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Crosstalk Analysis of Printed Circuits with Many Uncertain Parameters Using Sparse Polynomial Chaos Metamodels

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Abstract—This paper presents a metamodel based on the sparse polynomial chaos approach, well adapted to high-dimensional uncertainty quantification problems, applied for the analysis of crosstalk in printed circuit board microstrip traces. It enables to estimate, with a low computational cost compared to Monte Carlo (MC) simulation, statistical quantities and provides a sensitivity analysis of the crosstalk effects considering numerous uncertain variables. The approach is validated against MC simulation and shows a good efficiency and accuracy.

Index Terms—Circuit design, crosstalk, high dimensional problems, polynomial chaos, printed circuit board, sensitivity analysis, transmission lines, uncertainty quantification.

I. INTRODUCTION

Due to the increasing impact of variability in electronic devices, the assessment of uncertainties effect is becoming a major challenge. Indeed, the design phase of circuits should allow to take into account uncertain parameters, such as the temperature variations, intrinsic characteristics of materials, geometrical tolerances, since they may generate a large variability of output signals.

Since a few years, research studies have investigated the computation of several statistical quantities, providing an estimation of the central tendency [1]–[3] and/or a risk analysis [4]–[9] of a response depending on uncertain parameters. For example, various techniques based on polynomial chaos (PC) allow to efficiently estimate statistical moments and distribution functions for the analysis of signal and power integrity in high-speed interconnects [10]–[12]. These approaches aim at replacing a numerical model (which can be computationally expensive), from a limited set of its evaluations, by a metamodel (*i.e.* an analytic function) in order to predict the observed response. However, when the size of the problem increases, *i.e.* with a large number of uncertain input parameters, these techniques show some limitations since the number of computations of the numerical model blows up.

This paper introduces then an approach based on the *sparse PC* [13], aiming at substituting a numerical model in the context of high dimensional problems. First, the technique is presented in Section II. Next, an application case of a transmission line network with coupled lines is given in Section III. Finally, the results obtained by the sparse PC metamodel are given and discussed in Section IV.

II. SPARSE POLYNOMIAL CHAOS REPRESENTATION

A. Introduction

Let \mathbf{X} be a random vector of joint PDF $f_{\mathbf{X}}(\mathbf{x})$, including M random variables (X_1, \dots, X_M) assumed to be independent and representing the uncertain input parameters of the problem. Let $Y = \mathcal{M}(\mathbf{X})$ be the random response (supposed scalar) of a numerical model \mathcal{M} describing the physical system. Assuming that the random response Y has a finite variance, it may be written as [14]:

$$Y = \sum_{\lambda \in \mathbb{N}^M} a_{\lambda} \Phi_{\lambda}(\mathbf{X}), \quad (1)$$

where the a_{λ} 's are unknown deterministic coefficients and the Φ_{λ} 's represent a basis of multivariate polynomials, which are orthonormal with respect to the joint PDF $f_{\mathbf{X}}(\mathbf{x})$, *i.e.* $\mathbb{E}[\Phi_{\lambda}(\mathbf{X})\Phi_{\beta}(\mathbf{X})] = \delta_{\lambda\beta}$, with $\delta_{\lambda\beta} = 1$ if $\lambda = \beta$ and 0 otherwise. In practice, families of orthonormal polynomials are associated in terms of probability distributions of input random variables.

B. Classical Truncation Scheme

Let $\mathcal{X} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\}$ be a set of realizations of \mathbf{X} , called *experimental design* (ED), and $\mathcal{Y} = \{\mathcal{M}(\mathbf{x}^{(1)}), \dots, \mathcal{M}(\mathbf{x}^{(n)})\}$ be the associated set of model response quantities.

Using a set of the model evaluations \mathcal{Y} , the coefficients of the PC representation may be estimated by using non-intrusive techniques. Among these techniques, the ordinary least square regression [15] may be employed. It relies on the choice of a *truncation set*, *i.e.* $\mathcal{A} = \{\lambda_0, \dots, \lambda_{l-1}\} \subset \mathbb{N}^M$, containing the multi-indices of the basis of the remained polynomials $\{\Phi_{\lambda_0}, \dots, \Phi_{\lambda_{l-1}}\}$.

