Efficient variability analysis of photonic circuits by stochastic parametric building blocks

Abi Waqas, Daniele Melati, Bhawani Shankar Chowdhry and Andrea Melloni

***Abstract*—This paper presents a method to build stochastic parametric building blocks to be used in photonic process design kits. The building blocks are based on parametric macro-models computed by means of the generalized Polynomial Chaos Expansion technique. These macro-models can be built upfront and stored in process design kits. Being parametric, they do not have to be recalculated if the value of their design or statistical parameters change. It is shown that a single deterministic simulation performed with a classical circuit simulator is sufficient to perform the statistical analysis of any arbitrary photonic circuit realized combining these building blocks with different parameters, without the need of time-consuming Monte Carlo approach. Relevant numerical examples are used to demonstrate that the proposed macro-models are truly parametric, inherently stochastic and have greater simulation efficiency compared to Monte Carlo.**

***Index Terms*—photonic integrated circuits, variability analysis, building blocks, optical filters, stochastic process, fabrication yield, manufacturing tolerances, polynomial chaos (PC).**

I. Introduction

PROCESS design kits (PDKs) give the designers access to foundry-specific information relevant for the simulation, design and mask layout preparation of photonic circuits. PDKs relate to a given fabrication technology, and ideally include structure dimensions, material properties, layout, design rules, performance and functional behaviour of each building block (BB) [1]. Often, commercially available PDKs offer a deterministic mathematical macro-model of the behaviour of each BB for simulation, generally in the form of either a transmission or a scattering matrix. Exploiting PDKs, the designers can work on a higher abstraction level using circuit simulators for analysis and optimization and mask generators for layout preparation. However, inherent variabilities have to be considered as an unavoidable factor related to the tolerances of fabrication processes such as waveguide geometry deviation, gap opening issues, material composition fluctuations and surface roughness. This means that nominally identical devices may differ from one to another once fabricated as a result of the manufacturing process. The device response is thus no longer regarded as deterministic but is more suitably interpreted as a stochastic process [2], [3]. Incorporating the information on physical and behavioural uncertainties in the PDK and the availability of efficient computational strategies to predict the statistical behaviour of any circuit are hence not only desirable but essential for the realistic description of photonic integrated circuits.

A powerful technique to evaluate the impact of uncertainties on the functionality of circuits and to extract statistical information is the Monte Carlo (MC) method and all its variants [2], [4], [5]. Although effective, these approaches are often very time-consuming even for relatively simple circuits, as they require a large number of samples to estimate the stochastic moments. For this reason, the approaches based on surrogate modelling have been introduced in several application fields as an efficient alternative to the classical Monte Carlo methods. Generalized Polynomial Chaos Expansion (gPC), proposed several years ago [6], is a popular and classical choice to build stochastic surrogate models and several advanced techniques have been recently reported to deal also with a large number of variables and variable correlation [7]–[9]. A few gPC implementations have been proposed also for stochastic analysis of photonics devices [10]–[14]. As a drawback, both gPC and Monte Carlo based techniques are circuit-specific and the entire analysis has to be repeated each time the BB parameters or the circuit layout change, with a large expense of time and resources.

In a recent work [15], we took advantage of the concept of augmented macro-modelling recently introduced in electronics and microwave modelling [16]–[23]. We presented a method to use gPC expansion to build stochastic building blocks by substituting the scattering matrix-based deterministic models in the PDK with new augmented models. The augmented model is obtained combining non-intrusive sample-based and Galerkin projection methods. The new model is still based on a scattering-matrix formalism but it conveys stochastic information as gPC coefficients. Through the formulation presented in [15] these coefficients are not parametric and need to be recalculated for any change in the value of the parameters of the building block.

A possible solution to introduce design parameters that has been proposed in literature is the use of combined models where parameters are transformed in uniformely distributed random variables [24], [25]. On the other hand this approach comes at the cost of forming a gPC expansion over additional dimensions and it is applicable only for parameters with a bounded domain. Moreover, its use in the context of augmented models could be critical as additional random variables would further increase the size of the model matrices as detailed in Section II. In this work, we propose an alternative methodology to make the stochastic building blocks fully

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parametric exploiting the gPC approach in conjunction with spectral projection [26]. This approach does not require any assumption on the parameters value, does not increase the dimensionality of the gPC expansion, and does not affect the size of the augmented models. Since the new building block models are parametrized, they do not have to be recalculated if geometrical, physical and optical parameters of the BBs are changed. Each BB depends on its own set of design parameters and stochastic variables. Stochastic BBs can then be combined according to circuit connections to compute the stochastic properties of any photonic circuit (which will depend on the entire ensemble of parameters and variables) through a single run of a deterministic circuit simulator, enabling an unprecedented simulation efficiency compared to classical Monte Carlo techniques.

