Abstract—The author deals in the paper with simulations of stochastic EM fields dedicated especially to 5G frequency band for which FDTD calculation domain becomes relatively large. The PCE-based FDTD is considered in the paper. The author presents an approach for a relatively very fast calculation of PCE coefficients for the case when multiple FDTD simulations of a considered wireless scenario are required. This is the case when more than one set of probability densities of the scenario parameters need to be considered, e.g. different nominal (mean) positions of antenna and/or obstacles. The author proposes also a concept for an improvement of a PCE-FDTD code which provides a substantial decrease of a simulation time.

Index Terms — Stochastic simulation; polynomial chaos expansion (PCE); Finite-difference time-domain (FDTD).

I. INTRODUCTION

The author deals in the paper with FDTD simulations of stochastic electromagnetic fields in a wireless propagation channel for a 5G frequency band. The author bases on polynomial chaos expansion (PCE) [1] dedicated to FDTD. Consequently the uncertainties of geometrical (e.g. position of an antenna, size and/or position of an obstacle) and physical parameters (e.g. permittivity, conductivity of an obstacle) of a simulated scenario are modeled by random variables that are described by their probability densities (PDFs). In the area of stochastic EM fields analysis the most commonly used PDFs are Gaussian, Beta and Uniform distributions, while the latter is a special case of a Beta distribution.

The PCE together with the collocation method or a regression method have been used effectively in the area of stochastic EM fields analysis [2-5]. In PCE the stochastic EM field function is expanded using polynomials that are orthogonal with respect to considered PDFs of random parameters of a simulation scenario. The PCE coefficients are used then to find stochastic moments, PDF and cumulative distribution function of a considered stochastic EM field function. The two PCE-FDTD approaches was introduced in literature. The first one is non-intrusive approach which implements many full FDTD simulations for different realizations of random variables at the collocation points, e.g. [3]. The second approach is an intrusive approach which requires to reconfigure the update equations in the FDTD code, e.g. [4, 5]. Then only one full FDTD simulation is necessary to derive the desired PCE coefficients. The ideas and results presented by the author in the paper correspond to the latter approach.

Let us assume now that for a given simulation scenario we need to perform a stochastic EM field analysis for many sets of PDFs of a scenario parameters, e.g. when the nominal (mean) position of an antenna need to be updated. All of the nowadays PCE approaches require to run a new PCE-FDTD simulation for every change of joint PDF of a simulation scenario parameters. This process is very time-consuming especially for the case of full-wave simulations. The author proposes an approach that enables to solve the described problem. In particular this approach enables a relatively fast and accurate analysis of the:

- variations of stochastic EM fields distributions in a propagation channel with respect to antenna parameters changes (e.g. nominal position and its uncertainty) in predefined limits.
- sensitivity that regards to optimization of nominal parameters of antennas.
- variations of stochastic EM fields distributions with respect to changes of geometry and physical simulation scenario parameters in predefined limits.
- influence of PDF of a plane wave amplitude on indoor EM fields distributions for the case of an outdoor to indoor propagation scenario.

The author uses the so-called primary simulation and universal expansion coefficients (UECs). The UECs are analytical functions of parameters of PDFs (e.g. mean, standard deviation) of random variables of a considered simulation scenario. The UECs rely on information collected from the primary simulation what is described in Section III of the paper. In Section II of the paper the author presents briefly methodology for implementing the geometry uncertainty in a FDTD lattice for EM wave propagation. In Section IV the author gives a programming concept that rapidly
decreases the time of an execution of a PCE-FDTD algorithm. This is especially very beneficial for 5G frequency band for which the calculation volume is relatively large and the time step is very short to keep the stability condition of a FDTD algorithm. The proposed concept provides the speedup on the order of 10-20. The author presents a simulation example in section V and summarize the paper in Section VI.

II. GEOMETRY UNCERTAINTY FOR STUDY OF EM WAVE PROPAGATION

In this Section the author uses the concept of Yee lattice deformation described in [5] for representing the geometry uncertainty in a FDTD simulation of EM wave propagation. Two kinds of EM wave sources for 2D scenarios are considered in Fig. 1. The left figure shows a rectilinear Yee lattice deformation for including uncertainty in a point source position. This uncertainty is represented by random variables \( \xi_1 \) and \( \xi_2 \) in \( x \) and \( y \) dimension, respectively. The size of a distorted sector is \( (n_{1x}+n_{2x})\times(n_{1y}+n_{2y}) \). Figure 1b) shows one realization of an obstacle rotation with respect to plane wave incidence using curvilinear Yee lattice cells.

