Polynomial Chaos-Based Macromodeling of Multiport Systems using an Input-Output Approach

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SUMMARY

An innovative technique to build stochastic frequency-domain macromodels of generic linear multiport systems is presented. The proposed method calculates a macromodel of the system transfer function including its statistical properties, making it tailored for variability analysis. The combination of the modeling power of the Vector Fitting algorithm with the Polynomial Chaos expansion applied at an input-output level allows to accurately and efficiently describe the system variability features. Thanks to its versatility and automated order selection, the proposed technique is suitable to be applied to a large range of complex modern electrical systems (e.g. filters, interconnections) and can tackle the case of correlated random variables. The performance in terms of accuracy and computational efficiency of the proposed method are compared with respect to the standard Monte Carlo analysis for two pertinent numerical examples. Copyright © 2014 John Wiley & Sons, Ltd.

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1. INTRODUCTION

Nowadays, the analysis of the effects of geometrical or electrical parameters variability on the performance of integrated circuits is fundamental. Indeed, many techniques [1]-[6], based on the Polynomial Chaos (PC) expansion [7]-[11], were developed over the last years to study the stochastic variations of electrical circuits as alternative to the computationally cumbersome Monte Carlo (MC) based techniques. The MC analysis is considered the standard approach for variability analysis, thanks to its robustness and ease of implementation. The drawback of MC is its slow convergence rate, that forces the designers to perform a large number of simulations to obtain reliable results. Considering that both the operative bandwidth and complexity of modern electrical systems are constantly increasing, the high computational time required by the MC analysis is a clear limitation. The PC-based techniques proposed so far allow to overcome the computational cumbersomeness of the MC-based approaches, but they were designed for specific systems: multiconductor transmission lines [1]-[4] or lumped elements circuits [5], [6].

Recently, a PC-based technique was presented in [12] to perform variability analysis on a generic linear multiport system. This technique first builds a set of deterministic univariate frequency-domain models of the system transfer function, that can be expressed in different forms (e.g. scattering, impedance or admittance parameters), and then uses the PC expansion to perform the variability analysis. In particular, the PC expansion of the system transfer function is obtained by combining a deterministic set of system equations expressed in state-space form with the PC model of the system's state-space matrices, through the use of Galerkin projections [1]-[6]. This approach, while applicable to a large range of microwave systems, has a main drawback: the PC model of the system transfer function must be calculated for each frequency of interest solving

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a linear system. Note that, the set of frequency values of interest can be freely chosen over the frequency range of the initial set of deterministic univariate frequency-domain models of the system transfer function. Finally, despite its accuracy and efficiency, the technique [12] does not offer the possibility to enforce the stability of the calculated PC-based model.

The novel approach presented in this paper calculates a PC-based frequency-domain macromodel of a generic linear multiport system, described by its scattering parameters, which is suitable for variability analysis. Furthermore, the macromodel is obtained through the application of the PC expansion at an input-output level without intermediate state-space models as in [12], adopting an efficient model-building procedure that

- proposes an algorithm that adaptively chooses the number of basis functions of the PC model;
- it is straightforward to implement.

Finally, we propose a method to enforce the stability and check the passivity of the calculated PC-based macromodel.

The starting point of the proposed technique is the evaluation of the system scattering parameters on a discrete set of values of the frequency and the parameters involved in the variability analysis. Next, the PC model of the system transfer function for the chosen frequencies is calculated through an iterative procedure. Finally, a frequency-domain stochastic macromodel is built as weighted summation of frequency-dependent rational functions of the PC matrix coefficients by means of the Vector Fitting (VF) algorithm [13], [14].

This paper is structured as follows. First, an overview of PC properties is given in Section 2. The new frequency-domain macromodeling technique is described in Section 3, while its validation is described in Section 4 by means of two numerical examples. The conclusions are summed up in Section 5.

2. POLYNOMIAL CHAOS PROPERTIES

The PC expansion allows to express a stochastic process X with finite variance [7] as

$$X = \sum_{i=0}^{\infty} \alpha_i \varphi_i(\vec{\xi}) \quad (1)$$

where the terms α_i are scalar coefficients, $\vec{\xi}$ is a vector of normalized random variables and the basis functions $\varphi_i(\vec{\xi})$ are orthogonal polynomials with respect to the probability measure $W(\vec{\xi})$ with support Ω as [9]

$$\langle \varphi_i(\vec{\xi}), \varphi_j(\vec{\xi}) \rangle = \int_{\Omega} \varphi_i(\vec{\xi}) \varphi_j(\vec{\xi}) W(\vec{\xi}) d\vec{\xi} = a_i \delta_{ij} \quad (2)$$

where δ_{ij} is the Kronecker delta and a_i are positive numbers. Therefore, (1) expresses a stochastic process X as a series of orthogonal polynomials with suitable coefficients.

Of particular interest is the case of a stochastic process X composed of independent random variables. Indeed, the basis functions $\varphi_i(\vec{\xi})$ can be computed as products combinations of the orthogonal polynomials corresponding to each individual random variable ξ_i [11]. Furthermore, in this case it is possible to truncate (1) up to basis functions of a maximum degree P , called order of the expansion, and a maximum number of basis function $M + 1$ as

$$\varphi_i(\vec{\xi}) = \prod_{k=1}^N \phi_{j_k}(\xi_k) \quad \text{with} \quad \sum_{k=1}^N j_k \leq P \quad \text{and} \quad 0 \leq i \leq M \quad (3)$$

where $\phi_{j_k}(\xi_k)$ represent the polynomial function of degree j corresponding to the random variable ξ_k . It can be easily proven that, if the definition (3) is used, the total number of basis functions $M + 1$ used in the PC expansion is [8]

$$M + 1 = \frac{(N + P)!}{N!P!} \quad (4)$$

If the independent random variables $\vec{\xi}$ have arbitrary probability density functions (PDFs), the corresponding basis functions can be calculated numerically following the approach described in [9]. That approach allows to calculate the basis function $\varphi_i(\vec{\xi})$ under the condition that their weighting function $W(\vec{\xi})$ corresponds to the PDF of the associated random variable in standard form. Hence, an exponential convergence rate of the PC expansion can be achieved [9], and the basis

functions used are optimal. Furthermore, for random variables with specific PDFs (i.e. Gaussian, Uniform, Beta distribution) the optimal basis functions are the polynomials of the Wiener-Askey scheme [10]. In the sequel, these particular PDFs are referred as standard distributions.

