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A Polynomial Chaos Expansion based Building Block approach for stochastic analysis of photonic circuits

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ABSTRACT

The Building Block (BB) approach has recently emerged in photonic as a suitable strategy for the analysis and design of complex circuits. Each BB can be foundry related and contains a mathematical macro-model of its functionality. As well known, statistical variations in fabrication processes can have a strong effect on their functionality and ultimately affect the yield. In order to predict the statistical behavior of the circuit, proper analysis of the uncertainties effects is crucial. This paper presents a method to build a novel class of Stochastic Process Design Kits for the analysis of photonic circuits. The proposed design kits directly store the information on the stochastic behavior of each building block in the form of a generalized-polynomial-chaos-based augmented macro-model obtained by properly exploiting stochastic collocation and Galerkin methods. Using this approach, we demonstrate that the augmented macro-models of the BBs can be calculated once and stored in a BB (foundry dependent) library and then used for the analysis of any desired circuit. The main advantage of this approach, shown here for the first time in photonics, is that the stochastic moments of an arbitrary photonic circuit can be evaluated by a single simulation only, without the need for repeated simulations. The accuracy and the significant speed-up with respect to the classical Monte Carlo analysis are verified by means of classical photonic circuit example with multiple uncertain variables.

Keywords: Integrated photonic, building block, generalized polynomial chaos (gPC), stochastic process

1. INTRODUCTION

Recent advances in photonic integration are making possible the implementation of photonic circuits combining many functions on a single chip, significant production volumes and reduced fabrication costs [1]. As for electronics, the introduction of a building-block-based approach allowed for complex photonic integrated circuits to be conceived, designed, and realized by assembling a restricted number of building blocks (BBs) made available through a Process Design Kits (PDK). A PDK contains foundry specific technology information and provides a library of the offered building blocks incorporating all the information related to a particular device such as its schematic representation and the deterministic mathematical macro-model of its behavior, generally in the form of either a transmission or a scattering matrix. Once the BBs of a particular photonic foundry are available, the design and simulation of complex photonic can be carried out at a circuit level by simply combining the desired BBs according to given design rules [2, 3]. However, stochastic uncertainties related to unavoidable tolerances of the technological processes such as waveguide width or height variations, proper gap opening or changes in material composition can have a strong effect on the functionality of the fabricated circuits and ultimately affect the entire circuit performance [4-6]. The information on the expected variability is hence an essential aspect for each building block and the availability of efficient computational strategies is fundamental to quickly predict the statistical behavior of a circuits since the early stage of the design process.

In this regard, Monte Carlo is a robust, accurate, and easy-to-implement approach, and is often considered as the standard for stochastic analysis. However, its high computational cost can obstruct its application to the analysis of even relatively simple circuits because a large number of simulation runs (generally in the order of 10^4 - 10^5) is required to obtain reliable results. For this reason, the generalized polynomial chaos approach has been introduced in several application fields as an efficient alternative to the classical Monte Carlo method [7, 8], and recently it has been proposed also for the

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variability analysis of photonic devices [9, 10]. The generalized polynomial chaos technique allows approximating the dependence of the simulation output on the stochastic input parameters with a set of orthonormal polynomials. The computation of the coefficients of the basis functions is done either through intrusive methods (e.g. stochastic Galerkin [11] and stochastic testing [12]), that require modifying the internal code of an existing deterministic solver, or nonintrusive methods (i.e. sample-based methods), such as stochastic collocation [13], that use the deterministic solvers as black boxes.

The few implementations of the generalized polynomial chaos (gPC) described in literature for photonics applications are based on nonintrusive methods. Figure 1(a) schematically reports the common approach for stochastic analyses at circuit level. The building blocks made available by a process design kit are used by the designer to build a deterministic circuit model, depending on a set of random parameters. During simulations, the value of these parameters is sampled according to their probability density function and the circuit simulator is used iteratively to compute the response of the designed circuit for each sample exploiting the deterministic model (e.g. scattering matrices) included in each building block. The number of simulations depends on the problem, but it is generally smaller than few hundreds. This pool of initial Monte Carlo simulations is used to correctly approximate the stochastic behavior of the circuit through a generalized polynomial chaos expansion. This approach is obviously circuit-specific and has to be carried out each time the layout of the circuit changes.