II. Parametric models of stochastic building blocks

The starting point of the proposed method is the computation of a parametric gPC model of the building block's scattering parameters. For a passive and linear building block, the scattering matrix represents the relation between the complex amplitude of the outgoing field waves with respect to the complex amplitude of the incoming waves. When building block parameters are subjected to uncertainty, here represented as a vector of random variables $\vec{\xi}$, the corresponding scattering matrix depends also on $\vec{\xi}$. The scattering relations can thus be expressed as

$$\vec{b}(\vec{x},\vec{\xi}) = \vec{S}(\vec{x},\vec{\xi})\vec{a}(\vec{x},\vec{\xi}), \tag{1}$$

where $\vec{S} \in \mathbb{C}^{n_p \times n_p}$ is the scattering matrix of the building block, the vector $\vec{x}$ denotes a set of geometrical, physical and optical parameters and the vectors $\vec{a}$ and $\vec{b}$ of dimensions ($n_p \times 1$) are the complex input and output wave amplitudes at the n_p ports, respectively. According to the gPC method [26], the wave relation (1) can be represented as a truncated summation of basis functions with suitable coefficients,

$$\sum_{i=0}^{M} \vec{b_i}(\vec{x})\phi_i(\vec{\xi}) = \sum_{i=0}^{M}\sum_{j=0}^{M} \vec{S_i}(\vec{x})\vec{a_j}(\vec{x})\phi_i(\vec{\xi})\phi_j(\vec{\xi}), \tag{2}$$

where $\vec{a_j}$, $\vec{b_i}$ and $\vec{S_i}$ contain the gPC coefficients of the input and output wave amplitudes and the scattering parameters for each port, respectively. $\phi_i(\vec{\xi})$ are orthonormal polynomials with respect to a given probability measure. M+1= (N+P)!/N!P! is the number of coefficients that depends on the number N of uncertain parameters (the dimension of $\vec{\xi}$) and polynomials expansion order P. If the stochastic variables are indepedent, the orthonormal polynomials can be chosen according to the Wiener-Askey scheme [6] for the most common distributions. The computation of the gPC coefficients $\vec{S_i}(\vec{x})$ of the polynomial basis functions is the core task of the gPC approach.

In this work, we explicitly express the dependence of the gPC coefficients on the geometrical, physical and optical parameters $\vec{x}$ in order to obtain a parametric stochastic model of the building blocks. We calculate the parameters-dependent gPC coefficients by means of the classical spectral projection technique (non-intrusive method) [26], i.e., as an orthogonal projection onto the polynomial basis,

$$\vec{S_i}(\vec{x}) = \frac{\langle \vec{S}(\vec{x},\vec{\xi}), \phi_i(\vec{\xi})\rangle}{\langle \phi_i(\vec{\xi}), \phi_i(\vec{\xi})\rangle} = \frac{\int \vec{S}(\vec{x},\vec{\xi})\phi_i(\vec{\xi})W(\vec{\xi})d\vec{\xi}}{\alpha_i^2}. \tag{3}$$

where $\vec{S}(\vec{x},\vec{\xi})$ is the deterministic model of the building block, $W(\vec{\xi})$ is the probability measure of random variables and $\langle \phi_i(\vec{\xi}), \phi_i(\vec{\xi})\rangle = \alpha_i^2$ is a normalizing factor, equal to one when orthonormal polynomials are used. In general the elements of the matrix $\vec{S}(\vec{x},\vec{\xi})$ have a complex form or are unknown in their explicit form and the computation of the integral (3) has to be done numerically with a large cost in terms of time and computational resources. As such, this approach is rarely used and stochastic collocation is often preferred [10], [11], [26], [27]. On the other hand, in the case of a building block, the governing equations that describe its behaviour are relatively simple to manipulate, and the projection method becomes a convenient way to obtain the parametrized gPC coefficients $\vec{S_i}(\vec{x})$. Here, following the method presented in [15], the Galerkin projection is applied to expansion (2) to describe the relationship between the gPC coefficients of the incident and reflected waves as

$$\vec{b}_{\mathbf{PC}}(\vec{x}) = \vec{S}_{\mathbf{PC}}(\vec{x})\vec{a}_{\mathbf{PC}}(\vec{x}). \tag{4}$$

The vectors $\vec{a}_{\mathbf{PC}} \in \mathbb{C}^{(M+1)n_p \times 1}$ and $\vec{b}_{\mathbf{PC}} \in \mathbb{C}^{(M+1)n_p \times 1}$ contain the gPC coefficients of input and output waves, respectively, and $\vec{S}_{\mathbf{PC}} \in \mathbb{C}^{(M+1)n_p \times (M+1)n_p}$ is the augmented matrix of the building block obtained by the combination of gPC coefficients of scattering matrix in Eq. (2). Equation (4) describes the "parametric augmented model" of the building block. Compared to Eq.(9) in [15], this augmented model now explicitly depends on the considered geometrical, physical and optical parameters through an analytical expression. An example of derivation of a stochastic parametric model of a single waveguide building block is reported in the Appendix. Note that $\vec{S}_{\mathbf{PC}}(\vec{x})$ is (M + 1) times larger than the original deterministic scattering matrix in terms of number of ports and it is commonly sparse. It is important to mention that $\vec{S}_{\mathbf{PC}}(\vec{x})$ is still a unitary and loss-less scattering matrix and the use of orthonormal gPC basis functions preserves the symmetry (see Eq. (12) in Appendix).