The basis function in (1) can be calculated also in the more general case of correlated random variables with arbitrary PDFs, following the approaches described in [7]-[9], [11]. In this case, a variable transformation, such as the Nataf transformation [15] or the Karhunen-Loève expansion [16], can be used to achieve decorrelation, even if the PC expansion convergence rate may not be exponential.

Finally, upon determination of the $M + 1$ basis functions $\varphi_i(\vec{\xi})$, (1) is truncated as

$$X \approx \sum_{i=0}^M \alpha_i \varphi_i(\vec{\xi}) \quad (5)$$

where the only unknowns are the PC coefficients α_i that can be calculated following different approaches [8].

The most attractive feature of the PC expansion is the analytical representation of the system variability. Indeed, the mean μ and the variance σ^2 of the stochastic process X can be expressed as [8]

$$\mu = \alpha_0 \quad (6)$$

$$\sigma^2 = \sum_{i=1}^M \alpha_i^2 < \varphi_i(\vec{\xi}), \varphi_i(\vec{\xi}) > \quad (7)$$

Furthermore, apart from the others moments, more complex stochastic functions of X , such as the PDF, can be efficiently calculated following standard analytical formulas or numerical schemes [17].

Finally, the extension of the PC expansion to a stochastic process written in a matrix form $\mathbf{X}$ is straightforward. In this case, (5) becomes

$$\mathbf{X} \approx \sum_{i=0}^M \boldsymbol{\alpha}_i \varphi_i(\vec{\xi}) \quad (8)$$

where $\boldsymbol{\alpha}_i$ is the matrix of PC coefficients, corresponding to the i -th polynomial basis, calculated for each entry of $\mathbf{X}$. For an extensive reference to polynomial chaos theory, the reader may consult [7] – [11].

3. MACROMODELING STRATEGY

3.1. PC modeling of system transfer function

The scattering parameters are widely used to describe the broadband frequency behavior of microwave systems. Indeed, the use of the appropriate reference impedances to all system ports overcomes the difficulties in the measurement of impedance, admittance and hybrid parameters caused by short-circuit, open-circuit, and test-circuit parasitics at microwave frequencies [18].

Also, the scattering parameters have in general a smoother and more bounded behavior with respect to the impedance, admittance and hybrid parameters. This makes the scattering parameters particularly suitable to be efficiently modeled with a PC-based approach.

Therefore, the proposed technique aims at building a PC model for the scattering parameters of a generic multiport system of the form

$$\mathbf{S}(s, \vec{\xi}) \approx \sum_{i=0}^M \alpha_i(s) \varphi_i(\vec{\xi}) \quad (9)$$

where the matrix $\mathbf{S}$ represents the system scattering parameters and $\alpha_i(s)$ is a univariate frequency-domain rational model of the i -th PC coefficient matrix and s is the Laplace variable. As will be demonstrated in the sequel, this goal can be achieved by

- determining the basis function $\varphi_i(\vec{\xi})$;
- deciding on the number of basis functions M (4);
- calculating and solving an equivalent linear system for the coefficients of the PC expansion of $\mathbf{S}$;
- calculating a rational model for each PC coefficient matrix obtained.

Without loss of generality, in the sequel we will limit our attention to stochastic processes composed by independent random variables with the corresponding PDFs included in the standard distributions. Hence, the optimal basis functions are the polynomials of the Wiener-Askey scheme. Note, however, that in the most general case of correlated random variables with arbitrary

distributions, the corresponding basis functions can also be calculated using the techniques described in [7]-[9], [11].

The starting point of this work is the calculation of the scattering parameters $\mathbf{S}$ for a discrete set of values of the frequency $[f_l]_{l=1}^L$ corresponding to the Laplace variable $[s_l = j2\pi f_l]_{l=1}^L$ and the normalized random variables $[\vec{\xi}_j]_{j=1}^K$. Equation (9) can therefore be written as

$$\mathbf{S}(s_l, \vec{\xi}) \approx \sum_{i=0}^M \alpha_i(s_l) \varphi_i(\vec{\xi}) \quad (10)$$

where only the coefficients $\alpha_i(s_l)$ and the number of basis functions M must be estimated. Next, the linear regression technique [8] is used to obtain the desired PC coefficients. This approach allows to calculate the PC coefficients in (10) solving, for each value of the Laplace variable $[s_l]_{l=1}^L$, a least-square system [8] in the form

$$\Phi \alpha = \mathbf{R} \quad (11)$$

with

$$\begin{aligned} \Phi &= \begin{bmatrix} \varphi_0(\vec{\xi}_1) & \cdots & \varphi_M(\vec{\xi}_1) \\ \vdots & & \vdots \\ \varphi_0(\vec{\xi}_K) & \cdots & \varphi_M(\vec{\xi}_K) \end{bmatrix} \\ \alpha &= \begin{bmatrix} \alpha_0(s_l) \\ \vdots \\ \alpha_M(s_l) \end{bmatrix} \\ \mathbf{R} &= \begin{bmatrix} \mathbf{S}(s_l, \vec{\xi}_1) \\ \vdots \\ \mathbf{S}(s_l, \vec{\xi}_K) \end{bmatrix} \end{aligned} \quad (12)$$

and where α contains the matrices of the unknown PC coefficients $[\alpha_i(s_l)]_{i=0}^M$, the j -th row of the matrix Φ is formed by the elements of the multivariate polynomial basis $[\varphi_i]_{i=0}^M$ evaluated in $[\vec{\xi}_j]_{j=1}^K$ multiplied by the identity matrix of the same dimension of the scattering parameters, and the matrix $\mathbf{R}$ collects the corresponding set of scattering parameters values $\mathbf{S}(s_l, \vec{\xi}_j)$ for $[\vec{\xi}_j]_{j=1}^K$.

Note that the system (11) must be over-determined to be solved in a least-square sense. Therefore, the number of basis functions M must be chosen to evaluate the number of initial samples K needed to solve (11). Since the order of expansion P is limited for practical applications [10], several techniques [1]–[6], [12] choose upfront the number of basis function M , according to (4).