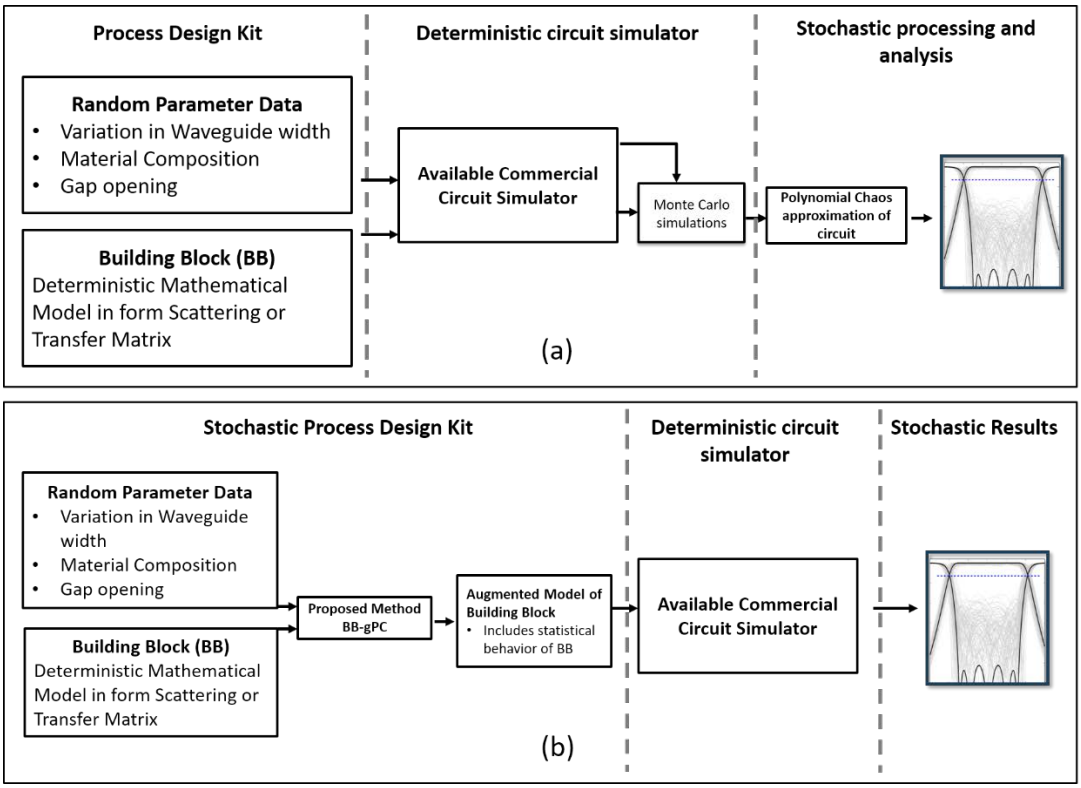


Figure 1. (a) Typical approach for the stochastic analysis of photonic circuit exploiting standard process design kits, Monte Carlo simulations and nonintrusive generalized polynomial chaos approximation. (b) Computation of the stochastic behavior of the circuit exploiting the proposed stochastic process design kits. In both cases PDK and stochastic PDK are circuit independent

In this work, the generalized polynomial chaos expansion is exploited in conjunction with the stochastic Galerkin method to efficiently build BB's model (augmented macro-models) directly embedding their statistical behavior. This new models retain the form of transmission or scattering matrices, are circuit independent and can be stored and replace the original deterministic models of the building blocks in the process design kit [see Fig.1(b)]. The augmented macro-models can hence combined according to the circuit connections to derive with a single deterministic simulation run an augmented matrix description of the whole circuit. The obtained gPC coefficients are related to the stochastic moments of the circuit such as mean, variance and Probability Density Function of a desired quantity of interest. Using this approach, we demonstrate that the augmented macro-models of the BBs can be calculated once and stored in a BB (foundry dependent)

library and then used for the analysis of any desired circuit. The main advantage of this approach, shown here for the first time in photonics, is that the stochastic moments of an arbitrary photonic circuit can be evaluated by a single simulation only, without the need for repeated simulations. The accuracy and the significant speed-up with respect to the classical Monte Carlo analysis are verified by means of a two-stage Mach-Zehnder filter with multiple uncertain variables.