The augmented scattering matrices describing different building blocks can thus be combined according to circuit layout by using the same classical techniques exploited by circuit simulators with deterministic scattering matrices. The augmented scattering matrix $\vec{S}_{\mathbf{T}}(\vec{x})$ of any arbitrary complex circuit is therefore calculated with a single deterministic simulation run, immediately providing a description of the stochastic properties of the entire circuit in the form of gPC coefficients. By construction, the first row or column of the augmented matrix $\vec{S}_{\mathbf{T}}(\vec{x})$ is formed by the gPC coefficients $\vec{S}_{\mathbf{i}}(\vec{x})$. From these coefficients, the first two stochastic moments, i.e., the mean $\mu(\vec{x}) = \vec{S}_{\mathbf{T}}^{\mathbf{00}}(\vec{x})$ and the standard deviation $\sigma^2(\vec{x}) = \sum_{i=1}^{M} \vec{S}_{\mathbf{T}}^{\boldsymbol{i}\mathbf{0}}(\vec{x})$ can be analytically computed

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[26]. The indices 00 and i0 indicate the very first element and the first row of matrix $\vec{S}_{\mathbf{T}}(\vec{x})$, respectively. The other statistical functions, such as the probability density function (PDF) or the cumulative distribution function (CDF) of any quantity of interest, can be calculated via inexpensive Monte Carlo sampling on the gPC approximation

$$\vec{S}(\vec{x},\vec{\xi}) = \sum_{i=0}^{M} \vec{S}_{\mathbf{T}}^{i0}(\vec{x})\phi(\vec{\xi}), \tag{5}$$

of the considered circuit, without further expensive circuit analysis.

Although we start here from analytical models, if these are not available the approach can still work. For example, the data obtained from iterative FDTD simulations of a component could be used to find the gPC coefficients using stochastic collocation method as described in [15]. The gPC coefficients can then be calculated for different values of design and stochastic parameters and be fitted to obtain a parametric stochastic augmented macro-model. Another possibility is to prepare an approximated parametric macro-model of a building block from simulation data with some assumptions and approximation techniques (e.g., Taylor expansion). This model can then be used to build the augmented parametric stochastic model as described in the Appendix. Lastly, if analytical models are not available design parameters could also be included through fictitious random variables generating combined gPC models [24].

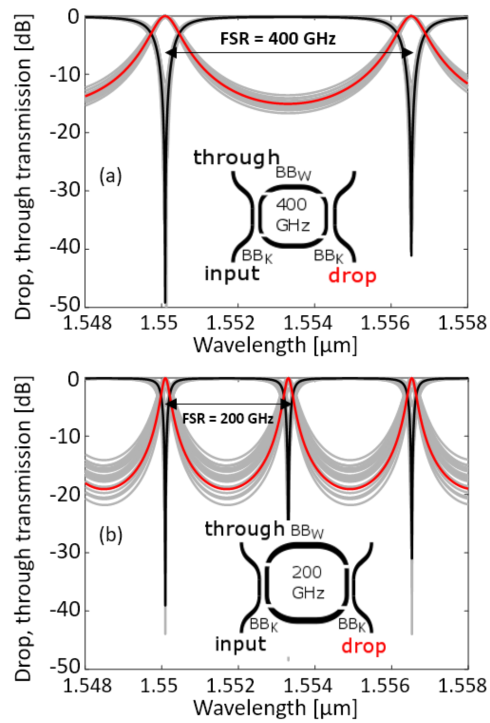

Fig. 1. Transfer functions of two different race track ring resonators (a) and (b) at drop (red) and through (black) ports. The thin grey lines show the effect of fabrication uncertainties on the waveguide widths and coupling coefficients.

III. Numerical Examples

As an example, the parametric stochastic model of a waveguide ($\mathrm{BB_W}$) and of a directional coupler ($\mathrm{BB_K}$) are here computed and stored by considering the effective refractive index and the coupling coefficient as uncertain parameters, respectively. The $\mathrm{BB_W}$ model is parametric with respect to waveguide length, wavelength, mean and standard deviation of the effective index n_{eff}. The $\mathrm{BB_K}$ model is parametric with respect to mean and standard deviation of coupling coefficient K. For both building blocks, an order of expansion P = 2 is considered. The uncertainties are considered as independent and Gaussian-distributed random variables and the corresponding basis functions are Hermite polynomials. In order to demonstrate the potential of the proposed approach, two different photonic circuits based on the same elementary building blocks $\mathrm{BB_W}$ and $\mathrm{BB_K}$ are considered: a racetrack ring resonator and a third-order Vernier coupled ring resonator filter. The complex frequency response (transfer function) of the photonic devices is considered as the stochastic process. The results obtained by parametric BB-gPC are compared with Monte Carlo analysis on 10^4 samples.