We propose a fully automatic procedure, explained in Algorithm 1, to determine the minimum order of expansion P that guarantees accurate results and, therefore, the estimated number of basis functions M (4).

Let us assume that the basis functions up to polynomials of order P' are calculated before starting Algorithm 1. P' is chosen, see (4), aimed at keeping the corresponding number of basis functions $M' + 1$ limited. At this point the number of initial samples $K > M' + 1$ can be chosen. In [19] it is recommended to use a number of samples equal to the double of the basis function used, i.e., $K \approx 2(M' + 1)$.

We will now describe in detail the iterative procedure summarized in Algorithm 1. Initially, the basis functions for polynomials of order one and two, indicated in Algorithm 1 with the symbols Φ^1 and Φ^2 , respectively, are selected. Next, the corresponding linear system (11) is solved for both PC expansion models. Following equations (6) and (7), it is now obvious to estimate the mean and the variance for the two PC models. Now, if the difference between the mean and variance of the two PC models exceeds a suitable threshold, then the PC model with polynomials up to order one is discarded and the basis functions corresponding to polynomials of order three are chosen. The procedure is repeated iteratively until the error between the mean and variance predicted by two consecutive PC models is lower than the chosen threshold. If the previous condition cannot be achieved upon calculation of the basis functions up to polynomials of order P' , the PC model of order P' is chosen. It is important to notice that, in Algorithm 1 the computation of the PC coefficients corresponding to basis functions of polynomials of increasing order is not nested: a linear system in the form (11) must be solved for each PC model computed up to a specific order of expansion.

Input: Basis function up to order P' : $[\Phi^1, \dots, \Phi^{P'}]$, $\mathbf{S}(s_l, \vec{\xi}_j)$

Output: PC model of order P : $Basis_{chosen}$, α_{chosen}

$Basis_1 = \Phi^1$;

$Basis_2 = \Phi^2$;

$\alpha_1 = \text{Solve (11) for } Basis_1$;

$\mu_1 = \text{Solve (6) for } Basis_1 \text{ and } \alpha_1$;

$\sigma_1 = \text{Solve (7) for } Basis_1 \text{ and } \alpha_1$;

$\alpha_2 = \text{Solve (11) for } Basis_2$;

$\mu_2 = \text{Solve (6) for } Basis_2 \text{ and } \alpha_2$;

$\sigma_2 = \text{Solve (7) for } Basis_2 \text{ and } \alpha_2$;

$Error(\mu) = \frac{\mu_2 - \mu_1}{\mu_2}$

$Error(\sigma) = \frac{\sigma_2 - \sigma_1}{\sigma_2}$

$i = 2$;

$Error = error_{chosen}$;

while $Error(\mu) > Error$ || $Error(\sigma) > Error$ **do**

if $i < P'$ **then**

$Basis_1 = Basis_2$;

$\alpha_1 = \alpha_2$;

$\mu_1 = \mu_2$;

$\sigma_1 = \sigma_2$;

$Basis_2 = \Phi^{i+1}$;

$\alpha_2 = \text{Solve (11) for } Basis_2$;

$\mu_2 = \text{Solve (6) for } Basis_2 \text{ and } \alpha_2$;

$\sigma_2 = \text{Solve (7) for } Basis_2 \text{ and } \alpha_2$;

$Error(\mu) = \frac{\mu_2 - \mu_1}{\mu_2}$

$Error(\sigma) = \frac{\sigma_2 - \sigma_1}{\sigma_2}$;

$i = i + 1$;

else

end while

end

end

if $Error(\mu) \leq Error$ && $Error(\sigma) \leq Error$ **then**

$Basis_{chosen} = Basis_1$;

$\alpha_{chosen} = \alpha_1$;

else

$Basis_{chosen} = Basis_2$;

$\alpha_{chosen} = \alpha_2$;

end

Algorithm 1: Iterative procedure to build the PC model.

Figure 1. Description of the proposed modeling strategy.

At this point, following the procedure described in Algorithm 1, we have calculated (10) for each sample $[s_l]_{l=1}^L$, using an iterative estimation of the expansion order and the linear regression method to calculate the PC coefficients. Next, to obtain the desired PC model in the form (9), the VF algorithm is applied to calculate a rational model for each PC coefficient matrix $[\alpha_i(s_l)]_{i=0}^M$ with $[s_l]_{l=1}^L$. The proposed modeling strategy is summarized in Fig. 1.

The technique described in this paper is easy to implement, it can be applied to any generic linear multiport system described by its scattering parameters, and it allows to perform the variability analysis with accuracy and efficiency in the frequency-domain. It produces a macromodel of a generic multiport system in the form of a PC model, where each PC coefficient matrix is expressed with a rational model in the frequency-domain. The proposed technique only requires an initial set of samples of the system transfer function for $[s_l]_{l=1}^L$ and $[\vec{\xi}_j]_{j=1}^K$, and therefore it can be applied to a large range of microwave systems. With respect to the technique presented in [12], the novel proposed method presents several advantages:

- it proposes an algorithm for the automatic choice of the minimum order of expansion;
- it offers a simple model generation procedure (see Algorithm 1).

- it does not require to calculate a deterministic model, e.g. state-space models as in [12], prior to the application of the PC expansion;
- it calculates a PC-based macromodel in the form of weighted summation of rational functions, therefore it is not required to solve a linear system to evaluate the obtained PC-based macromodel over a discrete set of frequencies as in [12];

It is worthwhile to notice that the proposed technique can calculate a stable frequency-domain macromodel. Indeed, the macromodel in the form (9) is expressed as a weighted sum of frequency-dependent rational functions. Since a weighted sum of stable frequency-dependent rational functions is also stable [20], the stability of the proposed macromodel can be ensured by calculating a stable rational model for each PC coefficient matrix $[\alpha_i(s_l)]_{i=0}^M$, using the VF algorithm. Furthermore, the passivity of the proposed macromodel can be checked by means of standard techniques (see Appendix 6.2 for further details).

Note that, the loads can be included in the variability analysis by means of the Galerkin projections [1]-[6], as shown in [12].

4. NUMERICAL EXAMPLES

In this Section, the proposed technique is applied to different structures. In each example, a comparison with the MC analysis is shown in order to validate the efficiency and accuracy of our novel technique. In particular, the results of the variability analysis obtained with the novel proposed method are compared with the corresponding results obtained with a MC analysis that requires a comparable computational cost as the proposed technique and with a MC analysis performed using a large set of samples.

