Analysis of the Influence of Roughness on the Propagation Constant of a Waveguide via Two Sparse Stochastic Methods

Ruben Waeytens, Dries Bosman, Martijn Huynen, Michiel Gossye, Hendrik Rogier, Dries Vande Ginste
Electromagnetics Group/IDLab, Department of Information Technology, Ghent University/imec, Gent, Belgium
Dries.VandeGinste@UGent.be

***Abstract*—The aim of this contribution is to study the effect of roughness on the propagation constant in interconnect structures. For this purpose, a stochastic framework is constructed around a full-wave electromagnetic field solver. To reduce the number of repeated calls to the full-wave simulator, two sparse stochastic techniques have been implemented and tested. A balance between calculation time and accuracy is sought for and found, which is demonstrated for a rough rectangular waveguide.**

***Index Terms*—Interconnect structures, line edge roughness, stochastic testing, sparse polynomial chaos**

I. INTRODUCTION

The need for smaller and faster electronics imposes serious challenges to their design, as previously negligible phenomena now influence their performance. One such example is line edge roughness (LER) [1], where the edges of electronic structures have a random, rough profile. This can be induced on purpose for improved adhesion or unintentionally by the nature of the production process. No matter its origin, the ever-increasing skin effect, pushing the current towards the edges of a conductor, only reinforces the influence of the LER, necessitating a rigorous study. A full-wave approach imposes itself to capture all emerging phenomena, entailing computational challenges. Full-wave electromagnetic simulations tend to be very time-consuming, while stochastic methods typically demand repeated runs of the electromagnetic field solver.

In this contribution, we investigate two stochastic methods to model the influence of roughness on the propagation constant of a waveguide. To keep the computational burden as small as possible, whilst still accurately capturing the relevant features, the two stochastics methods are sparse. More specifically, a novel sparse grid version of the well-known Stochastic Testing (ST), originally proposed by Zheng Zhang *et al.* in 2013 [2], is constructed and the sparse Polynomial Chaos (SPC) method, proposed by Blatman and Sudret in 2009 [3], is adapted to our waveguide problem. Both stochastic approaches require (a few) calls to a full-wave simulator, which in this contribution is a finite-element method (FEM) based solver. The obtained stochastic framework is applied to the variability analysis of the TE_{10} mode's propagation constant of a rectangular waveguide. The validation of the methods is provided by means of comparison with a brute-force Monte Carlo (MC) analysis.

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II. DETERMINISTIC PROBLEM AND FULL-WAVE SOLVER

We start from Maxwell's curl equations and assume, based on the longitudinal invariance encountered in waveguides (e.g., Fig. 1), a z-dependency of $e^{-j\beta z}$ for the electromagnetic fields, where the z-axis is the direction of invariance and β the propagation constant of the mode. A finite-element method (FEM) is employed to solve Maxwell's equations numerically. Approximating the electric field in the domain Ω by an appropriate set of hierarchical vector basis functions and applying a Galerkin weighting procedure eventually yields a quadratic eigenvalue problem

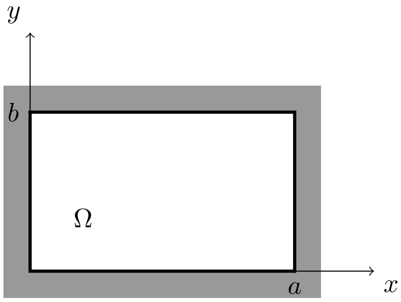

Fig. 1. An air-filled rectangular waveguide with perfectly conducting edges and dimensions a and b.

$$\left[\bar{\bar{M}}\beta^2 + \bar{\bar{C}}\beta + \bar{\bar{K}}\right]\bar{v} = 0. \tag{1}$$

The expressions for the matrices $\bar{\bar{M}}$, $\bar{\bar{C}}$, and $\bar{\bar{K}}$ are not detailed, as they are readily derived from the standard FEM procedure. Solving (1) yields the propagation constants β for the given geometry (and also the corresponding eigenvector $\bar{v}$).