2. POLYNOMIAL CHAOS BACKGROUND

The finite-variance stochastic process Y depending on a vector of normalised random variables $\vec{\boldsymbol{\xi}}$ can be described as a summation of basis functions $\varphi_i(\vec{\boldsymbol{\xi}})$ with suitable coefficients y_i as [14]

$$Y(\vec{\boldsymbol{\xi}}) = \sum_{i=0}^{\infty} y_i \varphi_i(\vec{\boldsymbol{\xi}}). \tag{1}$$

In this expression, $\vec{\boldsymbol{\xi}} = [\xi_1, \xi_2, ..., \xi_N]$ are independent standard normal random variables, N is number of uncertain parameters and φ_i are the orthonormal polynomials with respect to the probability measure $W(\vec{\xi})$ as

$$\langle \varphi_i(\vec{\boldsymbol{\xi}}), \varphi_j(\vec{\boldsymbol{\xi}}) \rangle = \int \varphi_i(\vec{\boldsymbol{\xi}})\, \varphi_j(\vec{\boldsymbol{\xi}}) W(\vec{\xi}) d\vec{\xi} = \delta_{ij}, \tag{2}$$

where δ_{ij} is the Kronecker delta. The construction of the gPC expansion (1) requires the following three-step process. The first step is to calculate the orthogonal polynomials. The second step is to truncate the series to a finite order, and last is to compute the gPC coefficients y_i. If the random variables $\vec{\boldsymbol{\xi}}$ are independent, the corresponding basis functions $\varphi_i(\vec{\boldsymbol{\xi}})$ can be computed as product combinations of the orthogonal polynomials corresponding to each individual random variable ξ_i. It is important to note that for random variables with specific distributions (i.e., Gaussian, Uniform and Beta), the basis functions are the polynomials described by the Wiener-Askey scheme [14]. For example, in the Gaussian PDF case, the basis functions are the Hermite polynomials. Consequently, equation (1) can be truncated for computational purposes. Considering all N-dimensional Hermite polynomials of order P, the response may be approximated as

$$Y(\vec{\boldsymbol{\xi}}) = \sum_{i=0}^{M} y_i \varphi_i(\vec{\boldsymbol{\xi}}). \tag{3}$$

The number of gPC basis function M in equation (3) with the order of the expansion P and the number of random variables N is

$$M + 1 = \frac{(N + P)!}{N!\, P!}. \tag{4}$$

After determination of basis functions and truncation of the series in equation (3), the $M + 1$ scaler coefficients y_i can be computed. In this work, to calculate the gPC coefficients y_i we have used the linear regression technique in which all the gPC coefficients are calculated solving a least square system.

$$\boldsymbol{\Psi} \mathbf{y_i} = \mathbf{R}. \tag{5}$$

Equation (5) is calculated for an initial small pool of K Monte Carlo simulations of the normalized random variables $\vec{\boldsymbol{\xi}}$, indicated as $[\vec{\boldsymbol{\xi}}_j]_1^K$. The jth row of the matrix $\boldsymbol{\Psi}$ contains the multivariate polynomial basis evaluated at $\vec{\boldsymbol{\xi}}_j$ and the matrix $\mathbf{R}$ represents the corresponding set of stochastic response values of process under consideration. The main feature of the gPC expansion is the efficient representation of the system variability: stochastic moments of Y, such as its mean μ and variance σ^2, can be analytically computed as

$$\mu = y_0, \tag{6}$$

$$\sigma^2 = \sum_{1}^{M} y_i \langle \varphi_i(\vec{\boldsymbol{\xi}}), \varphi_i(\vec{\boldsymbol{\xi}}) \rangle. \tag{7}$$