To calculate the PC model by means of the method described in Algorithm 1, the maximum relative error between the mean and the variance of two consecutive PC models with increasing order is set to 0.01. Furthermore, the rational model of each PC coefficient matrix $[\alpha_i(s_l)]_{i=0}^M$ for

$[s_l]_{l=1}^L$, is calculated with the VF algorithm with the following relative error measure

$$Err = \max_{r,c,l} \left(\frac{|\alpha_i^{rc}(s_l) - \tilde{\alpha}_i^{rc}(s_l)|}{\frac{1}{A^2 L} \sum_{r=1}^A \sum_{c=1}^A \sum_{l=1}^L |\alpha_i^{rc}(s_l)|} \right) \quad (13)$$

for $r, c = 1, \dots, A$; $l = 1, \dots, L$;

where the symbol $\alpha_i^{rc}(s_l)$ is the element (r, c) of the matrix $\alpha_i(s_l)$ of size $A \times A$, where A is the number of ports, and $\tilde{\alpha}_i^{rc}(s_l)$ is the corresponding value of the rational model. The simulations are performed with MATLAB[†] 2010a on a computer with an *Intel(R) Core(TM) i3* processor and 4 GB RAM.

4.1. Hairpin Filter, 3 Independent Random Variables

In the first example, a bandpass hairpin filter of length $L = 12$ mm has been modeled within the frequency range $[1.5 - 3.5]$ GHz. Its layout is shown in Fig. 2. The filter conductors have width $W_1 = 0.33$ mm, while $W_2 = 0.66$ mm is the width of the conductors at the input and output port. The spacing between the port and the filter conductors is $D_1 = D_2 = 0.3$ mm and the spacing between the filter conductors is $D_3 = 1$ mm. The distance C is equal to 2.5 mm. The substrate of thickness 0.635 mm has a relative dielectric constant $\epsilon_r = 9.9$.

Figure 2. Example A. Geometry of the bandpass hairpin filter.

Three parameters are considered as independent random variables with uniform PDFs: the spacing D_1 , D_2 , and D_3 , varying by $\pm 10\%$ with respect to their previously indicated nominal value.

[†]The Mathworks Inc., Natick, MA, USA.

The selected random variables are normalized as

$$D_1 = \mu_{D_1}(1 + \sigma_{D_1}\xi_1) \quad (14)$$

$$D_2 = \mu_{D_2}(1 + \sigma_{D_2}\xi_2) \quad (15)$$

$$D_3 = \mu_{D_3}(1 + \sigma_{D_3}\xi_3) \quad (16)$$

where ξ_1, ξ_2, ξ_3 are random variables with uniform PDFs over the interval $[-1, 1]$. The corresponding probability measure (2) is

$$W(\xi) = \begin{cases} 2^{-N}, & |\xi_i| \leq 1, \quad i = 1, \dots, N \\ 0, & elsewhere \end{cases} \quad (17)$$

and the optimal basis functions are products of the Legendre polynomials [11], shown in Table I[‡] for $M = 9$ and $P = 2$.

Table I. Legendre polynomials products for three independent random variables, with $M = 9$ and $P = 2$

index i	i -th basis function φ_i	$\langle \varphi_i, \varphi_i \rangle$
0	1	1
1	ξ_1	$\frac{1}{3}$
2	ξ_2	$\frac{1}{3}$
3	ξ_3	$\frac{1}{3}$
4	$\xi_1\xi_2$	$\frac{1}{9}$
5	$\xi_1\xi_3$	$\frac{1}{9}$
6	$\xi_2\xi_3$	$\frac{1}{9}$
7	$\frac{1}{2}(3\xi_1^2 - 1)$	$\frac{1}{5}$
8	$\frac{1}{2}(3\xi_2^2 - 1)$	$\frac{1}{5}$
9	$\frac{1}{2}(3\xi_3^2 - 1)$	$\frac{1}{5}$

The filter scattering parameters are evaluated using ADS Momentum[§] over a regular grid composed of 51 samples for the frequency and $4 \times 4 \times 4$ (D_1, D_2, D_3) samples for the geometrical

[‡]Based on the fact that $\int_{-1}^1 P_n(x)^2 dx = 2/(2n+1)$ where $P_n(x)$ are the Legendre polynomials.

[§]Momentum EEsof EDA, Agilent Technologies, Santa Rosa, CA.

Figure 3. Example A. Variability of the magnitude of S_{11} . The green thick line corresponds to the central value for (D_1, D_2, D_3) , while the blue lines are the results of the MC simulations performed using 10000 (D_1, D_2, D_3) samples.

parameters. The number K of initial samples for the geometrical parameters is chosen according to the relation $K \approx 2(M' + 1)$, considering a maximum number of basis function $M' = 34$ and a corresponding order $P' = 4$, according to (4). The frequency samples are divided in two groups: modeling points (26 samples) and validation points (25 samples). Figure 3 shows an example of the variability of the scattering parameters with respect to the chosen random variables.

To build the rational model of the PC coefficients, the VF algorithm is used targeting 0.01 as maximum error (13). The PC-based model calculated with the proposed technique has $P = 3$, according to Algorithm 1, and $M = 19$, according to (4), and it shows an excellent accuracy and superior efficiency compared with the standard MC analysis in computing system variability features. Indeed, an example of the comparison results for the proposed technique and the MC analysis can be seen in Figs. 4 - 6, while in Table II the computational time required by the two approaches is reported. In particular, Figs. 4 - 5 show the mean and the standard deviation of the real part of S_{11} for the validation frequencies obtained with the proposed technique, a MC analysis with a comparable computational cost (performed using 64 (D_1, D_2, D_3) samples) and a

MC analysis performed using 10000 (D_1, D_2, D_3) samples. It is important to notice that around the filter resonance frequency the accuracy of the MC method performed using 64 samples for the geometrical parameters is drastically reduced. Furthermore, the computation of higher order moments like the PDF and the CDF can not be performed accurately using such a reduced set of samples. Indeed, Fig. 6 describes the PDF and the CDF of S_{11} for the central frequency of the filter obtained with the proposed method and the MC analysis performed using a large set of samples. Finally, it is worth specifying that in Table II the total computational time of the proposed PC-based technique is split into two contributions: the time needed to calculate the initial samples over the modeling frequencies and to build the PC-based macromodel of the scattering parameters and evaluate it on the validation frequencies. Note that, the computational cost to build the PC-based macromodel shown in Table II includes the cost to compute the PC-model of the scattering parameters in the form (10) for all the orders $P \leq 4$ as described by Algorithm 1. Similar results can be obtained for the other entries of the scattering matrix.