The common truncation strategy used in the PC expansion, retains the polynomials of the basis having a total degree less than or equal to l , *i.e.* the truncation set $\mathcal{A}^{M,l} = \{\lambda \in \mathbb{N}^M : \|\lambda\|_1 = \sum_{i=1}^M \lambda_i \leq l\}$. With this strategy, the number of coefficients maintained, *i.e.* $L = \frac{(M+l)!}{M!l!}$, blows up for large values of M and l . To reduce the number of terms a_{λ} to estimate (and so the computational cost of the model \mathcal{M}), an improved truncation scheme is then introduced [13].

C. Improved Truncation Scheme

The scheme of the classical PC approximation consists in retaining the L terms contained in the finite set $\mathcal{A}^{M,l}$. An improved truncation scheme [13] based on k , $0 < k < 1$, is given by:

$$\mathcal{A}^{M,l,k} = \{\boldsymbol{\lambda} \in \mathbb{N}^M : \|\boldsymbol{\lambda}\|_k = \left(\sum_{i=1}^M \lambda_i^k \right)^{1/k} \leq l\}. \quad (2)$$

This truncation strategy favors the main effects and low-order interactions, which mainly impact the response quantity according to the *sparsity-of-effects principle* [16]. It is worth noting that the lower is k , the more high-rank interactions will be neglected. Moreover, when $k = 1$, this scheme is equivalent to the classical PC approximation defined by the truncation set $\mathcal{A}^{M,l}$. When $k < 1$, the remaining terms of the polynomial basis can be significantly reduced compared to L [13].

D. Adaptive Technique based on Least Angle Regression

The improved truncation strategy allows to represent the response quantity by a sparse PC approximation. However, the obtained number of terms of the polynomial basis may be even more reduced by using a variable selection algorithm, such as *Least Angle Regression* (LARS) [17].

This method is often used in statistics to deal with high dimensional problems, *i.e.* when the number of input random variables is large. It is a regression technique allowing to select the variables having the most impact on the model response Y . A sparse PC representation is then built, containing a small number R of terms compared to the full approximation, leading to the *sparsity index* $S = \frac{R}{L}$. However, the identification of an efficient number of polynomials basis in the truncation set $\mathcal{A}^{M,l}$ may be difficult. Thus, an adaptive technique allowing to adjust the truncation set is employed. It consists in evaluating a range of degrees l , and then retaining the best one from the leave-one-out error ϵ_{LOO} . This error criterion, often used in machine learning, is based on a cross validation technique. It is computed *a posteriori* without additional model evaluations. It allows to represent quite properly the response Y by a regression model while avoiding the over-fitting phenomenon [13]. It can be written as

$$\epsilon_{LOO} = \frac{\sum_{i=1}^N (\mathcal{M}(\mathbf{x}^{(i)}) - \mathcal{M}_{-i}^{PC}(\mathbf{x}^{(i)}))^2}{\sum_{i=1}^N \left(\mathcal{M}(\mathbf{x}^{(i)}) - \frac{1}{N} \sum_{i=1}^N \mathcal{M}(\mathbf{x}^{(i)}) \right)^2}, \quad (3)$$

where $\mathcal{M}_{-i}^{PC}(\mathbf{x}^{(i)})$ are N metamodels built up on the ED $\mathcal{X} \setminus \mathbf{x}^{(i)} = \{\mathbf{x}^{(q)}, q = 1, \dots, N, q \neq i\}$. From a range of degrees l , the adaptive technique selects the one minimizing the error ϵ_{LOO} . In the following, the quality of the metamodel will be computed via the Q^2 coefficient defined by $Q^2 = 1 - \epsilon_{LOO}$, $0 \leq Q^2 \leq 1$. Note that larger is Q^2 , the better is the prediction of the metamodel built up.