Apart from the first moments, complex stochastic information of Y, such as the probability density function (PDF) and the cumulative density function (CDF), can be computed following standard analytical formulae or by applying Monte Carlo sampling on the gPC approximation (3). In this work, we consider the complex frequency response (transfer function) of

photonic circuits as the stochastic process $\mathbf{Y}$, which can be handled by considering equation (3) for each wavelength and calculating the coefficients $\mathbf{y_i}$ as wavelength dependent.

3. AUGMENTED SYSTEM FOR THE BUILDING BLOCKS

The polynomial chaos formalism described in the previous section is exploited here to create an augmented-macro model of a building block embedding its stochastic behavior. For a given building block, a scattering matrix represents a convenient way to describe the relation between the complex amplitude of the input waves and the complex amplitude of the output waves. In this formalism, the behavior of a system with n_p ports can hence be expressed as

$$\vec{\mathbf{b}} = \vec{\mathbf{S}}\vec{\mathbf{a}}, \tag{9}$$

where vectors $\vec{\mathbf{a}} \in \mathbb{C}^{n_p \times 1}$ and $\vec{\mathbf{b}} \in \mathbb{C}^{n_p \times 1}$ are the complex input and output at all the n_p ports and $\vec{\mathbf{S}} \in \mathbb{C}^{n_p \times n_p}$ is the matrix containing scattering parameters of building block. If the building block described by the scattering matrix depends on a set of random variables $\vec{\boldsymbol{\xi}}$, equation (9) becomes

$$\vec{\mathbf{b}}(\vec{\boldsymbol{\xi}}) = \vec{\mathbf{S}}(\vec{\boldsymbol{\xi}})\vec{\mathbf{a}}(\vec{\boldsymbol{\xi}}). \tag{10}$$

Using the gPC expansion (3), the wave relation (10) becomes

$$\sum_{i=0}^{M} \vec{\mathbf{b}}_i \varphi_i(\vec{\boldsymbol{\xi}}) = \sum_{i=0}^{M}\sum_{j=0}^{M} \vec{\mathbf{S}}_i \vec{\mathbf{a}}_j \varphi_i(\vec{\boldsymbol{\xi}})\varphi_j(\vec{\boldsymbol{\xi}}), \tag{11}$$

where $\vec{\mathbf{a}}_i$, $\vec{\mathbf{b}}_i$ and $\vec{\mathbf{S}}_i$ are now the polynomial chaos coefficients of the input and output wave amplitudes and of the building block scattering parameters for each port, respectively. A non-intrusive approach can be used to obtain the gPC coefficient $\vec{\mathbf{S}}_i$ of a given building block similar to the method described in Section 2. In order to build the augmented scattering matrix of building block, using Galerkin method, projecting equation (11) on to the pth gPC basis function φ_p gives

$$\vec{\mathbf{b}}_p^k = \sum_{i=0}^{M}\sum_{j=0}^{M} \vec{\mathbf{S}}_i \vec{\mathbf{a}}_j \, \langle \varphi_i(\vec{\boldsymbol{\xi}})\, \varphi_j(\vec{\boldsymbol{\xi}}),\, \varphi_p(\vec{\boldsymbol{\xi}})\rangle, \tag{12}$$

where the elements $\vec{\mathbf{b}}_p^k$ represent the pth gPC coefficient at the kth port ($k = 1 \dots n_p$) for the output wave. The factors $\langle \varphi_i(\vec{\boldsymbol{\xi}})\, \varphi_j(\vec{\boldsymbol{\xi}}),\, \varphi_p(\vec{\boldsymbol{\xi}})\rangle$ arises in equation (12) are real scalar numbers and can be computed analytically solving multi-dimensional integrals and stored. Repeating this operation for all the $M + 1$ gPC basis functions lead to

$$\vec{\mathbf{b}}_{\mathbf{PC}} = \vec{\mathbf{S}}_{\mathbf{PC}}\vec{\mathbf{a}}_{\mathbf{PC}}. \tag{13}$$