Table II. Example A. Efficiency of the Proposed PC-based Technique

Technique	Computational time
Monte Carlo Analysis (10000 samples, validation frequencies)	165 h, 3 min, 28.94 s
Monte Carlo Analysis (64 samples, validation frequencies)	63 min, 22.94 s
PC-based technique	67 min, 21.01 s
Details PC-based technique	Computational time
Initial simulations EM (64 samples, modeling frequencies)	67 min, 14.16 s
PC model scattering parameters	6.85 s

Finally, the proposed technique is compared with respect to the PC-based method presented in [12]. The variability analysis performed with the technique [12] uses the same sampling for the geometrical parameters and frequency and adopts the same order of the expansion as for the proposed technique, leading to a PC model of order $P = 3$ and $M = 19$ basis functions.

Figure 4. Example A. The top plot shows a comparison between the mean of the real part of S_{11} obtained with the MC analysis performed using first 10000 (D_1, D_2, D_3) samples (full black line), then 64 (D_1, D_2, D_3) samples (dashed green line), and the proposed PC-based method (red circles: $\circ$) for the validation frequencies. The lower plot shows the corresponding absolute error.

Figure 5. Example A. The top plot shows a comparison between the standard deviation of the real part of S_{11} obtained with the MC analysis performed using first 10000 (D_1, D_2, D_3) samples (full black line), then 64 (D_1, D_2, D_3) samples (dashed green line), and the proposed PC-based method (red circles: $\circ$) for the validation frequencies. The lower plot shows the corresponding absolute error.

Figure 6. Example A. PDF and CDF of the magnitude of S_{11} at 2.5 GHz. Full black line: PDF computed using the novel technique; Dashed black line: CDF computed using the novel technique; Circles ($\circ$): PDF computed using the MC technique; Squares ($\square$): CDF computed using the MC technique.

First, state-space matrices (root macromodels) with common order are computed for all the $4 \times 4 \times 4$ (D_1, D_2, D_3) samples for the geometrical parameters over the modeling frequencies using the VF algorithm. In order to estimate the required number of poles, -50 dB is chosen as maximum absolute model error between the scattering parameters and the corresponding root macromodels. As a result, 8 poles are used to compute the root macromodels for all the $4 \times 4 \times 4$ (D_1, D_2, D_3) samples. Next, the PC coefficients of the root macromodels are estimated using the linear regression technique. Hence, the PC model of the state-vector is computed by solving a suitable linear system (see [12], equation (17)). Finally, the PC model of the filter scattering parameters over the validation frequencies can be directly computed starting from the PC model of the state-vector.

The proposed approach and the technique [12] have a similar accuracy and computational cost in computing the filter variability features, as shown in Fig. 7 and Table III, respectively.

The calculation of the initial samples via EM simulations is the principal component of the computational time for the proposed approach and the technique [12], as shown in Tables II and III. However, the proposed approach requires the half of the time to compute the PC model of the

Figure 7. Example A. The top plot shows a comparison between the standard deviation of the imaginary part of S_{12} obtained with the MC analysis performed using 10000 (D_1, D_2, D_3) samples (full black line), the technique [12] (dashed magenta line), and the proposed PC-based method (red circles: $\circ$) for the validation frequencies. The lower plot shows the corresponding absolute error.

Table III. Example A. Efficiency of the PC-based Technique [12]

PC-based technique [12]	Computational time
Initial simulations EM (64 samples, modeling frequencies)	67 min, 14.16 s
PC model scattering parameters	13.27 s
Total computational time	67 min, 27.43 s

filter scattering parameters for the evaluation frequencies, see the element “PC model scattering parameters” in Tables II and III, despite the proposed approach uses an adaptive model order selection and it computes the PC-models of the scattering parameters in the form (10) for all the orders $P \leq 4$ as described by Algorithm 1. This superior efficiency is obtained thanks to the simpler model building procedure of the proposed approach.

The technique [12] requires the computation of a set of root macromodels in a state-space form with common order for each (D_1, D_2, D_3) sample prior to the application of the PC expansion.

Then, the desired PC model of the scattering parameters over the evaluation frequencies is obtained by solving an augmented system of dimension 320×320 (see [12], equation (17)) for each validation frequency sample. Building such a system required the computation of 8000 triple integrals depending on the normalized variables (ξ_1, ξ_2, ξ_3) obtained via Galerkin projections [1]-[6]. Note that these projections are frequency-independent, can be calculated upfront and can be used for each problem involving three uniform random variables since they depend on normalized random variables (ξ_1, ξ_2, ξ_3) . Hence, the corresponding computational time is not included in Table III.

4.2. Distributed Microstrip Bandstop Filter, 2 Correlated Random Variables

In the second example, a distributed microstrip bandstop filter has been modeled within the frequency range [100 Hz – 2.5 GHz]. Its layout is shown in Fig. 8.

The filter is realized using four open stubs connected by three microstrips. The length of all the lines is $L = 4$ cm and is related to the central wavelength of the filter λ_0 as

$$L = \frac{\lambda_0}{4}$$

The substrate is *FR4* of thickness $h = 130 \mu\text{m}$ with a relative dielectric constant ϵ_r and a loss tangent $\tan\delta$ characterized by a dispersive and causal model [21]. All the microstrips have copper conductors (conductivity $\sigma = 5.8 \cdot 10^7$ S/m) of thickness $t = 10 \mu\text{m}$, but with different widths. In

Figure 8. Example B. Geometry of the distributed microstrip bandstop filter.

particular the lines M_2 , M_4 and M_6 have a conductor of width $w = 120 \mu\text{m}$; for the lines M_1 and M_7 the conductor width is $w = 20 \mu\text{m}$, while $w = 160 \mu\text{m}$ for the lines M_3 and M_5 .