A. Racetrack Ring Resonator

To demonstrate that the building blocks are truly parametric and inherently stochastic we start with considering two racetrack ring resonators with different characteristics and uncertainties, the schematic being in the inset of Fig. 1(a) and 1(b). The ring considered in Fig. 1(a) has FSR = 400 GHz, mean effective index $\mathrm{n_{eff,a}}$ = 2.2315 and mean coupling coefficient $\mathrm{K_a}$ = 0.3 for both couplers. For simplicity and without loss of generality the group index is assumed equal to the effective index. The standard deviation of $\mathrm{n_{eff,a}}$ and $\mathrm{K_a}$ is $\sigma_{\mathrm{n_{eff,a}}} = 4\times10^{-5}$ and $\sigma_{\mathrm{K_a}}$ = 0.03, respectively. The ring in Fig. 1(b) has the same mean effective index $\mathrm{n_{eff,b}}$ = 2.2315 but FSR = 200 GHz and mean coupling coefficient $\mathrm{K_b}$ of both couplers equal to 0.2. The standard deviation of $\mathrm{n_{eff,b}}$ and $\mathrm{K_b}$ is also changed to $\sigma_{\mathrm{n_{eff,b}}} = 2\times10^{-5}$ and $\sigma_{\mathrm{K_a}}$ = 0.06, respectively. Figure 1 shows, in addition to the nominal responses at drop and through ports (red and black solid lines, respectively), several examples of spectral transfer functions of the two racetrack ring resonators at the drop and through ports (grey lines) obtained by classical Monte Carlo analysis with aligned resonances. It can be clearly seen that the transfer function of the original nominal design (bold lines) is largely affected even by the small considered uncertainties with fluctuations in both the pass-band and the in-band isolation.

For both racetrack ring resonators $\mathrm{BB_W}$ and $\mathrm{BB_K}$ are considered independent of each other, therefore, the number of random variables is $N = 3$ (see insets of Fig. 1). The augmented scattering matrices of $\mathrm{BB_W}$ and $\mathrm{BB_K}$ are combined and the augmented matrix description of the whole circuit is readily obtained with only one simulation. As mentioned, the first row or column of the computed overall augmented scattering matrix $\mathrm{S_T}$ contains the gPC coefficients which are used to compute the circuit statistical behaviour. Figures 2(a) and 2(b) show the mean of the absolute value and standard deviation of the transfer function for both racetrack ring resonators at

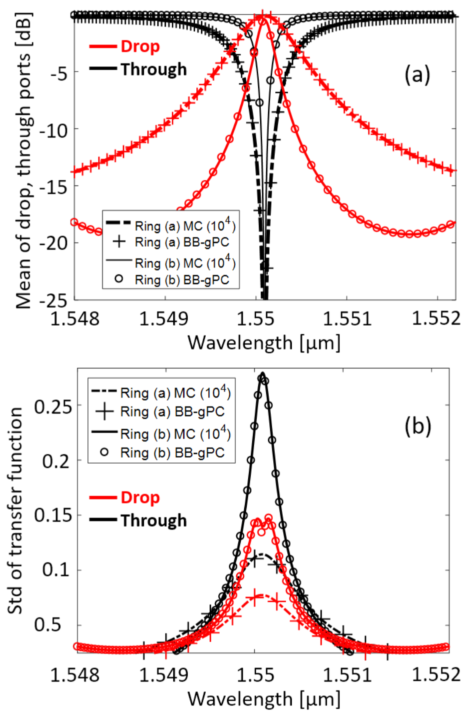

Fig. 2. Comparison between (a) the mean and (b) the standard deviation of the transfer function of drop (red) and through (black) ports of the racetrack ring resonator obtained with parametric BB-gPC and MC analysis.

drop (red) and through (black) ports, respectively. Dash-dot line (MC analysis) and plus marker (BB-gPC) represent the result of the ring in Fig. 1(a) while solid line (MC analysis) and circle marker (BB-gPC) represent the result of the ring in Fig. 1(b). The proposed parametric BB-gPC technique is in excellent agreement compared with the classical MC analysis in computing mean and standard deviation for both racetrack ring resonators and shows the validity of the approach, that consider the building blocks parametric in terms of design variables and statistical parameters. The direct MC analysis took about 1 hour, while the proposed technique took around 12 seconds to build the parametric augmented model, to retrieve gPC approximation of the entire circuit and to run 10^4 MC samples analysis (which might be needed to obtain high order moments).

B. Vernier Coupled Ring Resonator Filter

To further demonstrate the reliability of the method, we used the same elementary building blocks $\mathrm{BB_W}$ and $\mathrm{BB_K}$ to investigate a third order Vernier coupled ring resonator filter, schematically illustrated in Fig. 3(a), consisting of three rings and four couplers.