E. Post-processing

Once the coefficients of PC expansion are obtained, it is possible to carry out a post-processing at a negligible cost to evaluate a quantity of interest. For example, the orthonormality

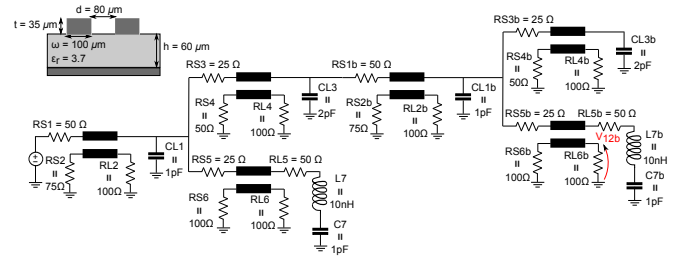


Fig. 1. Transmission line network with coupled microstrip traces and associated line cross section.

of the basis allows to obtain directly the expectation and the variance of the response Y from the coefficients:

$$\mathbb{E}[Y] = a_0 \quad (4)$$

$$\mathbb{V}[Y] = \sum_{\lambda \in \mathcal{A} \setminus \{0\}} a_\lambda^2 \quad (5)$$

In addition, it is also possible, at a lower cost, to estimate the so-called *Sobol' sensitivity indices* [18] aiming at quantifying the impact of input uncertainties on the output variability. For instance, the *total sensitivity indices* allowing at estimating the global effect of the random variable X_i on the model response Y , can be estimated by [19]:

$$S_{T,i} = \frac{\sum_{\lambda \in \mathcal{A}_{T,i}} a_\lambda^2}{\mathbb{V}[Y]} \quad (6)$$

where $\mathcal{A}_{T,i} = \{\boldsymbol{\lambda} \in \mathcal{A} : \lambda_i \neq 0\}$.

III. TRANSMISSION LINE NETWORK WITH COUPLED LINES

In this section, a lossless transmission line network illustrated in Fig. 1, is considered to evaluate the impact of input uncertainties on signal propagation. The structure is extracted from [11], but the size has been raised. The transmission line network is fed by a sine wave voltage source with a magnitude of 1 V and sweeping the frequency band [100 MHz - 10 GHz]. The segments of coupled microstrip transmission line have a mean length of 3 cm. The randomness of the structure is provided by all RLC components, and all parameters of the cross section, *i.e.* copper trace widths w , trace thicknesses t , trace-to-trace separation d , substrate dielectric relative permittivity ϵ_r and substrate thicknesses h . This leads to 33 uncertain parameters, which are considered as uniform random variables with 20% of uncertainty around their nominal values given in Fig. 1.

In this study, we are interested in estimating the far-end crosstalk voltage V_{12b} in the transmission line network. We aim at building a sparse PC metamodel of the voltage V_{12b} in order to reduce the computational cost of the numerical model. Moreover, we provide a hierarchization of uncertain input parameters with respect to their influence on the voltage V_{12b} .

IV. NUMERICAL RESULTS AND DISCUSSION

The statistical results given in this section have been obtained via the UQLAB toolbox (Uncertainty Quantification toolbox in MATLAB) [20].

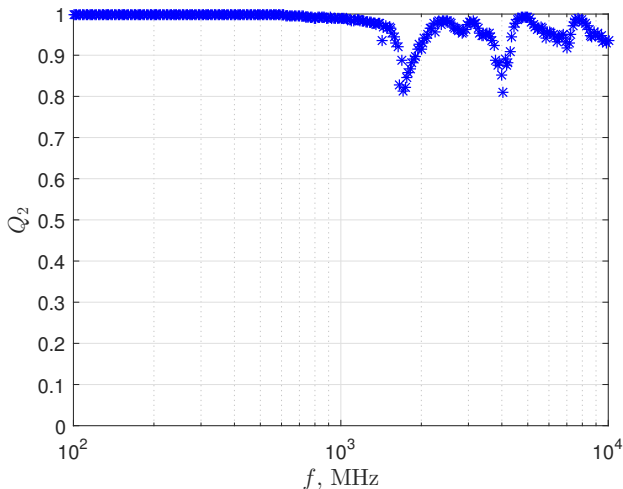


Fig. 2. Evolution of the Q^2 coefficient of the sparse PC metamodel over the frequency band [100 MHz - 10 GHz].

A. Metamodeling by Sparse PC

In order to study the impact of uncertain input parameters, we consider the crosstalk voltage V_{12b} over the frequency band [100 MHz - 10 GHz]. We build a sparse PC with 200 realizations from Latin Hypercube Sampling [21] with an adaptive degree l between 1 and 10. The choice of a large range of degrees is carried out in order to properly approximate the voltage V_{12b} at high frequencies, since it can be particularly irregular in resonance regime. The k parameter introduced in (2) is set to 0.6. This allows to obtain a reduced number of polynomial basis coefficients while providing a good approximation of the model response.