The scattering parameters are considered as a stochastic process that depends on two correlated random variables with Gaussian PDFs: the length L of the microstrip M_2 and the width w of the shunt M_1 . Assuming a worst case analysis, the correlation coefficient is chosen equal to $\rho = 0.9$ and, for both the random variables (L, w) , the normalized standard deviation is $\pm 5\%$ with respect to their nominal value, indicated in the following with the symbols L_0 for the length and w_0 for the width. The corresponding correlation matrix is

$$\mathbf{C} = \begin{bmatrix} (L_0\sigma_L)^2 & \rho L_0\sigma_L w_0\sigma_w \\ \rho L_0\sigma_L w_0\sigma_w & (w_0\sigma_w)^2 \end{bmatrix}$$

where σ_L and σ_w represent the normalized standard deviations of the length and the width, respectively. In this case $\mathbf{C}$ is positive-definite, hence the couple of random variables (L, w) follow the non-degenerate multivariate normal distribution [22]

$$W_{\vec{\eta}} = \frac{1}{2\pi \det(\mathbf{C})^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\vec{\eta} - \vec{\mu})^T \mathbf{C}^{-1}(\vec{\eta} - \vec{\mu})\right) \quad (18)$$

where the symbol $\det(\cdot)$ is used to represent the matrix determinant, while $\vec{\eta} = [L, w]^T$ and $\vec{\mu} = [L_0, w_0]^T$.

Applying the Karhunen-Loève expansion [16], the scattering parameters can be considered as a stochastic process with respect to the pair of uncorrelated Gaussian random variables with zero mean and unit variance (ξ_1, ξ_2) . In particular, the vector of correlated random variables $\vec{\eta}$ can be expressed with respect to the vector of uncorrelated random variables $\vec{\xi}$ as

$$\vec{\eta} = \vec{\mu} + \mathbf{U}\mathbf{\Lambda}^{\frac{1}{2}}\vec{\xi} \quad (19)$$

where $\mathbf{\Lambda}$ is a diagonal matrix containing the eigenvalues of the correlation matrix $\mathbf{C}$ and $\mathbf{U}$ is the matrix of the corresponding eigenvectors. See Appendix 6.1 for further details. Therefore, due to the use of the Karhunen-Loève expansion, it is possible to express the scattering parameters as a stochastic process that depends on the pair of uncorrelated random variables $\vec{\xi} = [\xi_1, \xi_2]^T$ and,

since the variables ξ_1 and ξ_2 are Gaussian, they are also independent. Hence, the corresponding basis functions are products of the Hermite polynomials [11], as shown in Table IV for $M = 5$ and $P = 2$, while the probability measure (2) is

$$W(\vec{\xi}) = \frac{1}{2\pi} \exp\left(-\frac{1}{2}\vec{\xi}^T \vec{\xi}\right) \quad (20)$$

The evaluation of the scattering parameters is performed using a quasi-analytical model [23] over a regular grid composed of 81 samples for the frequency and 8×8 samples for the geometrical parameters (L, w) . Again, the number K of initial samples for the couple of geometrical parameters is chosen according to the relation $K \approx 2(M' + 1)$, considering a maximum order of expansion $P' = 6$ and a corresponding number of basis functions $M' = 27$, according to (4). Next, the frequency samples are divided in two groups: modeling points (41 samples) and validation points (40 samples).

This second example represents a particular difficult structure to model since, as shown in Fig. 9, the random variables chosen have a high impact on the scattering parameters of the structure: the range of the stop-band frequencies is influenced by the random variables chosen and in the band-pass frequencies the magnitude of the element S_{11} has a high variability, often over -20 dB, compromising the correct behavior of the filter.

Table IV. Hermite polynomials products for two independent random variables, with $M = 5$ and $P = 2$ [2]

index i	i -th basis function φ_i	$\langle \varphi_i, \varphi_i \rangle$
0	1	1
1	ξ_1	1
2	ξ_2	1
3	$\xi_1^2 - 1$	2
4	$\xi_1 \xi_2$	1
5	$\xi_2^2 - 1$	2

Figure 9. Example B. Variability of the magnitude of S_{11} . The green thick line corresponds to the nominal value for (L, w) , while the blue lines are the results of the MC simulations performed using 10000 (L, w) samples.

We note that, the variability analysis shown in this example cannot be performed with previous developed techniques [1]-[4], even if the filter is realized using only microstrips. Indeed, the techniques [1]-[4] employ a stochastic model of the per-unit-length parameters and the length of a line cannot be assumed as parameter for the variability analysis.

The PC model of the scattering parameters for the modeling frequencies has order $P = 5$, according to Algorithm 1, and $M = 20$, according to (4), while 0.01 is targeted as maximum error (13) between the PC coefficients and the corresponding rational models. The obtained PC-based model shows an excellent accuracy compared with the classical MC analysis in computing system variability features, as shown in Figs. 10 - 12. In particular, Figs. 10 - 11 show the mean and the standard deviation of the imaginary part of the element S_{12} for the validation frequencies computed with the proposed method, a MC analysis with the similar computational cost (performed using 64 (L, w) samples) and a MC analysis performed using 10000 (L, w) samples. It is important to notice that for this highly dynamic system the PC method offers a much higher accuracy in estimating these statistical moments than the MC analysis with the similar computational cost. Finally, Fig. 12

Figure 10. Example B. The top plot shows a comparison between the mean of the imaginary part of S_{12} obtained with the MC analysis performed using first 10000 (D_1, D_2, D_3) samples (full black line), then 64 (D_1, D_2, D_3) samples (dashed green line), and the proposed PC-based method (red circles: (o)) for the validation frequencies. The lower plot shows the corresponding absolute error.

describes the PDF and the CDF of S_{11} at the frequency of 281.25 MHz. Note that similar results can be obtained for the other entries of the scattering matrix.

The proposed technique offers a great computational efficiency in addition to its accuracy; in Table V the computational time needed for the MC analysis (performed on the validation frequencies using 64 and 10000 (L, w) samples) and the proposed PC-based technique is reported. As in the previous example, in Table V the computational time of the new PC-based technique is explicitly divided into the time needed to calculate the initial samples and to build the polynomial model of the scattering parameters (including the computational cost to build the PC-model of the scattering parameters in the form (10) for all the orders $P \leq 6$, as described by Algorithm 1) and evaluate it on the validation frequencies.