For the sake of clarity only the vertical domain is considered in Fig. 3. This domain is divided into 4 segments having \( n_1 \), \( n_2 \), \( n_3 \) and \( n_4 \) rows with cells of height \( \Delta y_{14}(\xi_1) \), \( \Delta y_{21}(\xi_1,\xi_2) \), \( \Delta y_{32}(\xi_1,\xi_2) \) and \( \Delta y_{43}(\xi_1) \), respectively. The nominal realization of this division is shown in Fig. 3. There are two uncertainties represented in Fig. 3. The first is the uncertainty of obstacle position which is modeled by \( \xi_1 \) while the second is the uncertainty of the source position which is modeled by \( \xi_2 \). The nominal vertical sizes of Yee lattice cells for the consecutive sectors in Fig. 3 are: \( \Delta y_{14}(0) \), \( \Delta y_{21}(0,0) \), \( \Delta y_{32}(0,0) \), \( \Delta y_{43}(0) \). Then the random functions of these sizes can be written as follows:

\[
\Delta y_{1/4}(\xi_1) = \Delta y_{1/4}(0) \pm \frac{\xi_1}{n_{1/4}}
\]

\[
\Delta y_{2/3}(\xi_1,\xi_2) = \Delta y_{2/3}(0,0) \pm \frac{\xi_2 - \xi_1}{n_{2/3}}
\]

When for at least for one of realisations of \( \xi_1 \) and \( \xi_2 \) the dashed blue lines in Fig. 3 interleave or coincide then curvilinear Yee lattice cells must be applied [5].

III. THE NEW APPROACH TO PCE-FDTD SIMULATIONS

In PCE theory the considered EM field function, which depends on a vector of random variables \( \xi \) and can be named by \( Y(\xi) \), is expanded using orthogonal basis of multivariate polynomials with respect to joint PDF \( p(\xi) \). If we have \( N \) independent random variables this vector is \( \xi = [\xi_0, \xi_1, ..., \xi_N] \). The PCE of \( Y(\xi) \) can be formulated as follows:

\[
Y(\xi) = \sum_{p=0}^{P} \gamma_p \cdot \psi_p(\xi)
\]

where \( p \) is the number of \( p \)-th row in the multi-index array that follows the Askey scheme [1] and \( \gamma_p \) are the PCE coefficients. The multivariate orthogonal polynomials must fulfill the following orthogonality condition:

\[
\langle \psi_m(\xi), \psi_l(\xi) \rangle = \begin{cases} 0 & \text{if } m \neq l \\ \gamma_m & \text{if } m = l \end{cases}
\]

where \( \gamma_m \) is a normalisation factor [1] and:

\[
\langle \psi_m(\xi), \mu(\xi) \rangle = \int_{\Omega} \psi_m(\xi) \mu(\xi) d\xi
\]

where \( \Omega \) is the support of \( \xi \) while multivariate polynomial \( \mu(\xi) \) is the product of univariate polynomials, e.g. Hermite polynomials or a Jacobi polynomials depending on the PDF of a single random variable [1]. The stochastic moments of \( Y(\xi) \) are calculated using PCE coefficients of \( Y(\xi) \) [1]. In practical applications the expansion (3) is truncated to finite number, e.g. \( P+1 \) PCE coefficients.
The author assumes in the paper that FDTD simulation scenario have two dimensions and an electric field have only z-component. Under these assumptions, as an example, we can formulate the PCE of an electric field at time step \((n+1)\Delta t\) and Yee lattice cell number \(i, j\) with respect to random variables \(\xi\) as follows:

\[
E_{z, i,j}^{n+1} \approx \sum_{p=0}^{P} e_{i,j}^{n+1} \psi_p(\xi) \tag{6}
\]