The coefficient of quality Q^2 (see Section II) of the sparse PC in the frequency band [100 MHz - 10 GHz], is illustrated in Fig. 2. We observe that the coefficient Q^2 is very close to 1 from 100 MHz to 1 GHz, and then from 1 GHz to 10 GHz, it oscillates between 0.8 and 1. This shows that the quality of the sparse PC metamodel in the frequency band [100 MHz - 1 GHz] is very high, while it decreases somewhat over the frequency band [1 GHz - 10 GHz]. This may be explained by the strong variability of the voltage V_{12b} in the resonance domain. In order to illustrate it, we compare in Fig. 3 the predictions of the sparse PC metamodel $\mathcal{M}^{PC}(\mathbf{x}^{(i)})$ (circles) and the evaluations of the numerical model $\mathcal{M}(\mathbf{x}^{(i)})$ (solid line) with 3 realizations from MC simulation. As expected, we observe a very good agreement between the two curves, despite small differences between 1 GHz and 10 GHz, related to the resonances of the voltage V_{12b} . Indeed, we see that the behaviour of the voltage V_{12b} is rather smooth over [100 MHz - 1 GHz], and becomes irregular over [1 GHz - 10 GHz] with resonance peaks. This explains the variation of the Q^2 coefficient in Fig. 2 in this last frequency band.

We now choose to illustrate the accuracy of the sparse PC metamodel in low and high frequency domain, *e.g.* at the frequencies of 100 MHz and 9.1 GHz, for which $Q^2_{100\text{ MHz}} = 99.97\%$ and $Q^2_{9.1\text{ GHz}} = 95.42\%$. Thus, we represented, by means of 10000 MC realizations, the PDF's of the crosstalk voltage V_{12b} obtained by sparse PC (red dashed-line) and by

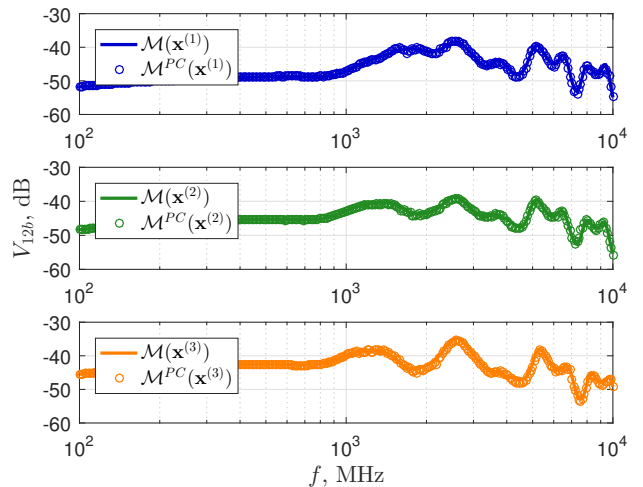


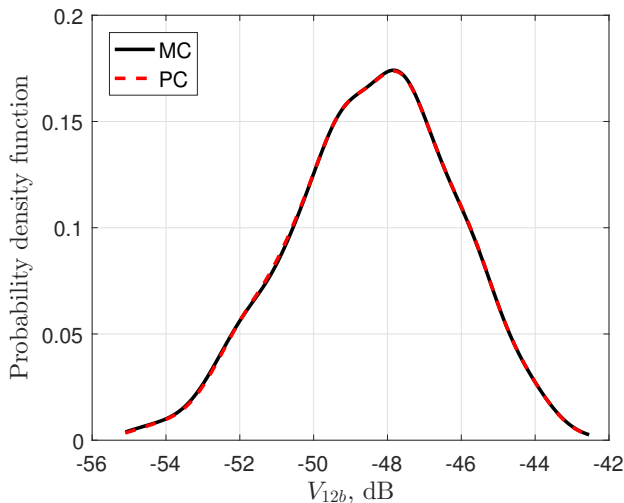
Fig. 3. Evolution of the crosstalk voltage V_{12b} in the frequency band [100 MHz - 10 GHz]. From a set of 3 realizations obtained by MC simulation, the crosstalk voltage V_{12b} is computed by the sparse PC metamodel \mathcal{M}^{PC} (circles) and by the numerical model \mathcal{M} (solid line).