The Vernier operation is usually employed to extend the FSR by arranging ring resonators with unequal radii (i.e $\mathrm{FSR_1} \neq \mathrm{FSR_2}$). The overall FSR is equal to $N * FSR_1 = M * FSR_2$ where N and M are the number of rings with $\mathrm{FSR_1}$ and $\mathrm{FSR_2}$, respectively. The filter is designed according to the synthesis technique described in reference [28], [29]. With a nominal bandwidth BW_0 = 28.5 GHz, the resulting nominal

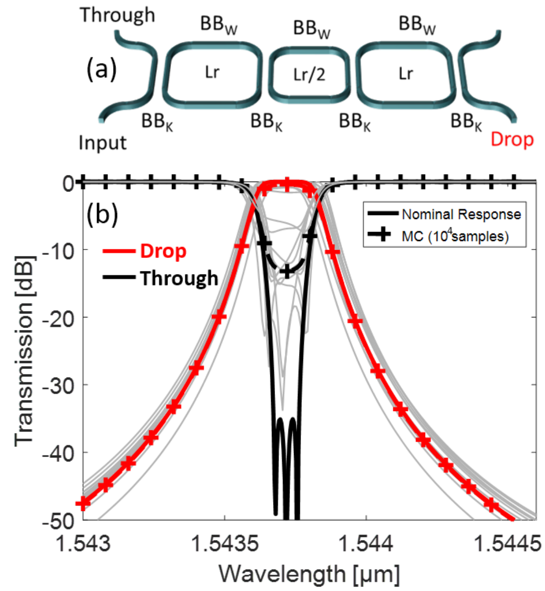

Fig. 3. (a) Schematic of third order Vernier coupled ring resonator filter (b) Nominal response of the filter compared with mean response obtain through MC technique using 10^4 samples. Thin grey lines (few MC samples) shows the effect of fabrication uncertainties on the filter response.

coupling coefficients for the four directional couplers are $\mathrm{K_1} = \mathrm{K_4}$ = 0.337 and $\mathrm{K_2} = \mathrm{K_3}$ = 0.12, providing an in-band isolation larger than 40 dB. The first and third ring have a length of 336.2 μm which is twice that of the second ring and corresponds to FSR = 800 GHz. All three rings have the same nominal effective refractive index $\mathrm{n_{eff,i}}$ = 2.2315 (i= 1 - 3). The nominal response of the filter is shown in Fig. 3(b) (solid red and black lines). In the stochastic analysis, the $\mathrm{n_{eff}}$, i and the $\mathrm{K_i}$ are assumed as independent normally distributed random variables with standard deviation $\sigma_{n_{eff,i}} = 2 \times 10^{-5}$ and $\sigma_{K,i} = 0.03$, respectively, and mean values corresponding to nominal design values. In addition to the nominal response Fig.3(b) also reports mean (dash lines with plus marker) and several spectral transfer function (thin grey line) obtained with classical Monte Carlo technique using 10^4 samples. For the given design variables and statistical parameters, the scattering matrices of stochastic building blocks ($\mathrm{BB_W}$ and $\mathrm{BB_K}$) are combined to obtain the augmented matrix description of the whole circuit and the gPC approximation in the form of Eq. (5).

Results relative to the Vernier ring filter obtained both with classical Monte Carlo method and with the proposed parametric BB-gPC method are shown in Fig. 4. Solid lines refer to Monte Carlo while markers report the result obtained by BB-gPC. The comparison shows a very good agreement. Figs. 4(a) and 4(b) show, respectively, the mean of the absolute value and standard deviation of transfer function at drop (red) and through (black) ports. It is worth to note that the mean transfer function differs from the nominal response, especially for the in-band rejection and the out of band spurious peak, as clearly indicated by the large standard deviation of Fig. 4(b) around these wavelengths. For the Vernier coupled ring resonator filter, the Monte Carlo analysis took about 1.5 hour for 10^4

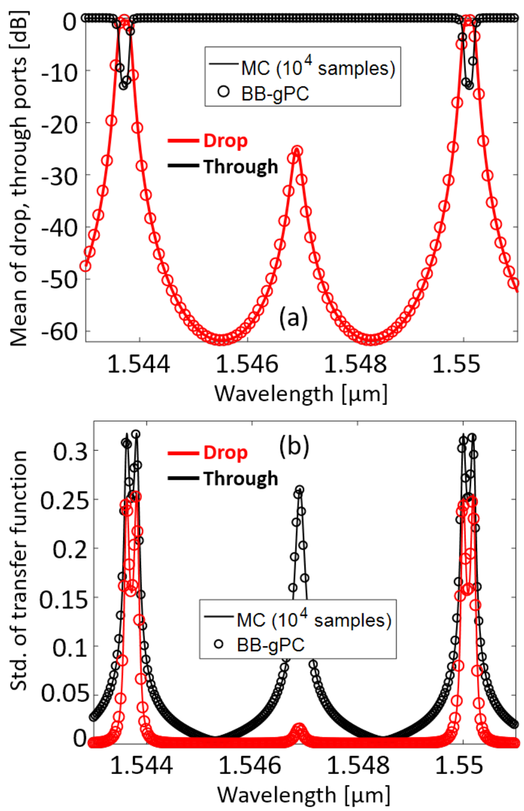

Fig. 4. Comparison of (a) the mean of the absolute value and (b) the standard deviation of the transfer function of drop (red) and through (black) ports of the Vernier filter obtained using MC and parametric BB-gPC techniques.