The vectors $\vec{\mathbf{a}}_{PC} \in \mathbb{C}^{(M+1)n_p \times 1}$ and $\vec{\mathbf{b}}_{PC} \in \mathbb{C}^{(M+1)n_p \times 1}$ contains the gPC coefficient of input and output waves respectively, while the augmented matrix $\vec{\mathbf{S}}_{PC} \in \mathbb{C}^{(M+1)n_p \times (M+1)n_p}$ of the building block is the weighted combination of gPC coefficients. Equation (13) describes the "augmented model" of the building block which depends on the considered random variables. It is important to mention that $\vec{\mathbf{S}}_{PC}$ is still a unitary and loss-less scattering matrix and the use of orthonormal gPC basis functions preserves the symmetry. The augmented scattering parameters $\vec{\mathbf{S}}_{PC}$ can be used to generate the stochastic scattering parameters. The gPC coefficients are contained in the augmented matrices. It can be seen from the definition of augmented matrices (12) that the entries of the first row of an augmented matrix contain the corresponding expansion coefficients. Next, the procedure can be repeated for all the needed frequency points in a given frequency range to obtain frequency-dependent augmented models $\vec{\mathbf{S}}_{\mathbf{PC}}(\mathbf{f_l})$ for $l = 1, \dots, L$.

The library of building blocks modeled by frequency-dependent augmented matrices in form of equation (6) realize a Stochastic Process Design Kit. Using standard procedures [2], the BBs augmented scattering matrices can be combined according to the circuit layout with a single simulation run of available deterministic circuit simulators and the stochastic behavior of any arbitrary circuit is obtained.

4. CASCADED MACH-ZEHNDER FILTER

In this section, the proposed approach is applied to compute the augmented models of two different building blocks, that are a directional coupler (BB_K) and a waveguide (BB_W), that are exploited to analyze the stochastic behaviour of a two-stage Mac-Zehnder filter. To build the second-order Mach-Zehnder filter, we use the two building blocks as schematically shown in Fig. 2(a). We consider as a reference a standard silicon-on-insulator technology. The nominal design of the filter

was obtained with the synthesis technique described in reference [15]. The Mach-Zehnder filter has a nominal 3-dB bandwidth of $BW_o = 62$ GHz and the corresponding coupling coefficients for the three directional couplers are $K_1 = K_3 = 0.865$ and $K_2 = 0.532$, with an in-band isolation larger than 20 dB. For the directional coupler building blocks, the considered nominal gap distance is $g_i = 0.3$ µm. For the waveguide building blocks the nominal waveguide width is $W_i = 407.7$ nm and thickness is 220 nm, corresponding to an effective and group indices of about 2.23 and 4.402. Both building blocks have the same unbalance lengths of 680.8 µm, corresponding to a free spectral range of 100 GHz. Figure 2(b) shows the ideal transfer function of the Mach-Zehnder filter at the bar (bold black) and the cross (bold red) ports respectively. Although these results already represent high-quality designs, they do not take into account the unavoidable process variations affecting real fabricated circuits. For BB_w the waveguide width (ΔW_i) and for BB_K the gap (Δg_i) of the couplers are assumed as independent standard Gaussian distributed random variable with standard deviation $\sigma_W = 10$ pm and $\sigma_g = 5$ nm respectively. Figure 2b shows, in addition to the nominal response, several spectral transfer function of the Mach-Zehnder filter at bar and cross ports (grey lines) obtained for reference by classical Monte Carlo analysis. It can be clearly seen that the transfer function of the original nominal design (bold lines) is largely distorted even is the case small considered uncertainty, with fluctuations of both the pass band and the in-band isolation.