MC simulation (black solid line) at the frequencies of 100 MHz and 9.1 GHz in Fig. 4(a) and Fig. 4(b), respectively.

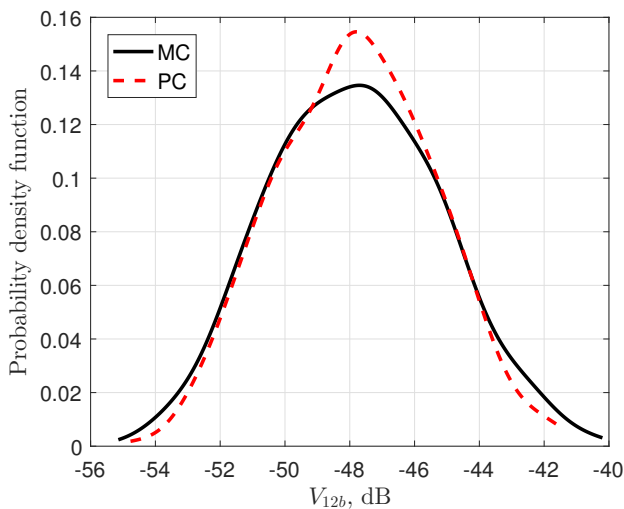
On the one hand, we observe in Fig. 4(a), a perfect agreement between the two curves confirming a high quality level of the sparse PC metamodel at 100 MHz. The estimation of the mean and the standard deviation of V_{12b} given by sparse PC and MC simulation are very close, *i.e.* $\mu^{PC} = -48.46$ dB, $\sigma^{PC} = 2.20$ dB and $\mu^{MC} = -48.47$ dB, $\sigma^{MC} = 2.21$ dB, respectively. The sparse PC requires an optimal degree equal to 4, with 78 polynomial basis out of 661 terms of the full basis, *i.e.* a sparsity index $S = \frac{78}{611} = 11.80\%$.

On the other hand, we see a slight difference between the two curves in Fig. 4(b), underlining a less good accuracy of the sparse PC metamodel at 9.1 GHz. In this case, the difference between the mean and the standard deviation of V_{12b} computed by sparse PC and MC simulation is larger, *i.e.* $\mu^{PC} = -47.85$ dB, $\sigma^{PC} = 2.48$ dB and $\mu^{MC} = -47.82$ dB, $\sigma^{MC} = 2.72$ dB, respectively. The best degree needed by the sparse PC is 6, using 60 terms of the polynomial basis out of 1783 of the complete basis, leading to a sparsity index $S = \frac{60}{1783} = 3.37\%$.

As expected, we notice at 9.1 GHz, that the sparse PC is less accurate, and requires a higher optimal degree and thus a larger number of terms of the full polynomial basis. It is relevant to point out that the spread of the crosstalk voltage V_{12b} is more important ($\sigma^{MC} = 2.72$ dB), underlining a larger variability of the response model. However, the sparsity index is lower, although the complexity of the problem increases, which highlights that the main contribution of the response variation is explained by a reduced number of terms of the polynomial basis. Regarding the computational cost associated to the evaluation of the crosstalk voltage V_{12b} in the frequency band [100 MHz - 10 GHz], 10000 MC realizations took 65 min, whereas the sparse PC required 4.08 s. The achieved speed up of the metamodel is about 956 times with respect to the MC technique.



(a)



(b)

Fig. 4. PDF of the crosstalk voltage V_{12b} obtained by sparse PC (red dashed-line) and by MC simulation (black solid line) at the frequencies of (a) 100 MHz and of (b) 9.1 GHz.

B. Sensitivity Analysis

As mentioned in Section II-E, the sparse PC metamodel allows, at a negligible computational cost, to obtain a sensitivity analysis of the response model. Thus, we represented in Fig. 5 the total Sobol indices of the crosstalk voltage V_{12b} in the frequency band [100 MHz - 10 GHz].