III. RANDOM PROBLEM AND SPARSE TECHNIQUES

A. Roughness and Karhunen-Loève transform (KLT)

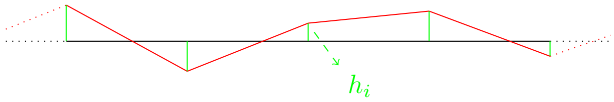

Fig. 2. Generation of a rough edge (red) by shifting k points along the nominal edge (black) over a random distance h_i ($i = 1, \ldots, k$) (green) along the outward pointing normal to that edge.

As shown in Fig. 2, we model the rough edge by a multivariate Gaussian distribution, similar as in [4]:

$$P(\bar{h}) = \frac{1}{\sqrt{| (2\pi)^k \bar{\bar{\Sigma}} |}} \exp(-\frac{1}{2}\bar{h}^T \bar{\bar{\Sigma}}^{-1} \bar{h}). \tag{2}$$

The $\bar{h}$-vector collects the deviations of k points on the edge $\partial\Omega$, measured along the outward pointing normal to the edge. $\bar{\bar{\Sigma}}$ is the correlation matrix, for which a Gaussian relationship on the distance between two points, measured along the edge, is chosen:

$$\bar{\bar{\Sigma}}_{ij} = \sigma_r^2 \exp\left(-\frac{|| \vec{r}_i - \vec{r}_j ||^2_{\partial\Omega}}{L_c^2}\right). \tag{3}$$

The parameter σ_r determines by how much points on the edge can deviate from their nominal position, while the correlation length, L_c, is a measure for how much the heights of neighbouring nodes depend on each other. The Karhunen-Loève transform (KLT) approximates the distribution of $\bar{h}$ by

$$\bar{h}(\bar{\xi}) \approx \bar{\bar{V}}\, \bar{\bar{\Lambda}}^{1/2}_{N_{\text{RV}}}\, \bar{\xi}, \tag{4}$$

where $\bar{\xi}$ contains a set of N_{RV} stochastically independent standard normal random variables (RVs). $\bar{\bar{\Lambda}}_{N_{\text{RV}}}$ has on its diagonal the first N_{RV} eigenvalues, λ_n, of $\bar{\bar{\Sigma}}$, in descending order. The columns of $\bar{\bar{V}}$ are the corresponding eigenvectors. A measure for the fraction of variability that is captured by this approximation is given by:

$$\Theta = \frac{\sum_{n=1}^{N_{\text{RV}}} \lambda_n}{\sum_{n=1}^{k} \lambda_n}. \tag{5}$$

B. Polynomial chaos expansion (PCE)

A relationship between the rough edge and a set of RVs has been established by the KLT. The distribution of the propagation constant β will be provided through a spectral decomposition into a set of $P+1$ orthonormal polynomials, $\phi_i(\bar{\xi})$, given by:

$$\beta(\bar{\xi}) \approx \sum_{i=0}^{P} a_i \phi_i(\bar{\xi}). \tag{6}$$

The focus now shifts towards determining the expansion coefficients a_i $(i = 0, \ldots, P)$ in this polynomial chaos expansion (PCE). These can be found in several ways.

C. Sparse grid Stochastic Testing (ST) method

A popular technique, able to deal with a large number of RVs, is stochastic testing (ST) [2]. Within ST, (6) is tested for a certain number of 'interesting' values of $\bar{\xi}_i \in \{\bar{\xi}_i\}_{\text{test}}$:

$$\begin{aligned} \beta(\bar{\xi}_j) &= \sum_{i=0}^{P} a_i \phi_i(\bar{\xi}_j) \quad \forall j \in \{0, ..., P\} \\ \Rightarrow \bar{\beta} &= \bar{\bar{\Phi}} \cdot \bar{a}, \end{aligned} \tag{7}$$

where the number of testing nodes is equal to the number of basis functions. Calculating the expansion coefficients is now equivalent to solving a matrix equation. The selection of 'interesting' testing nodes results from a node picking algorithm [2]. In this algorithm, first a tensor grid of nodes is constructed, based on quadrature rules. Then, nodes with a higher weight are favored and selected, in the meantime guaranteeing the well-conditionedness of (7).