As a first step, the augmented macro-models of these two building blocks are calculated once and stored as described in section 3. The complex frequency response (transfer function) of the photonic circuit is considered as the stochastic process under investigation. In order to calculate the augmented macro-models, we computed the following steps:

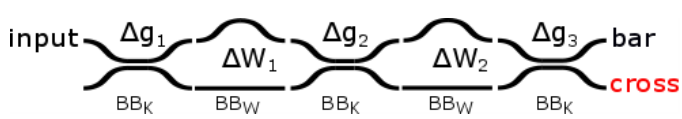
1. The gPC model of the directional coupler (BB_K) and the waveguide (BB_W) are calculated for 250 wavelength samples between 1.549 µm and 1.551 µm in the form of equation (11) considering the order of expansion $P = 2$ and a number of uncertain parameters $N = 1$. The gap of the coupler and the waveguide width are the uncertain parameter for BB_K and BB_W respectively. The random parameters are modelled with Gaussian random variables and corresponding basis functions are Hermite polynomials. The gPC coefficients are calculated with $K = 30$ Monte Carlo samples for each BB.
2. The $\vec{\mathbf{S}}_{\mathbf{PC}}$ Matrix in the form of equation (13) is built via Galarkin projection for both elementary BBs for each wavelength considering the uncertain parameters of the whole circuit. Both building blocks have $n_p = 2$ ports.
3. The matrices of the directional coupler and waveguides are combined to obtain the final matrix of the circuit. The first row of the final matrix contains the coefficient of gPC approximation of whole circuit.

The obtained wavelength-dependent gPC coefficients allow to calculate the stochastic moments, such as mean and variance using equations (6) and (7). Stochastic functions such as the probability density function (PDF) and the cumulative density function (CDF) can be computed following standard analytical formulae or by applying Monte Carlo sampling on the gPC approximation (14) of the circuit.

$$\vec{S}(\lambda, \vec{\xi}) = \sum_{i=0}^{M} \vec{\mathbf{S}}_{PC}^{i0}(\lambda)\varphi_i(\vec{\boldsymbol{\xi}}). \tag{8}$$

Since BB_K and BB_W are used three and two times, respectively, and they are considered independent of each other, for the whole circuit the number of random variables is $N = 5$. This makes the size of the augmented matrix BB_W 42 × 42 with M = 21, $n_p = 2$ and BB_K 84 × 84 with $n_p = 4$ and same M. The BB_K and BB_W are combined accordingly to build an augmented matrix description of the whole circuit in which first row or column contains the gPC coefficients. Using these coefficients the gPC approximation in form of equation (14) is obtained.

(a)



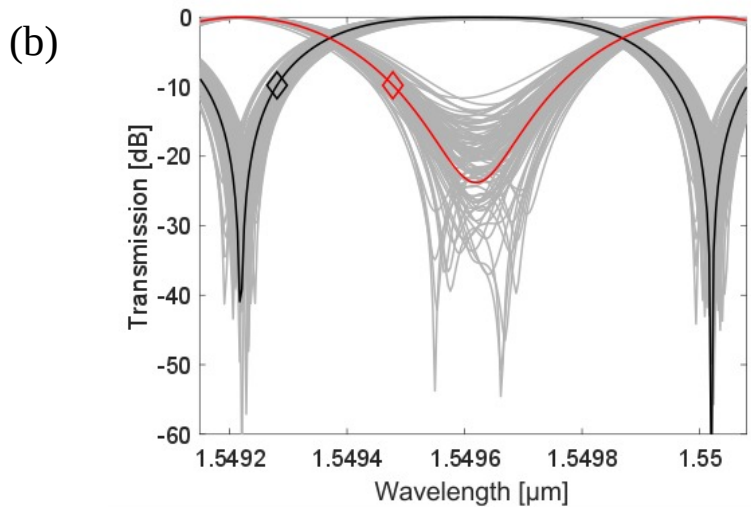


Figure 2: (a) Schematic of the second-order Mach-Zehnder filter (b) Transfer function of the Mach-Zehnder filter at the bar (black) and the cross (red) ports for the nominal design. Thin grey lines show the effect of fabrication uncertainties on the waveguide widths and the gap of couplers

