{\mathrm{P_{out}}} \end{bmatrix} = \begin{bmatrix} y(\mathbf{x}_0) \\ y(\mathbf{x}_1) \\ \vdots \\ y(\mathbf{x}_{\mathrm{P_{out}}}) \end{bmatrix}, \quad (6)$$

with $\mathbf{x}_0 = \{x_{1,i}, x_{2,i}, \dots, x_{N,i}\}$. The mean and the variance of y satisfy:

$$\mu_y = \alpha_0 \|\Phi_0\|, \qquad \sigma_y^2 = \sum_{i=1}^{\mathrm{P_{out}}} \alpha_i^2 \|\Phi_i^2\|. \quad (7)$$

B. Construction of orthogonal polynomials for an arbitrary distribution.

As already mentioned aPC is a moment-based method. Therefore, the next step is to express the polynomial basis Φ_i in terms of the statistical moments of $\boldsymbol{x}$. To do so we first write Φ_i in terms of univariate orthogonal polynomials using a multi-index I_j^i as:

$$\Phi_i(x_1, x_2, \dots, x_N) = \sum_{j=1}^{N} P_j^{\left(I_j^i\right)}(x_j). \quad (8)$$

$P_j^{(k)}$ refers to the jth univariate polynomial of degree k. It has the form:

$$P_j^{(k)}(x_j) = \sum_{i=0}^{k} p_{i,j}^{(k)} x_j^i, \quad (9)$$

with $p_{i,j}^{(k)}$ being the polynomial coefficients. In [6], it is shown that with straight forward algebra Eqs. (1), (2), and (4) can be used to find the coefficients $p_{i,j}^{(k)}$ in terms of the input moments. This relation is given by the matrix:

$$\begin{bmatrix} \mu_{0,j} & \mu_{1,j} & \cdots & \mu_{k,j} \\ \mu_{1,j} & \mu_{2,j} & \cdots & \mu_{k+1,j} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{k-1,j} & \mu_{k,j} & \cdots & \mu_{2k-1,j} \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} p_{0,j}^{(k)} \\ p_{1,j}^{(k)} \\ \vdots \\ p_{k-1,j}^{(k)} \\ p_{k,j}^{(k)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}. \quad (10)$$

The moment matrix in Eq. (10) may become ill-conditioned when high order polynomials are required. One way to reduce the order of the polynomials without affecting the accuracy of the solutions is by using the multi-element approach [7,8].

C. Error estimation

In data-driven applications an input variable x_i is given as a set of M samples. The l-th realization of the input sample set can be represented as:

$$x_i(l) = \{x_{i,1}(l), x_{i,2}(l), \dots, x_{i,M}(l)\}, \quad l = 1,2,\dots,L, \quad (11)$$

where L is the total number of realizations. Let $Z_{Approx}(l)$ be an output measure computed for the l-th realization. According to the central limit theorem when both M and L are big Z_{Approx} can be approximated by a normal distribution with a mean value $\mu_{Z_{Approx}}$ and a standard deviation $\sigma_{Z_{Approx}}$. Given that, the relative error of the output satisfy the bound:

$$P_r\left(\epsilon \leq \frac{max\{\left\|\mu_{Z_{Approx}} \pm 3\sigma_{Z_{Approx}}\right\| - Z_{Exact}\}}{Z_{Exact}}\right) = 0.9973. \quad (12)$$

P_r and ϵ refer to the probability operator and the relative error of the output, respectively. Z_{Exact} is computed by the exact distribution. In a simpler form the error in Eq. (12) can be approximated by the expression:

$$\epsilon \approx \frac{max\{\left\|\mu_{Z_{Approx}} \pm 3\sigma_{Z_{Approx}}\right\| - Z_{Exact}\}}{Z_{Exact}}. \quad (13)$$

IV. NUMERICAL EXAMPLES

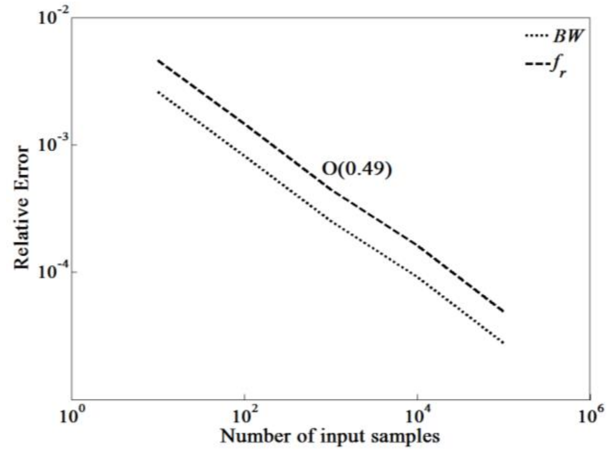
A. Uncertainty in width

First we consider variations in the patch size w (see Fig. 1 (b)). In this case w follows a normal distribution $w \sim N(\mu_w, \sigma_w^2)$, truncated at $3\sigma_w$, i.e., $\Delta w = \pm 3\sigma_w$. μ_w and the other parameters of the filter are fixed at the values provided in Section II. Figure 3 shows the maximum relative error obtained for the expected value and the standard deviation of the model outputs vs. number of input samples computed at $P_{out} = 2$ and $\Delta w = \pm 0.1t$ (t is the patch thickness). As the convergence rate in both cases is of order ~ 0.5, it is clear that the error is due to the statistical sampling used to generate the input sets. However, the results show that acceptable accuracies are achievable with relatively small input sets ($100 \leq M \leq 1000$). For this example, Eq. (6) shows that only 3 input points are required to obtain the model coefficients. Thus, it is clear that the time consumption in aPC is substantially lower when compared with Monte Carlo simulations.