We observe in Fig. 5, that the variability of V_{12b} in the frequency band [100 MHz - 1 GHz] is mainly due to the substrate thickness h , the trace-to-trace separation d , and with less effect, to the trace width w and the components $RS1$, $RS1b$, $RS6b$ and $RL6b$. We notice also, between 700 MHz and 1 GHz, a slight effect of various components $RS3$, $RS5$, $RS3b$, $RS5b$, and $RL5b$, which appears at frequencies close to the first resonance peak of 1.5 GHz. In the frequency band [1 GHz - 10 GHz], the variability of the crosstalk voltage V_{12b} is explained by a larger number of input variables. Among them, the variable having the main contribution on the variations of the voltage V_{12b} , is the relative permittivity ϵ_r , whose greatest impact is around 5 GHz and 8 GHz. Several RLC components

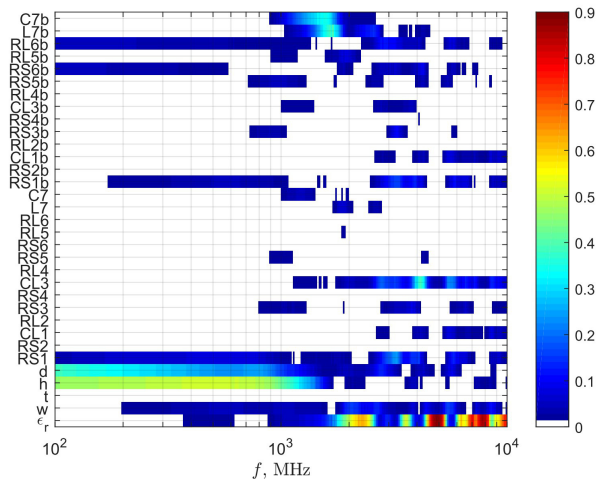


Fig. 5. Total Sobol indices of the crosstalk voltage V_{12b} in the frequency band [100 MHz - 10 GHz].

such as $RS1$, $CL3$, $RS1b$, $RS6b$, $RL6b$, $L7b$ and $C7b$, as well as the trace width w and the trace-to-trace separation d , play a significant role on the variability of V_{12b} . The rest of input variables have a little or no influence in this frequency band. It is also interesting to point out that the number of RLC components impacting the variability of the crosstalk voltage V_{12b} , is much more important in high frequency regime than in the frequency band [100 MHz - 1 GHz]. This is related to the resonance regime of the transmission line network illustrated in Fig 3, which is more sensitive to different RLC components.

C. Construction of Simplified Models from the Sensitivity Analysis Provided by Sparse PC

1) Analysis in the frequency band [100 MHz - 10 GHz]:

In this section, we exploit the sensitivity analysis of the crosstalk voltage V_{12b} , carried out in Section IV-B, in order to reduce the number of input random variables. From Fig. 5, we notice that 11 uncertain variables, *i.e.* the trace thickness t , and the components $RS2$, $RL2$, $RS4$, $RL4$, $RS6$, $RL6$, $RS2b$, $RL2b$, $RS4b$ and $RL4b$, have non significant impact on the variability of the crosstalk voltage V_{12b} . These lumped elements are end impedances of pieces of transmission lines that are coupled with the source through crosstalk effects. The fact that these impedance variations have a non significant influence on the response V_{12b} seems to indicate that the line coupling is weak, according to the well known Paul's hypothesis [22]. Therefore, we propose to neglect them by considering a simplified transmission line network, given in Fig. 6, and represented by a reduced model \mathcal{M}^r depending on $33 - 10 = 23$ uncertain variables. In order to check the validity of this reduced model \mathcal{M}^r , Fig. 7 represents, from 3 MC realizations $x^{(i)}$ and $\hat{x}^{(i)}$ of 33 and 23 uncertain variables, respectively, the crosstalk voltage V_{12b} obtained by the initial model \mathcal{M} (solid line) and the reduced model \mathcal{M}^r (dotted-line). We see that the two models are quite close between 100 MHz and almost 3 GHz, and then, from 3 GHz to 10 GHz, the magnitude and the occurrence of the resonance peaks of V_{12b} diverge. This highlights that the approximation,

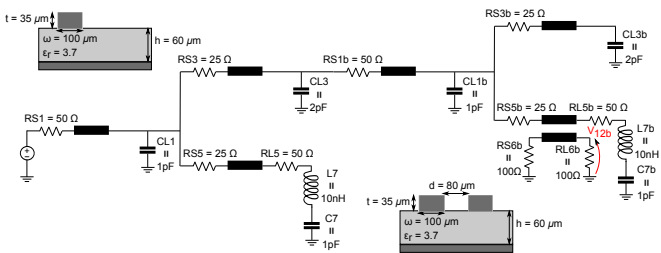


Fig. 6. Transmission line network with mixed single and coupled microstrip traces and corresponding line cross section.