When applying this approach to the analysis of roughness in waveguides, the standard ST procedure still entails too many realizations $\beta(\bar{\xi}_j)$, and thus calls to the full-wave FEM solver. The exponential growth in the number of function evaluations is due to the tensor product of univariate quadratures to integrate a multivariate function. Whereas in integration routines such a procedure is said to be second-order accurate, albeit component-wise, it turns out, however, that nodes can be omitted without sacrificing on accuracy. Removing these redundant nodes from the tensor grid, is the crux of so-called sparse grid techniques [5].

In this contribution, we apply a novel sparse grid ST algorithm, which is conceptually quite simple, yet effective. The procedure is similar to the one proposed by Gossye *et al.* [6] to analyze statistically spatially varying dielectric-property profiles. Starting from a sparse grid, we apply the rules of the standard ST algorithm to pick the interesting nodes, i.e., favoring nodes with a higher weight and guaranteeing that the matrix (7) remains well-conditioned. This reduces the number of calls to the FEM solver drastically, whilst maintaining accuracy, as demonstrated in Section IV.

D. Sparse Polynomial Chaos (SPC)

It can be shown that the standard ST and the sparse grid ST techniques boil down to the observation that not all basis functions $\phi_i(\bar{\xi})$ in the polynomial chaos expansion (PCE) (6) are equally relevant. Therefore, we will also compare our sparse grid ST technique with another sparse technique, i.e., sparse polynomial chaos (SPC). SPC is explored as a possible technique to exploit the aforementioned observation to the fullest. The SPC algorithm further reduces the required number of full-wave runs, while extracting the most important terms in the expansion. Several algorithms, attempting to construct a sparse polynomial chaos expansion, exist in literature. In this contribution, the algorithm described by Blatman and Sudret [3] is adapted to our needs. The basic idea is to perform a fixed number of runs once and for all. Afterwards, an adaptive sparse set of basis functions is selected to construct a PCE. The decision whether or not to add or remove a basis function to this sparse set, is based on solving subsequent overdetermined systems. After several iterations of adding and removing basis functions to a temporary set of basis functions, a sparse set of relevant basis functions is retained.

IV. APPLICATION TO A ROUGH RECTANGULAR WAVEGUIDE

We now apply the two sparse stochastic techniques to the rectangular waveguide of Fig. 1, where we focus on the variability of the TE_{10} lowest-order propagation constant, further denoted β. As values for a and b, we choose $2l$ and $1l$, respectively, with l an arbitrary length unit. The free-space wavenumber is given by $k_0 = 10l^{-1}$, leading to a discretization of Ω into 1094 triangles. A second-order expansion leads to a finite-element linear system in 5745 unknowns. The roughness profile is generated by varying $k = 82$ uniformly spaced nodes along the edge $\partial\Omega$. Additionally, the following constants were assigned for the KLT: $L_c = 0.5l$, $\sigma_r = 0.01l$, and $\Theta = 0.85$, yielding $N_{\text{RV}} = 8$ RVs collected in the vector $\bar{\xi}$.

We compare the results of the two sparse algorithms to a standard Monte Carlo (MC) approach. MC is here considered as the golden standard, given its guaranteed albeit slow $1/\sqrt{N_{\text{MC}}}$-convergence, with N_{MC} the number of samples drawn. For the particular example, it is observed that for $N_{\text{MC}} = 50000$, the average of the propagation constant β has converged up to a relative error of $6 \cdot 10^{-6}$ and its standard deviation up to a relative error of $2 \cdot 10^{-2}$. Specifically, the following values are obtained: $\mu_\beta = \left(9.87589 \pm 6 \cdot 10^{-5}\right) l^{-1}$ and $\sigma_\beta = \left(0.00192 \pm 4 \cdot 10^{-5}\right) l^{-1}$.