As for the previous numerical example, the proposed technique is compared with respect to the PC-based method presented in [12]. The comparison of the accuracy and efficiency of the two PC-based techniques is performed using the same sampling for the geometrical parameters and

Figure 11. Example B. The top plot shows a comparison between the standard deviation of the imaginary part of S_{12} obtained with the MC analysis performed using first 10000 (D_1, D_2, D_3) samples (full black line), then 64 (D_1, D_2, D_3) samples (dashed green line), and the proposed PC-based method (red circles: ($\circ$)) for the validation frequencies. The lower plot shows the corresponding absolute error.

Figure 12. Example B. PDF and CDF of the magnitude of S_{11} at 281.25 MHz. Full black line: PDF computed using the novel technique; Dashed black line: CDF computed using the novel technique; Circles ($\circ$): PDF computed using the MC technique; Squares ($\square$): CDF computed using the MC technique.

Table V. Example B. Efficiency of the Proposed PC-based Technique

Technique	Computational time
Monte Carlo Analysis (10000 samples, validation frequencies)	7 h 36 min, 43.7 s
Monte Carlo Analysis (64 samples, validation frequencies)	2 min, 55.38 s
PC-based technique	3 min 32.82 s
Details PC-based technique	Computational time
Initial simulations (64 samples, modeling frequencies)	3 min 1.36 s
PC model scattering parameters	31.46 s

frequency and adopting the same order of the expansion as for the proposed technique, leading to a PC model of order $P = 5$ and $M = 20$ basis functions.

The state-space matrices are calculated using the VF algorithm, targeting -40 dB as maximum absolute model error between the scattering parameters and the corresponding root macromodels in order to estimate the required number of poles. As a result, 35 poles are used to compute the root macromodels for all the 8×8 samples of the geometrical parameters (L, w) . Note that trying to impose a better accuracy (< -40 dB) does not provide good results, since the VF state-space matrices become nonsmooth as functions of the stochastic parameters.

Again, the proposed approach and the technique [12] have a similar accuracy in estimating the filter variability features, as shown in Fig. 13, and both show a great efficiency with respect to the MC analysis, as described in Tables V and VI.

Table VI. Example B. Efficiency of the PC-based Technique [12]

PC-based technique [12]	Computational time
Initial simulations (64 samples, modeling frequencies)	3 min 1.36 s
PC model scattering parameters	1 min 30.76 s
Total computational time	4 min, 32.12 s

Figure 13. Example B. The top plot shows a comparison between the mean of the real part of S_{11} obtained with the MC analysis performed using 10000 (L, w) samples (full black line), the technique [12] (dashed magenta line), and the proposed PC-based method (red circles: $(\circ)$) for the validation frequencies. The lower plot shows the corresponding absolute error.

However, the efficient model building procedure of the proposed approach leads to a superior efficiency with respect to the technique [12] in calculating the PC model of the filter scattering parameters for the evaluation frequencies, see the element “PC model scattering parameters” in Tables V and VI. It is worth to remark that the element “PC model scattering parameters” in Table V includes the computational cost to build the PC-model of the scattering parameters in the form (10) for all the orders $P \leq 6$, as described by Algorithm 1, while the technique [12] does not use an adaptive model order selection.

The technique [12] requires the computation of 64 root macromodels in a state-space form with common order corresponding to each (L, w) sample prior to the application of the PC expansion. Next, an augmented system in the form of equation (17) in [12] has dimension 1470×1470 for each one of the validation frequency samples. Building such a system required the computation of 9261 double integrals depending on the normalized variables (ξ_1, ξ_2) obtained via Galerkin projections [1]–[6]. Again, these projections are calculated upfront and the corresponding computational time is not included in Table VI.

5. CONCLUSIONS

In this paper, we present an innovative technique to calculate frequency-domain macromodels for efficient variability analysis of general multiport systems. It is based on the use of the PC expansion, applied at an input-output level, to describe the system variability features in combination with rational identification in the frequency-domain. The presented technique is straightforward to implement, it selects the PC expansion order automatically, and it can be applied to a large range of microwave systems. Comparisons with the standard MC approach and with the PC-based technique [12] are performed for two pertinent numerical examples, validating the accuracy and efficiency of the proposed method.

6. APPENDIX

6.1. Karhunen-Loève expansion and Correlated Gaussian Random Variables

If the correlation matrix $\mathbf{C}^{N \times N}$ is symmetric and positive-definite, then it has N orthogonal eigenvectors $[\vec{u}_i]_{i=1}^N$, and can be diagonalized as

$$\mathbf{C} = \mathbf{U} \mathbf{\Lambda} \mathbf{U}^T \quad (21)$$

where $\mathbf{\Lambda}$ is the diagonal matrix of the eigenvalues of $\mathbf{C}$, the symbol ^{T} indicates the matrix transpose and $\mathbf{U}$ is the orthogonal matrix defined as $\mathbf{U} = [\vec{u}_1, \dots, \vec{u}_N]$. Using (21) in (18) leads to

$$W_{\vec{\eta}} = \frac{1}{2\pi \det(\mathbf{\Lambda})^{\frac{1}{2}}} \exp \left(-\frac{1}{2} (\vec{\eta} - \vec{\mu})^T \mathbf{U} \mathbf{\Lambda}^{-1} \mathbf{U}^T (\vec{\eta} - \vec{\mu}) \right) \quad (22)$$

Therefore, for correlated Gaussian random variables that follow the non-degenerate multivariate normal distribution (18), the Karhunen-Loève expansion is a simple change of variables. The joint probability density (22) can be written with respect to a vector of independent Gaussian random variable $\vec{x}$, with zero mean and variance equal to $[\mathbf{\Lambda}_{ii}]_{i=1}^N$, as

$$W_{\vec{x}} = \frac{1}{2\pi \det(\mathbf{\Lambda})^{\frac{1}{2}}} \exp \left(-\frac{1}{2} \vec{x}^T \mathbf{\Lambda}^{-1} \vec{x} \right) \quad (23)$$

where

$$\vec{x} = \mathbf{U}^T (\vec{\eta} - \vec{\mu}) \quad (24)$$

Next, the vector $\vec{x}$ can be expressed with respect to the vector of normalized Gaussian random variables $\vec{\xi}$ with zero mean and unitary variance as

$$\vec{x} = \mathbf{\Lambda}^{\frac{1}{2}} \vec{\xi} \quad (25)$$

Combining (24) and (25) leads to (19).