In order to calculate \(P+1\) coefficients for an update equation (6) we can formulate the following matrix relation:

\[
E_{z, i,j}^{n+1} = E_{z, i,j}^{n} \cdot A_{(i,j)} + (H_y^{n+1/2,j} - H_y^{n+1/2,j}) \cdot B_{(i,j)} - (H_x^{n+1/2,j} - H_x^{n+1/2,j-1/2}) \cdot \Gamma_{(i,j)} \tag{7}
\]

where \(E_z, H_y, H_x\) are \((P+1)\)-element row-vectors and \(A, B\) and \(\Gamma\) are \((P+1)x(P+1)\) matrices, for which according to \([4, 5]\)

\[
A_{(i,j),p,q} = \left\{ \begin{array}{l} 2\varepsilon_{i,j}\sigma_{i,j}^{\Delta t} - \sigma_{i,j}^{\Delta t} \Delta t \psi_{i,j}^{p}(\xi) \psi_{i,j}^{q}(\xi) \\ 2\varepsilon_{i,j}\sigma_{i,j}^{\Delta t} + \sigma_{i,j}^{\Delta t} \Delta t \psi_{i,j}^{p}(\xi) \psi_{i,j}^{q}(\xi) \end{array} \right\} \psi_{i,j}^{p}(\xi)^T \tag{8}
\]

\[
B_{(i,j),p,q} = \left\{ \begin{array}{l} 2\Delta t \psi_{i,j}^{p}(\xi)^T \psi_{i,j}^{q}(\xi) \\ \psi_{i,j}^{p}(\xi)^T \psi_{i,j}^{q}(\xi) \end{array} \right\} \tag{9}
\]

\[
\Gamma_{(i,j),p,q} = \left\{ \begin{array}{l} 2\Delta t \psi_{i,j}^{p}(\xi)^T \psi_{i,j}^{q}(\xi) \\ \psi_{i,j}^{p}(\xi)^T \psi_{i,j}^{q}(\xi) \end{array} \right\} \tag{10}
\]

where \(\varepsilon\) and \(\sigma\) denote relative permittivity and conductivity for cell no. \(i, j\), respectively. These parameters can be also assumed as stochastic.

It should be noted that all the inner products in (8) - (10) for each Yee lattice cell can be calculated before running the PCE-FDTD algorithm. As a result of an execution of PCE-FDTD algorithm in the described form we obtain a PCE expansion of e.g. electric field for each spatial and time domain samples for a given set of PDFs of \(\xi\).

The PCE-FDTD simulation can be repeated for each change (update) of parameters of \(\xi\), e.g. nominal EM wave source position. However such operation is very time-consuming, especially for the case of 5G frequency band. As was stated in Section I the author propose an approach that enables to solve this problem. The approach have the following steps.

The first step is to perform the primary simulation during which the considered scenario is simulated for uniform PDFs with support \(\Omega\). The support \(\Omega\) have to comprise all supports \(\Omega^k\) \((k=1,2,3,\ldots)\) in (5) of \(k\)-th set of PDFs which is considered for a simulation scenario. Supports \(\Omega^k\) should be a-priori known by the simulation designer. The order of PCE expansion for support \(\Omega\) should be usually bigger than for support \(\Omega^k\), if \(\Omega_0\) is significantly larger than \(\Omega^k\). We can denote the order of PCE for support \(\Omega_0\) using letter \(Q\). The goal of the primary simulation is to obtain a primary approximation of e.g. (6) for support \(\Omega_0\) as follows.

\[
E_{z, i,j}^{n+1} = \sum_{q=0}^{Q} q_{i,j}^{n+1} \psi_q(\xi) \tag{11}
\]

After the approximation (11) is found for \(\Omega_0\) support, the analytical formulas for universal expansion coefficients (UECs) for all supports kept within \(\Omega_0\) can be derived. It can be shown that when univariate Jacobi polynomials used in the primary approximation are decomposed into Hermite polynomials a multivariate form of UEC can be written as follows.

\[
e_{i,j}^{n+1} = \frac{1}{\gamma_{p,q}} \sum_{\alpha=0}^{\gamma_{p,q}} \int_{\Omega} \frac{(h^{\alpha}_{\text{Gauss}})^{\gamma_{p,q} - 1}}{(h^{\alpha}_{\text{Beta}})^{\gamma_{p,q} - 1}} Q(p,q,p_{\alpha}) \sum_{\text{index } a} I_a \tag{12}
\]