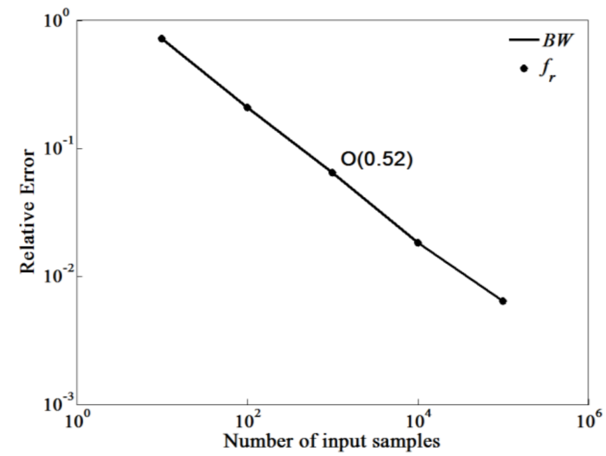
B. Uncertainty in corners

In this second example we study imperfections in the corners of the patch. To do so, a corner is approximated by a cylinder of radius r_i, where $i = 1,2,\dots,4$. The configuration of this problem is shown in Fig. 4. The radius of the cylinders is assumed to follow a normal distribution $r_i \sim N(0, w^2/16)$, truncated on $[0, 3w/4]$.

The univariate polynomials used in this example are of order 2. Since this is 4-th dimensional problem, the system response in Eq. (6) is computed at 15 points (i.e., $P_{out} = 15$). Figure 5 shows the maximum relative error obtained for the expected value and the standard deviation of the model outputs vs. the total number of input samples generated for the 4 corners. As in the previous example the output error in this case study is also dominated by the sampling process (i.e., the convergence rate is of order ~ 0.5). The results here also show that good accuracies can be achieved with a relatively small number of input samples.



(a) Expected value



(b) Standard deviation

Fig. 3. Convergence rate of expected value and standard deviation vs. number of w samples, with $\Delta w = \pm 0.1t$ and $P_{out} = 2$.

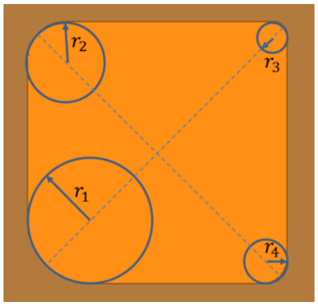
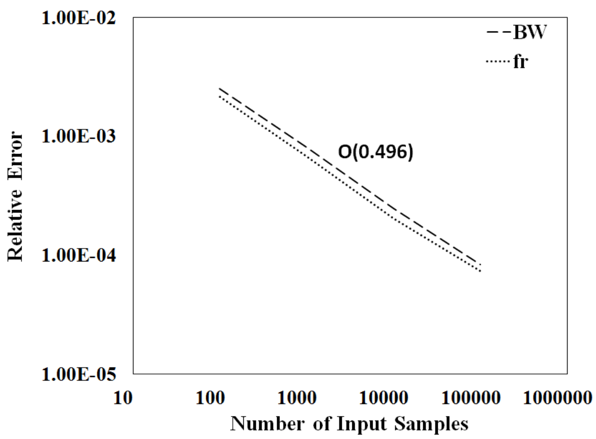
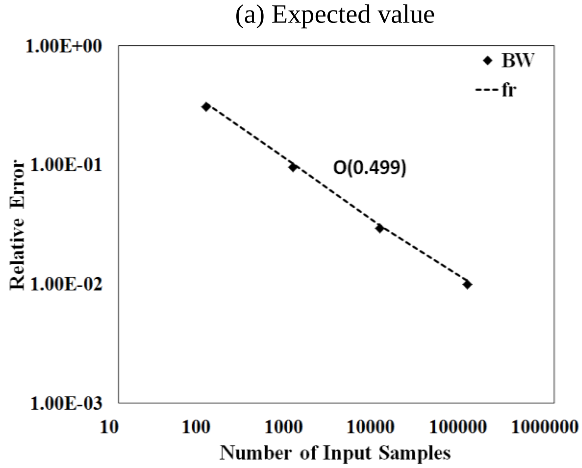


Fig. 4. MSEBG patch with imperfections in corners.



(a) Expected value



(b) Standard deviation

Fig. 5. Convergence rate of expected value and standard deviation vs. the total number of r_i samples, with $i = 4$ and $P_{out} = 15$.

V. CONCLUSION

A procedure based on data-driven arbitrary polynomial chaos (aPC) is introduced for uncertainty quantification (UQ) in filters. The filter imperfections are presented in terms of data samples. The main advantage of using this procedure is that the construction of the chaos polynomials is done by evaluating the input moments directly from the input samples without necessarily knowing the input distributions. In this work the samples are provided by distribution sampling. However, in real-world problems they are obtained by measurements. The aPC approach is validated with a model problem of a band stop filter. Two case studies addressing geometrical imperfections induced during the manufacturing process are considered. The results show that even with low-order polynomials the accuracy of the approach is dominated by sampling process. Therefore, the convergence rate of this approach is of order ~0.5.

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