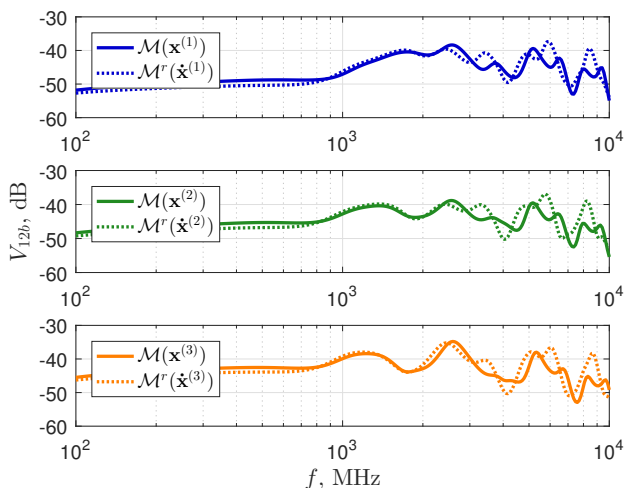


Fig. 7. Computation of the crosstalk voltage V_{12b} in the frequency band [100 MHz - 10 GHz]. The crosstalk voltage V_{12b} is evaluated by the numerical model \mathcal{M} (solid line) and the reduced model \mathcal{M}^r (dotted-line) from a set of 3 MC realizations $\mathbf{x}^{(i)}$ and $\tilde{\mathbf{x}}^{(i)}$ of the initial (33) and a reduced (23) number of uncertain variables, respectively.

consisting in neglecting the feedback of the coupled lines, may be acceptable at low frequencies only.

We propose then an alternative manner to obtain a reduced model of the initial model \mathcal{M} . As mentioned previously, 11 uncertain variables have a negligible effect on the variations of the crosstalk voltage V_{12b} . Going back to the initial transmission line network, we set them to their mean values given in Fig. 1. Then, we are interested in evaluating the numerical model \mathcal{M} on a reduced number of input random variables, *i.e.* $33 - 11 = 22$, whose realizations are denoted $\tilde{\mathbf{x}}^{(i)}$. We illustrate in Fig. 8, the crosstalk voltage V_{12b} evaluated by the numerical model \mathcal{M} from 3 MC realizations $\mathbf{x}^{(i)}$ and $\tilde{\mathbf{x}}^{(i)}$ of 33 and 22 uncertain variables, respectively. Fig. 8 shows, a very good agreement between the crosstalk voltage V_{12b} computed by $\mathcal{M}(\mathbf{x}^{(i)})$ and by $\mathcal{M}(\tilde{\mathbf{x}}^{(i)})$, represented by a solid line and squares, respectively. This allows to verify that the 11 input random variables, acting as parameters, have a negligible effect on the variability of the crosstalk voltage V_{12b} . Thus, it allows about a 30 % reduction in the number of uncertain input variables without altering the variability of the crosstalk voltage V_{12b} in the frequency band [100 MHz - 10 GHz].

2) *Study at 9.1 GHz:* Performing the same reasoning, we can also reduce the number of uncertain variables of the problem at the frequency of 9.1 GHz. Indeed, from the sensitivity analysis of Fig. 5, we see at 9.1 GHz, that only 9