samples while the proposed technique took about 24 seconds to build the augmented model of the circuit, to retrieve the gPC coefficient of the entire circuit (combining scattering matrices) and to run 10^4 MC analysis on the gPC approximation (5). Hence the proposed technique offers a greater efficiency with respect to Monte Carlo analysis achieving a speed up factor of $\times$ 225. The advantage in terms of computational effort increases with the circuit dimension. Concerning the range of the parameters of the parametric stochastic model of building blocks, there is no particular restriction as long as gPC approximation is valid and applicable. For example, for the case of the lossless waveguide detailed in Appendix, the parameters L_g and $\sigma_{n_{eff}}$ appear as product in Eq. (7). When this product grows so does the variability of the BB response and higher order polynomials could be necessary to accurately represent this variability.

A remarkable advantage of the parametric BB-gPC technique is that the probability density function of any quantity of interest can be obtained by inexpensive Monte Carlo sampling of the circuit approximation (5). Figure 5(a) shows the probability density function (PDF) of the intensity at the drop (red) and through (black) ports of the filter at the centre wavelength 1.5437 μm. Figure 5(b) shows the probability density function of the 3-dB bandwidth. For comparison, 10^4 iterative Monte Carlo simulations are performed sampling the variables $\mathrm{n_{eff,i}}$ and $\mathrm{K_i}$ according to their distribution and directly calculating each time the circuit response via circuit simulation. All the responses are then used to calculate the PDFs, which are shown in Fig. 5. The PDF of both transfer functions at drop and through ports of the ring filter are asymmetric. Note that the intensity at the through port suffers from a broader deviation when compared to drop port of the filter for the same process uncertainties. The distributions shown in Fig. 5(a) and 5(b) allow to estimate other key information such as the yield. For example, it results that 58.25 % (88.25 %) of the realizations have a bandwidth that differs less than $\pm$ 10 % ($\pm$ 20 %) from the nominal value as marked in Fig. 5(b). Similarly, 41.80 % of the filters guarantee an in-band rejection larger than -15 dB (see the shaded grey area Fig. 5(a)). Similar results can be obtained in a very simple way also for other filter characteristics such as the group delay response, the polarization dependence or even in the time domain as the eye aperture or the constellation distortion in optical communications systems [30].

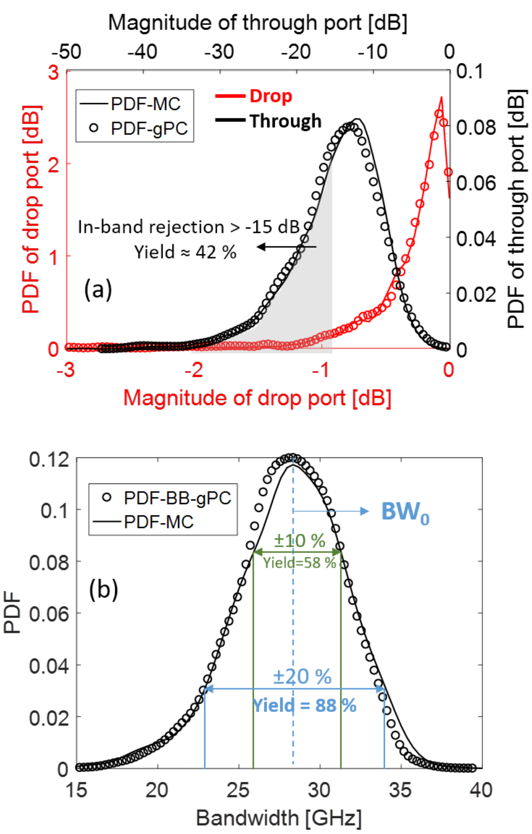

Fig. 5. (a) PDF of the intensity response at the drop (red) and through (black) ports of the filter at the center wavelength 1.5437 μm (b) PDF of the 3-dB bandwidth at the drop port of the filter.

IV. Conclusion

In this work, we have proposed a method to build a parametric stochastic augmented model of building blocks that allows a very efficient stochastic analysis of arbitrary photonic circuits. Although only in the limited case of waveguides and directional couplers, we demonstrated that once the augmented macro-model of the BBs are stored in the PDK, they can be directly used for the stochastic analysis of different photonic circuits with arbitrary design variables and statistical parameters. With only a single deterministic simulation run, the estimated statistical feature (e.g., mean, variance, probability density function, etc.) of the photonic circuits considered as examples could be obtained with an accuracy comparable to Monte Carlo and with a speed up factor of two orders of magnitude. This approach will play a critical role in building reliable PDK for future photonic foundries.