When \(\xi_{\alpha}\) is a random variable having Gauss PDF:

\[
S_{p_{\alpha}q}(\xi_{\alpha}) = \left( \frac{h^{\alpha}_{\text{Gauss}}}{h^{\alpha}_{\text{Beta}}} \right)^{\gamma_{p,q}} \sum_{j=0}^{n} \int_{\Omega} \frac{(g^{\alpha}_{\text{Gauss}})^{\gamma_{p,q} - 1}}{(g^{\alpha}_{\text{Beta}})^{\gamma_{p,q} - 1}} Q(p,q,p_{\alpha}) \sum_{\text{index } a} I_a \tag{13}
\]

and when \(\xi_{\alpha}\) is a random variable having Beta PDF:

\[
S_{p_{\alpha}q}(\xi_{\alpha}) = \sum_{j=0}^{n} \frac{q_{\alpha}}{\gamma_{p,q}} H_{j}(h^{\alpha}_{\text{Beta}})(g^{\alpha}_{\text{Beta}})^{\gamma_{p,q} - 1} \tag{14}
\]

Interpretation and calculation of expressions \(h^{\alpha}_{\text{Gauss}}, g^{\alpha}_{\text{Beta}}, Q(p,q,p_{\alpha}), h^{\alpha}_{\text{Beta}}, g^{\alpha}_{\text{Beta}}\) and \(I_a\) can be deduced referring to formulas (10), (11), (15) in [6], (12), (13) (19 - 20) in [7], respectively. Indices \(p_{\alpha}\) and \(q_{\alpha}\) are the \(n\)-th elements of \(p\)-th and \(q\)-th row, respectively in a multi-index array that follows the Askey scheme [1]. It should be noted that (13) is a function of a mean and a standard deviation of a Gauss PDF and (14) is a function of \(\alpha, \beta\) parameters and support limits of a Beta PDF. The uniform PDF is a special case of a Beta PDF when \(\alpha = \beta = 0\). Having UECs in the form of simple analytical formulas the PCE coefficients for every set of random variables for which we need to test considered simulation scenario (having in mind that \(\Omega^k\) must subset of \(\Omega_0\)) can be calculated very fast. We need of course to spent some initial time to run a primary simulation to find (11).

IV. IMPROVEMENT OF A PCE-FDTD CODE

The author propose a programming concept for a PCE-FDTD algorithm which to the best knowledge of the author was not published before and which provides a speedup of PCE-FDTD simulation on the order of 10-20. The speedup is calculated as a division of a simulation time of a reference simulation by a time of simulation that uses the author’s concept. The reference
simulation includes the loop sequence for a spatial domain. The speedup was tested on a platform with single 17 family CPU. The new concept enables to apply e.g. update equation (7) for every spatial sample using one matrix operation scheme instead of a loop sequence. In order to do this the spatial samples are reorganized into a vector. If 2D case is considered the coordinates $j$, $i$ of a given spatial point are mapped into 1D indices $\text{dim}_y(i{-}1)+j$, $1 \leq i \leq \text{dim}_x$, $1 \leq j \leq \text{dim}_y$ where $\text{dim}_x$ and $\text{dim}_y$ are the maximum indices in $x$ and $y$ domain, respectively. For clarity of explanation it can be assumed that in a results 4-element 1D vector of indices is obtained $1 \leq d \leq 4$. It can be assumed also that PCE order is 2. Let us focus now on the first component of right side of (7) for the new spatial index:

$$E A_{i,n}^{0} = E_{i}^{n} \cdot A_{(i)}^{(n)}$$

(15)

In order to calculate the first PCE coefficient for each spatial index the following can be formulated:

$$E A_{i,n}^{0} = E_{i}^{n} \cdot A_{(i)}^{(n)}$$

(16)

The product in (16) is element-wise product, while:

$$E_{z}^{n}_{(i)} = E_{z}^{n}_{(i,1), i}$$

(17)

$$A_{(i)}^{(n)} = A_{(i,0), i}$$

(18)

When column-wise sum of (16) is performed the row-vector of first PCE coefficients of (15) is obtained. In order to find the rest of PCE coefficients (16) – (18) must corrected in the following way. Matrix (17) must be copied 3 times. The copies should be appended at the right side of (17). Then the 3 matrices analogous to (18) should be found for $p=1$ and $p=2$ and appended in the mentioned order at the right side of (18). Now the element-wise product, subsequent column-wise sum followed by reshaping of a row-vector into a matrix would give the PCE coefficients of (15) for all of the spatial points. It should be noted that this concept requires more memory resources than the approach implementing loop sequence for a spatial domain.