Employing the novel advocated sparse grid ST technique, combined with a PCE, demands only 45 runs of the full-wave solver. This is a speed-up by a factor of more than 1000 compared to the brute force MC method. Note that the time needed for node picking is negligible compared to one full-wave simulation. The sparse grid ST predicts $\mu_\beta = 9.87590\, l^{-1}$ and $\sigma_\beta = 0.00196\, l^{-1}$. Hence, both values are within the bounds determined by the MC simulation. Furthermore, Fig. 3 compares the distribution of β obtained by the MC method and sparse grid ST. To construct the distribution by means of sparse grid ST, we sample our surrogate model (6) through a MC simulation, which only requires simple arithmetic. Thus, constructing such a distribution is also expedited tremendously. To quantify the good correspondence, we also performed a Cramèr-von Mises (CvM) test [7], which delivers a p-value of 0.18. This value shows that both datasets indeed originate from the same distribution.

We also apply the aforementioned SPC algorithm to the rough rectangular waveguide. For this simulation, the number of full-wave calculations could be further reduced from 45 to 30, cutting off a third from the calculation time. The computational cost of the iterative procedure to select the pertinent basis functions for the PCE is negligible compared to one full-wave run. SPC predicts $\mu_\beta = 9.87589\, l^{-1}$ and $\sigma_\beta = 0.00196\, l^{-1}$, which is again within the bounds set by the MC simulation. These results are also summarized in Table I. Moreover, the obtained distribution for β is added to the plot in Fig. 3. This distribution predicted by SPC is again plotted by employing the corresponding PCE as a surrogate model. A good qualitative resemblance is clearly visible and a CvM test was carried out as well, resulting in a p-value of 0.1241. It is therefore safe to assume that both the MC and SPC simulation also originate from the same distribution.

V. CONCLUSIONS

The goal of this contribution was to evaluate the influence of roughness on the propagation characteristics of interconnect structures. Given the computational burden of a single full-wave simulation, two sparse stochastic methods were implemented, in conjunction with a finite-elements full-wave solver. The methods were applied to the computation of the TE_{10} propagation constant of a rectangular waveguide. It was shown that the methods reduce the computational burden, whilst still accurately predicting the influence of the roughness profile.

In future research, both sparse techniques will be further explored and improved, pushing the number of RVs to the limit. Other roughness profiles and waveguide structures, including, e.g., lossy microstrip interconnects, will be investigated too.

	$\mu_\beta\ [l^{-1}]$	$\sigma_\beta\ [l^{-1}]$
MC	$9.87589 \pm 6 \cdot 10^{-5}$	$0.00192 \pm 4 \cdot 10^{-5}$
ST	9.87590	0.00196
SPCE	9.87589	0.00196

TABLE I

STATISTICS OF THE TE_{10} PROPAGATION CONSTANT β, OBTAINED BY MC SIMULATION, SPARSE GRID ST AND SPC.

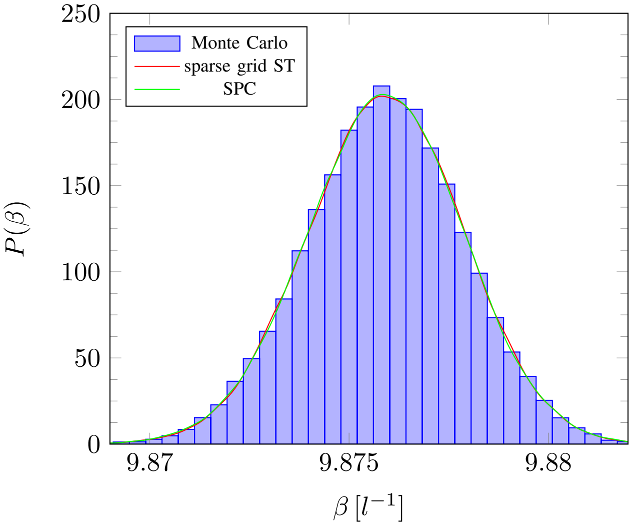

Fig. 3. Comparison of the distribution of the TE_{10} propagation constant β of a rectangular waveguide, obtained by MC, sparse grid ST and SPC.

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