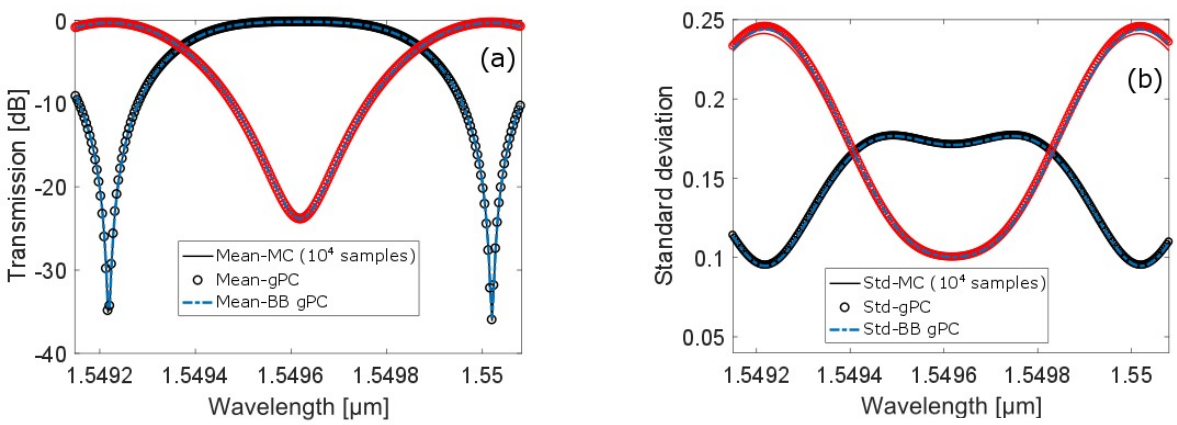


Figure 3: Comparison between (a) the mean and (b) the standard deviation of the magnitude of drop (black colour) and through (red colour) port of the filter obtained with the BB-PCE (blue dashed-dotted line), MC analysis (solid line) and the PC-based method (circles). The MC analysis is carried out using 10^4 samples, the PC-based analysis is carried out using 80 samples and 30 samples are used for the proposed BB-PCE method.

Using the proposed method (BB-gPC), the circuit statistical behavior is computed in terms of mean and variance with only one single simulation. A comparison between the direct Monte Carlo, classical gPC analysis and BB-gPC is shown in Figure 3 and 4. For both classical gPC and BB-gPC, the probability density function of any quantity of interest can be obtained by Monte Carlo sampling of the approximation of the circuit at a negligible computational cost. We used 10^4 samples for every Monte Carlo analysis. To build the gPC approximation through the classical approach in the form of equation (3) [see Section 2] we used K = 80 samples for linear regression at the output ports (bar and cross in Fig.1a) at each wavelength. Figures 3a and 3b shows the mean and the standard deviation of the transmission at the bar (black) and the cross (red) ports of the filter. Blue dash-dot lines represent the result obtained by the proposed technique while full line and circles shows the result obtained using Monte Carlo and gPC analysis, respectively. The BB-gPC method is in good agreement compared with the classical MC and gPC analysis in computing mean and standard deviation of the circuit.

Figure 4a describes the probability density function of the intensity transfer function at the bar (black color) and the cross port (red color) of the filter at a wavelength around 1.5493 μm (shown by a black marker in Fig. 2b) and 1.5495 μm

(shown by red marker in Fig. 2b) respectively. Blue desh-dot line represents proposed techiniqe while full line and circles shows the results of classical MC and gPC respectively. Note that the cross port of the filter suffers from a broader deviation of the intensity, while the bar port is more robust for the same process uncertainties. The obtained gPC approximation (14) can be used to perform the analysis of other desired quantities of interest, for example the 3-dB bandwidth of the filter. The transfer functions obtained with MC analysis on the original circuit and on both classical gPC and BB-gPC approximations are used to calculate the PDF of the 3-dB bandwidth of the filter at the bar port as shown in Fig. 4b. It is interesting to note that the bandwidth PDF is asymmetric and this behaviour is consistently described with all the three considered methods. The results obtained with all the three methods are in good agreement demonstrating that the BB-gPC provides reliable results not only for simple stochastic moments such as mean and variance but also for complex stochastic moments as the probability density function of any quantity of interest.