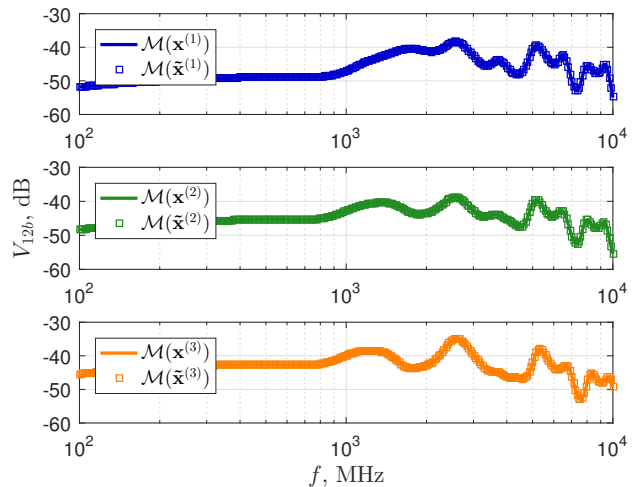


Fig. 8. Representation of the crosstalk voltage V_{12b} in the frequency band [100 MHz - 10 GHz]. The crosstalk voltage V_{12b} is computed by the numerical model \mathcal{M} from a set of 3 MC realizations $\mathbf{x}^{(i)}$ (solid line) and $\tilde{\mathbf{x}}^{(i)}$ (squares) of the total (33) and reduced (22) uncertain variables, respectively.

input random variables, *i.e.* the relative permittivity ϵ_r of the substrate, the trace width w and the components $RS1$, $CL1$, $RS3$, $CL3$, $RS1b$, $CL1b$ and $RL6b$, impact the variations of the crosstalk voltage V_{12b} . As done before, we set $33 - 9 = 24$ variables to their mean values given in Fig. 1. Fig. 9 represents then at 9.1 GHz, the PDF's of the crosstalk voltage V_{12b} computed by sparse PC (red dashed-line) in Section IV-A, and estimated by MC simulation from a set of 10000 realizations $\mathbf{x}^{(i)}$ (black) and $\tilde{\mathbf{x}}^{(i)}$ (pink dashed-line) of 33 and 9 uncertain variables, respectively. Keeping only a reduced number of uncertain variables, we notice that the PDF of the crosstalk voltage V_{12b} (pink dashed-line) is closer to the reference one (black) than that of the sparse PC (red dashed-line). This shows that, exploiting the sensitivity analysis given by the sparse PC, it is possible to simplify the initial model \mathcal{M} in reducing significantly the number of uncertain variables, while preserving the variations of the response V_{12b} .

V. CONCLUSION

In this paper, we have proposed a sparse PC metamodel, allowing to estimate the response model depending on many uncertain parameters. This metamodel, at a low computational cost compared to MC simulation, provides a very good estimation of the smooth part of the output model. However, when the behaviour of the output becomes more complex with strong irregularities, the sparse PC metamodel is less accurate to predict the model response.

Beside the fact that the sparse PC is well adapted to high dimensional problems, one of its advantages is, that it allows, at a negligible computational cost, to derive statistical moments and a sensitivity analysis of the output. These information are very useful for the circuit designer, since they enable him to quantify and to hierarchize the effects of uncertain parameters on the response variability of the system. We showed, in particular, that the sensitivity analysis may be used to derive simplified and still accurate new models of the initial problem.

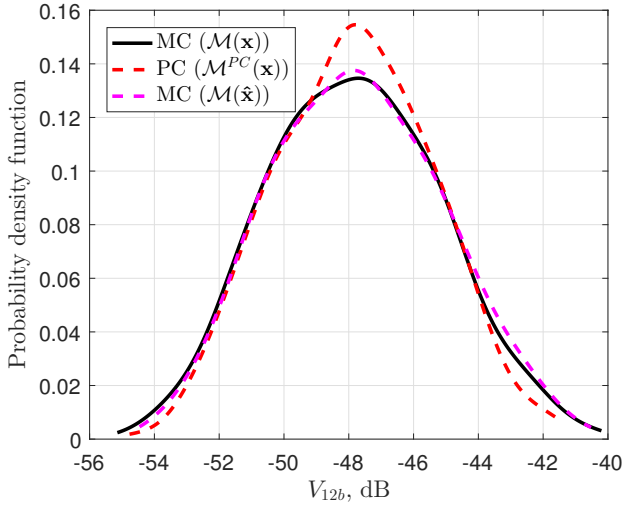


Fig. 9. PDF of the crosstalk voltage V_{12b} , at 9.1 GHz, given by sparse PC metamodel (red-dashed line), and by MC simulation considering the total number (33, black line) and a reduced number (9, pink dashed-line) of uncertain variables.

Dealing with a crosstalk problem consisting of about thirty uncertain input parameters, allowed us to obtain a quite efficient sparse PC metamodel. The robustness of this metamodel for even larger dimension problems will be the object of future investigations.

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