In addition to the above discussed advantages, the method proposed in this work can significantly support the generation of competitive PDK for photonic related production processes. It can help building a design environment where a designer can exploit already available tools (e.g., circuit simulators) to efficiently perform stochastic analysis or optimization of quantities such as the yield. The estimation of the statistical features of the circuit (such as mean, variance, yield) of the parameters (either physical or functional) can be used to identify the appropriate strategies (e.g., thermal tuning) to compensate such variations, and the cost for such compensation se.gtrategies (e.g., power consumption) can also be determined. It is further possible to exploit the framework to identify the most critical components of the circuit [3] which should either be carefully controlled by foundry or carefully optimized. This will help a designer to understand the effect of stochastic uncertainties on designed circuit and take better decisions based on the statistical information provided by framework to either continue for circuit fabrication step (if all the design specifications are met) or consider redesign or optimize the circuit‘s design to achieve better performance.

Besides the discussed advantages, the shortcoming of the proposed method is that the augmented macro-models of the BBs are large since scattering matrices must be scaled by a factor (M+1) for each port. However, these matrices are highly sparse with many entries equal to zero. The additional overhead required to handle these sparse augmented matrices, at least for the few tens of stochastic variables, is negligible compared to the time required to run many Monte Carlo simulations. The viability of the proposed approach for very large circuits with many stochastic variables and design parameters, as well as the possibility to include variable correlation will be treated in a future work.

Appendix
Preparation of stochastic parametric model of a single waveguide building block

In this appendix we provide the details of the preparation of the stochastic parametric model for a lossless waveguide (BB_W in the main text). The calculation of the model of other BBs follows an identical procedure.

For a waveguide building block, the wave relation can be written as

$$\vec{b}(\vec{x}) = \vec{S}(\vec{x})\vec{a}(\vec{x}), \tag{6}$$

where

$$\vec{S}(\vec{x}) = \begin{bmatrix} 0 & \mathrm{e}^{-\mathrm{j}\frac{2\pi}{\lambda}\mathrm{n_{eff}}\mathrm{L_g}} \\ \mathrm{e}^{-\mathrm{j}\frac{2\pi}{\lambda}\mathrm{n_{eff}}\mathrm{L_g}} & 0 \end{bmatrix}, \tag{7}$$

is the deterministic scattering matrix of a single-mode waveguide, L_g is its geometrical length, λ is the wavelength, n_{eff} is effective index, $\vec{x}$ represents the design variables (e.g., wavelength and geometrical length) and $\vec{a}$ and $\vec{b}$ are the complex amplitudes of the input and output waves. Effects such as waveguide attenuation, polarization coupling and back scattering are not considered in Eq. 7 but can be included straightforwardly. The wave relation under the effect of a vector of random variables $\vec{\xi}$ can be written as

$$\vec{b}(\vec{x},\vec{\xi}) = \vec{S}(\vec{x},\vec{\xi})\vec{a}(\vec{x},\vec{\xi}). \tag{8}$$

Considering the effective refractive as uncertain parameter, the vector of random parameters is the simple scalar ξ (normally distributed with zero mean and unitary standard deviation) that determines the effective index as $n_{eff} = [\mu_{neff}+\sigma_{neff}\xi]$ with mean and standard deviation $\mu_{n_{eff}}$ and $\sigma_{n_{eff}}$, respectively. The design variables are represented by the vector $\vec{x} = [L_g, \lambda, \mu_{n_{eff}}, \sigma_{n_{eff}}]$. The scattering matrix $\vec{S}(\vec{x},\vec{\xi})$ is given by

$$\vec{S}(\vec{x},\vec{\xi}) = \begin{bmatrix} 0 & \mathrm{e}^{-\mathrm{j}\frac{2\pi}{\lambda}(\mu_{\mathrm{neff}}+\sigma_{\mathrm{neff}}\xi)\mathrm{L_g}} \\ \mathrm{e}^{-\mathrm{j}\frac{2\pi}{\lambda}(\mu_{\mathrm{neff}}+\sigma_{\mathrm{neff}}\xi)\mathrm{L_g}} & 0 \end{bmatrix}. \tag{9}$$

By applying the gPC method as described in section II with order of expansion P = 2 and N = 1 random variables, each element of scattering matrix (9) can be written as

$$\begin{aligned} b_0\phi_0 + b_1\phi_1 + b_2\phi_2 = {} & S_0(\vec{x})a_0\phi_0\phi_0 + S_0(\vec{x})a_1\phi_0\phi_1 \\ & + S_0(\vec{x})a_2\phi_0\phi_2 + S_1(\vec{x})a_0\phi_1\phi_0 \\ & + S_1(\vec{x})a_1\phi_1\phi_1 + S_1(\vec{x})a_2\phi_1\phi_2 \\ & + S_2(\vec{x})a_0\phi_2\phi_0 + S_2(\vec{x})a_1\phi_2\phi_1 \\ & + S_2(\vec{x})a_2\phi_2\phi_2. \end{aligned} \tag{10}$$