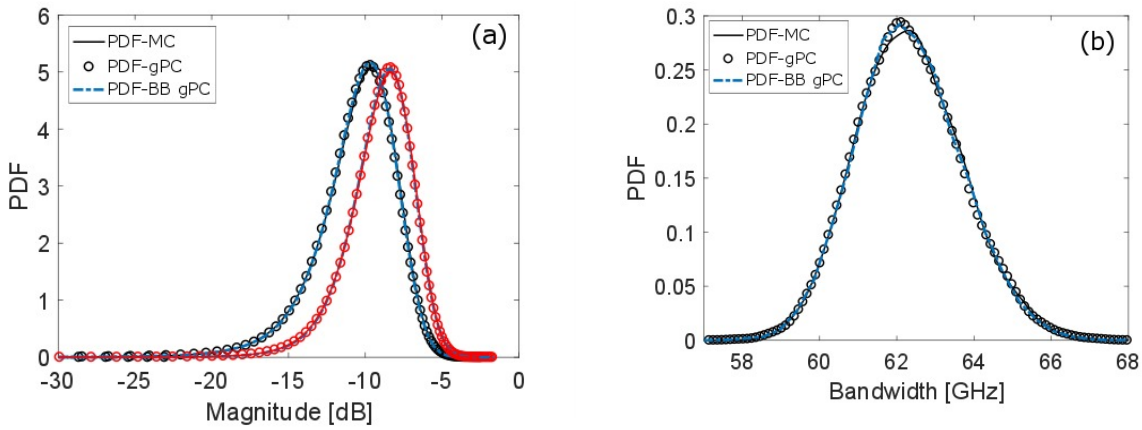


Figure 4: (a) PDF of the intensity transfer function at the bar (black colour) and cross (red colour) ports of the filter at a wavelength around 1.5493 µm (shown by a black marker in Fig. 4b) and 1.5495 µm (shown by red marker in Fig. 4b), respectively. (b) PDF of the bandwidth at bar port of the filter. Blue dash-dot line: PDF compute using the proposed BB-PCE method. Full line: PDF computed using the MC technique. Circles: PDF computed using the PC-based method.

The computational time of the test case described above is summarized in Table I. The Monte Carlo analysis took about 11 hours while classical gPC technique took around 5 minutes and 26 seconds using 80 samples. On the contrary, the proposed method required 3 minutes 9 seconds to compute gPC model using initial 30 samples for each BB in form of equation (7). This computation is required to be performed only once and used to obtain the statistical information of any circuit layout. The actual computational cost to retrieve the gPC approximation of the entire circuit is only 5.6 seconds.

Table 1: Efficiency of BB-gPC

Technique	**Computational time**
Frequency domain MC analysis [10^4 samples]	10 hour 58 minutes
gPC analysis [80 samples]	5 minutes 26 seconds
BB-gPC analysis	5.6 seconds
Preparation of stochastic models of BBs (one-time)	3 minutes and 9 seconds

5. CONCLUSION

In this paper, stochastic process design kits for efficient variability analysis of arbitrary photonic circuit using building block approach is presented. In the proposed framework the generalised polynomial chaos expansion is exploited in conjunction with the stochastic Galerkin method to efficiently build augmented macro-models of each BB directly embedding their statistical behaviour. Such augmented macro-model is calculated once and stored in BB library. Using

these augmented BB models, stochastic moments of an arbitrary photonic circuit can be evaluated by a single simulation only, without the need for repeated simulations. The efficiency and flexibility of the framework are illustrated using a relevant numerical example.

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