V. SIMULATION EXAMPLE

In this section the exemplary simulation scenario is presented. The spatial values corresponding to the nominal geometry of the simulation scenario are shown in Fig. 3. The geometry uncertainties are also indicated in Fig. 3. Three uncertainties are included in the simulation scenario. They are represented by random variables $\xi_1$, $\xi_2$ and $\xi_3$.

Fig. 3. The geometry of a 2D simulation scenario indicating the geometry uncertainties for upper window position (blue color) - $\xi_1$, EM wave source - $\xi_2$ and position of the door (black color) - $\xi_3$.

The first is the uncertainty of the upper window position, the second corresponds to the EM wave source position and the third to the door position. The associated "moveable" dashed blue lines introduced in Fig. 2 are also visible in Fig. 3. The cell sizing is also indicated in Fig. 3. The relative permittivity and conductivity of walls (green color), windows (blue color) and door (black color) are assumed to be deterministic. The relative permittivity of walls, windows and the door are 6, 5, and 3, respectively. The conductivity of walls is 2S/m and 0 for windows and the door. The stochastic attenuation of an amplitude of an electric field is considered. The observation points are distributed along the line defined within the $x$ limits $2.3 \leq x \leq 2.8$m and $y=6.25$m. Five different joint PDFs of random variables are considered for the simulation. The supports of the first and the third random variables are the same for all 5 joint PDFs: $-0.02m \leq \xi_1 \leq 0.02m$, $-0.05m \leq \xi_2 \leq 0.05m$. The support of the EM wave source position has the same width equal to 0.06m for all 5 cases however the nominal source position is different for each case. All of the random variables have a uniform PDF. The support for a primary simulation in (11) is $-0.1m \leq \xi_1 \leq 0.1m$, $-0.1m \leq \xi_2 \leq 0.1m$, $-0.2m \leq \xi_3 \leq 0.2m$. The value of $P$ in (6) is 8, while the value of $Q$ in (11) is 12 to obtain an accurate PCE expansions. The results of simulations are shown in Fig. 4 (the mean of electric field attenuation) and Fig. 5 (the standard deviation of an electric field attenuation). The reference results (one execution of PCE-FDTD code for each of 5 joint PDFs) are represented by the dashed and solid lines. The results obtained with the primary simulation and analytical UECs are indicated by the circle and asterisk graphs. For the sake of space saving issue only two set of PDFs are considered in Figs. 4-5. The nominal $y$ position of the EM wave source for the first example is 6.25m and for the second example 6.30m.
The frequency of an EM wave is 6GHz. Each PCE-FDTD simulation lasts 600 periods. At least 20 samples along a wavelength are calculated.

The results of simulation obtained with the UEC approach are in a very good agreement with the reference results in Figs. 4-5. The same type of agreement could be shown for the remaining 3 sets of PDFs what indicates the accuracy of the proposed UEC approach. The comparison of times consumed by simulations are presented in Table I. The title "No. of Sim." in Table I means the number of executed PCE-FDTD simulations. The results corresponding to the UEC approach are denoted by "UEC time" in Table I, which shows that only for the case of one and two PCE-FDTD simulations the reference method is faster than the proposed UEC approach.

VI. CONCLUSIONS

The UEC approach implementing the primary approximation are a good candidate for PCE-FDTD simulations of stochastic EM fields for the case when many joint PDFs of input random variables need to be considered (see Section I). The proposed approach provides accurate simulation results in a relatively short time what is indicated in Figs 4-5 and Table I. The programming concept introduced in Section IV enables a rapid decrease of PCE-FDTD simulation time. Its application lets to obtain the stochastic EM fields results for 5G frequency band for the case of 2D scenario in a reasonable time using single CPU cores. However simulation of 3D scenario requires the use GPU cores.

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