For the sake of clarity, the dependence of the orthonormal polynomial ϕ_i on the random vector $\vec{\xi}$ is omitted. In Eq. (10), $S_i(\vec{x})$ are the parameter-dependent gPC coefficients, a_i and b_i are the gPC coefficients of input and output waves, respectively. Here we considered the n_{eff} as a normally distributed random variable therefore the orthonormal polynomials are the Hermite polynomials $\phi_0(\boldsymbol{\xi}) = 1$,$\phi_1(\boldsymbol{\xi}) = \xi$ and $\phi_2(\boldsymbol{\xi}) = (\xi^2-1)/\sqrt{2}$. Using Eq. (3), gPC coefficients $S_i(\vec{x})$ for the two off-diagonal elements of the scattering matrix (9) can be analytically calculated as,

$$
\begin{aligned}
S_0(\vec{\boldsymbol{x}}) &= \int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{j}\frac{2\pi}{\lambda}(\mu_{\mathrm{neff}}+\sigma_{\mathrm{neff}}\xi)\mathrm{L_g}} 1 \frac{\mathrm{e}^{\frac{-\xi^2}{2}}}{\sqrt{2\pi}} d\xi \\
&= \mathrm{e}^{-\frac{2\pi L_g^2 \sigma_{neff}^2}{\lambda^2}} \mathrm{e}^{-j\frac{2\pi L_g \mu_{neff}}{\lambda}}, \\
S_1(\vec{\boldsymbol{x}}) &= \int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{j}\frac{2\pi}{\lambda}(\mu_{\mathrm{neff}}+\sigma_{\mathrm{neff}}\xi)\mathrm{L_g}} \xi \frac{\mathrm{e}^{\frac{-\xi^2}{2}}}{\sqrt{2\pi}} d\xi \\
&= j\frac{2\pi L_g \sigma_{neff}}{\lambda} \mathrm{e}^{-\frac{2\pi L_g^2 \sigma_{neff}^2}{\lambda^2}} \mathrm{e}^{-j\frac{2\pi L_g \mu_{neff}}{\lambda}}, \\
S_2(\vec{\boldsymbol{x}}) &= \int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{j}\frac{2\pi}{\lambda}(\mu_{\mathrm{neff}}+\sigma_{\mathrm{neff}}\mathrm{L_g})} \frac{\xi^2-1}{\sqrt{2}} \frac{\mathrm{e}^{\frac{-\xi^2}{2}}}{\sqrt{2\pi}} d\xi \\
&= -\frac{2\sqrt{2}\pi^2 L_g^2 \sigma_{neff}^2}{\lambda^2} \mathrm{e}^{-\frac{2\pi L_g^2 \sigma_{neff}^2}{\lambda^2}} \mathrm{e}^{-j\frac{2\pi L_g \mu_{neff}}{\lambda}}.
\end{aligned} \tag{11}
$$

Note that the gPC coefficients $S_i(\vec{\boldsymbol{x}})$ are parametric with respect to L_g, λ, μ_{neff} and σ_{neff}. It is important to mention here that the integral of coefficients S_0, S_1 and S_2 needs to be evaluated only once and then stored. In case of more complex scatter coefficients that do not allow an analytical solution, integrals in the form of (11) can be evaluated numerically. Once the gPC coefficients are known, a classical Galerkin projection technique is used to obtain the parametric augmented scattering matrix (S_{PC}) of the waveguide building block. By projecting Eq. (10) on ϕ_0, ϕ_1 and ϕ_2 the augmented scattering matrix relating the expansion coefficients of the input to the coefficients of the output for the lossless waveguide results as .

$$
S_{\mathrm{PC}}(\vec{\boldsymbol{x}}) = \begin{bmatrix} S_0(\vec{\boldsymbol{x}}) & S_1(\vec{\boldsymbol{x}}) & S_2(\vec{\boldsymbol{x}}) \\ S_1(\vec{\boldsymbol{x}}) & S_0(\vec{\boldsymbol{x}})+\sqrt{2}S_2(\vec{\boldsymbol{x}}) & \sqrt{2}S_1(\vec{\boldsymbol{x}}) \\ S_2(\vec{\boldsymbol{x}}) & \sqrt{2}S_1(\vec{\boldsymbol{x}}) & S_0(\vec{\boldsymbol{x}})+2\sqrt{2}S_2(\vec{\boldsymbol{x}}) \end{bmatrix}. \tag{12}
$$

Equation 12 (whose generalized formalism is provided in reference [15]) describes the "parametric augmented model" of the BB, which depends on the considered parameters.

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