6.2. Passivity Verification of the PC-based Macromodel

The proposed technique does not guarantee the passivity of the frequency-domain macromodel in the form (9). However, the passivity of the proposed macromodel can be verified, since the matrix coefficients $[\alpha_i(s)]_{i=0}^M$ in (9) are rational functions of the Laplace variable s . Hence, the coefficients $\alpha_i(s)$ can be written as transfer functions:

$$\alpha_i(s) = \mathbf{C}_i (s\mathbf{I}_i - \mathbf{A}_i)^{-1} \mathbf{B}_i + \mathbf{D}_i$$

where $\mathbf{I}_i$ is the identity matrix with the same dimensions as the matrix $\mathbf{A}_i$. The state space matrices $[\mathbf{A}_i, \mathbf{B}_i, \mathbf{C}_i, \mathbf{D}_i]_{i=0}^M$ are obtained for each $\alpha_i(s)$ by means of system identification techniques such as VF. It should be noted that VF can enforce stability by pole flipping techniques.

Equation (9) can therefore be rewritten as

$$\mathbf{S}(s, \vec{\xi}) \approx \sum_{i=0}^M \left(\mathbf{C}_i (s\mathbf{I}_i - \mathbf{A}_i)^{-1} \mathbf{B}_i + \mathbf{D}_i \right) \varphi_i(\vec{\xi}) \quad (26)$$

Since (26) is a weighted sum of rational transfer functions, it is itself a rational transfer function, i.e.,

$$\mathbf{S}(s, \vec{\xi}) \approx \widehat{\mathbf{C}} \left(s\widehat{\mathbf{I}} - \widehat{\mathbf{A}} \right)^{-1} \widehat{\mathbf{B}}(\vec{\xi}) + \widehat{\mathbf{D}}(\vec{\xi}) \quad (27)$$

where

$$\begin{aligned}\widehat{\mathbf{A}} &= \text{blockdiagonal}(\mathbf{A}_0, \mathbf{A}_1, \dots, \mathbf{A}_M) \\ \widehat{\mathbf{B}}(\vec{\xi}) &= \begin{bmatrix} \mathbf{B}_0 \varphi_0(\vec{\xi}) \\ \mathbf{B}_1 \varphi_1(\vec{\xi}) \\ \vdots \\ \mathbf{B}_M \varphi_M(\vec{\xi}) \end{bmatrix} \\ \widehat{\mathbf{C}} &= \begin{bmatrix} \mathbf{C}_0 & \mathbf{C}_1 & \dots & \mathbf{C}_M \end{bmatrix} \\ \widehat{\mathbf{D}}(\vec{\xi}) &= \sum_{i=0}^M \mathbf{D}_i \varphi_i(\vec{\xi})\end{aligned}$$

Here $\text{blockdiagonal}(\cdot)$ represents the blockdiagonal matrix with blocks $[\mathbf{A}_i]_{i=0}^M$ on the main diagonal and $\widehat{\mathbf{I}}$ is the identity matrix with the same dimensions as the matrix $\widehat{\mathbf{A}}$.

The passivity of the macromodel (27), and of the corresponding form (9), can be assessed by computing the following Hamiltonian matrix [24, 25] :

$$\begin{bmatrix} \widehat{\mathbf{A}} - \widehat{\mathbf{B}}(\vec{\xi}) \widehat{\mathbf{R}}(\vec{\xi}) \widehat{\mathbf{D}}(\vec{\xi})^T \widehat{\mathbf{C}} & -\widehat{\mathbf{B}}(\vec{\xi}) \widehat{\mathbf{R}}(\vec{\xi}) \widehat{\mathbf{B}}(\vec{\xi})^T \\ \widehat{\mathbf{C}}^T \widehat{\mathbf{S}}(\vec{\xi}) \widehat{\mathbf{C}} & -\widehat{\mathbf{A}}^T + \widehat{\mathbf{C}}^T \widehat{\mathbf{D}}(\vec{\xi}) \widehat{\mathbf{R}}(\vec{\xi}) \widehat{\mathbf{B}}(\vec{\xi})^T \end{bmatrix} \quad (28)$$

where ^{T} stands for the matrix transpose and

$$\widehat{\mathbf{R}}(\vec{\xi}) = \left(\widehat{\mathbf{D}}(\vec{\xi})^T \widehat{\mathbf{D}}(\vec{\xi}) - \mathbf{I} \right)^{-1}, \quad \widehat{\mathbf{S}}(\vec{\xi}) = \left(\widehat{\mathbf{D}}(\vec{\xi}) \widehat{\mathbf{D}}(\vec{\xi})^T - \mathbf{I} \right)^{-1}$$

The transfer function $\mathbf{S}(s, \vec{\xi})$ is passive if and only if the Hamiltonian matrix (28) does not admit purely imaginary eigenvalues. It is important to note that the Hamiltonian matrix (28) only depends on the normalized random variables $\vec{\xi}$. Therefore, it is always possible to identify a compact smooth region $\Xi \subset \Omega$ where the macromodel (9) is passive, if the corresponding macromodel (27) is passive for the values of $\vec{\xi}$ corresponding with the nominal values of the parameters under consideration, in other words for the operating point.

Note that, the passivity region $\Xi \subset \Omega$ corresponds with all points $\vec{\xi} \in \Omega$ where the Hamiltonian matrix (28) does not admit purely imaginary eigenvalues. Equivalently, the passivity region $\Xi \subset \Omega$

can be found [26] by selecting the points $\vec{\xi} \in \Omega$ where the $\mathcal{H}_\infty$ norm $\|\mathbf{S}(s, \vec{\xi})\|_\infty \leq 1$.[¶] Finally, if one wants a parameter span or closed hyper-rectangle inside the passivity region Ξ , this can always be obtained, since if a point (here the operating point) is in the interior of a smooth compact region Ξ , then one can always find a closed hyper-rectangle inside Ξ containing that interior point.

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[¶]Note that this proves in fact that the passivity region Ξ is smooth and compact, since norms are continuous functions of their argument and $\mathbf{S}(s, \vec{\xi})$ is by construction a continuous function of its arguments.

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