ABSTRACT

In this paper we present an efficient and fully error controlled algorithm for yield estimation and yield optimization. Yield estimation is used to quantify the impact of uncertainty in a manufacturing process. Since computational efficiency is one main issue in uncertainty quantification, we propose a hybrid method, where a large part of a Monte Carlo (MC) sample is evaluated with a surrogate model, and only a small subset of the sample is re-evaluated with a high fidelity finite element model. In order to determine this critical fraction of the sample, an adjoint error indicator is used for both the surrogate error and the finite element error. For yield optimization we propose an adaptive Newton-MC method. We reduce computational effort and control the MC error by adaptively increasing the sample size. The proposed method minimizes the impact of uncertainty by optimizing the yield. It allows to control the finite element error, surrogate error and MC error. At the same time it is much more efficient than standard MC approaches combined with standard Newton algorithms.

Keywords Yield Analysis, Failure Probability, Uncertainty quantification, Stochastic sparse grid collocation, Adaptivity, Monte Carlo, Stochastic optimizations

1 Introduction

There are many applications where uncertainty quantification and optimization under uncertainty is important. Uncertainty in the manufacturing process may lead to deviations in the design parameters, i.e. geometrical or material parameters, which may lead in turn to rejections due to malfunctioning. In this context, malfunctioning means that predefined performance feature specifications are not fulfilled. In order to quantify the impact of uncertainty we define the yield according to [1] as the percentage of functioning realizations in a manufacturing process. Thus, yield is mathematically equivalent to the concept of reliability and the relation between yield and failure probability is given in the form $\text{yield} = 1 - \text{failure probability}$. The topic of yield optimization is motivated by high frequency electromagnetics and circuit design.

In general, it is not possible to carry out yield calculations exactly. Hence, many algorithms have been introduced to this end and the Monte Carlo (MC) method is probably the most popular one [2]. The main challenge of yield estimation is its high computational cost, since it requires numerous evaluations of the underlying model. In practice, these models are often given by partial differential equations (PDE) of high complexity and can only be solved numerically, with the finite element method (FEM), for instance. Since each high fidelity evaluation with FEM itself may be computationally challenging, a standard MC analysis becomes rapidly prohibitive due to limits of computational and / or time resources. In this paper we present a hybrid approach for yield estimation combining the efficiency of stochastic collocation with the accuracy of MC for probability estimation. We then present an algorithm for yield maximization, based on a globalized Newton method.

The classical MC approach consists in sampling the original high fidelity model, i.e., the highly resolved random FE model. The efficiency of this approach is independent of the number of uncertain parameters and the method does not suffer from the “curse of dimensionality”. Still, the sample size required for accurate estimation can be quite large [3]. There is a lot of research on reducing the computational effort of failure probability or yield estimation. The common goal is to reduce the number of high fidelity evaluations. There are sampling-free methods such as the first order reliability method (FORM) or the second order reliability method (SORM). These methods determine the most probable
point, which is the closest point from the parameter domain origin to the separating surface between the failure region and the safe region, and employ approximations of the limit state function around this point \( \Phi \) \cite{4,5}. Investigations in the context of sampling have led to a sample size reduction, e.g., through importance sampling \cite{6} or subset simulation \cite{7,8}. Alternatively, or complementarily, the computational effort has been reduced for each sample point, e.g., with surrogate-based approaches. In these surrogate methods an approximation (surrogate / response surface) of the original model is built using high-fidelity evaluations of a subset of training points followed by MC sampling of the surrogate model \cite{9}. In order to build the surrogate different methods have been employed, e.g., linear regression \cite{10}, Gaussian process regression \cite{11} or stochastic collocation \cite{12}. In this case, however, the accuracy of the surrogate depends on the size of the training set and on the number of uncertainty parameters. For a large number of uncertain parameters, the computational costs can exceed the costs for MC \cite{13}. Furthermore, as shown in \cite{14}, there are examples where the surrogate model is highly accurate, measured by classical norms or pointwise, but the yield estimator fails drastically. In \cite{14} a hybrid approach is proposed. Sample points which are close to the limit state function are evaluated based on the high-fidelity model, for all remaining sample points the surrogate model is used. Here, the assessment of whether a point is close to the interface between failure and safe domain is crucial for the accuracy and efficiency of the algorithm. To this end, a method using an adjoint error indicator has been presented in \cite{15}. Yield optimization has been carried out in \cite{16}, where a Newton method for optimization was presented, which was combined with the standard MC method.

In this paper, we present an algorithm for efficient yield estimation and optimization. For yield estimation we propose a hybrid approach similar to \cite{14,15}. Contrary to the approach presented in \cite{14} we use an adjoint error indicator to identify the aforementioned critical MC sample points. Also, contrary to \cite{15} we build a polynomial surrogate model based on stochastic collocation. Furthermore, we consider the FE error in addition to the surrogate error as hybrid distinction criterion. If required, we refine the FE model for a subset of sample points. We then integrate this hybrid approach into the yield estimation and optimization framework. The optimization algorithm proposed in this paper is based on a globalized Newton method by \cite{16}. For yield estimation, which is necessary in each iteration, we use our previously mentioned hybrid method, and during optimization we adaptively adjust the MC sample size. To the best of our knowledge, these are new elements in the context of yield optimization and we call the resulting algorithm adaptive Newton-MC. It guarantees an a-priori defined accuracy of the result and significantly reduces computational effort. Furthermore, we show the applicability of the presented estimation and optimization approaches to problems where the performance feature specifications are restrictions involving partial differential equations describing electromagnetic fields, i.e., Maxwell’s equations in frequency domain.

This paper is structured as follows. After setting up the problem in Section 2 we will focus on yield estimation. We briefly review standard MC and stochastic collocation. We then present the hybrid approach combining the two previous ones. In Section 4 we propose the new adaptive Newton-MC method for yield optimization, including the numerical algorithm. Numerical results for the application of electromagnetic field simulation are presented in Section 5 before the paper is concluded in Section 6.

2 Problem setting

In this paper we consider a PDE with uncertainty in the input data. Details on the differential operator, geometry and boundary conditions will be postponed to a later chapter, which allows us to focus on the main algorithmic aspects for yield estimation and optimization. The starting point is the parametric model problem

\[
L_{p,r}u_r(p) = g_r \quad \text{on } D,
\]

where \( L_{p,r} \) is a linear parametric differential operator, \( g \) a forcing term, \( D \subset \mathbb{R}^d \) a simply connected bounded domain, \( p \in \mathbb{R}^n \) the input parameter vector and \( r \) the range parameter. The range parameter may refer to frequency or to a temperature for instance, which are not affected by uncertainties. We assume that the boundary of \( D \) and \( g \) are sufficiently regular, such that a unique solution exists for all \( p \). Moreover, we assume that \( p \mapsto u(p) \) is a smooth function, which is often parametrized for parametrized differential equations, see \cite{17} for the case of elliptic problems and \cite{18} for other problem classes, for instance. Design objectives are frequently expressed through global quantities, which are modeled in our case as linear functionals of the solution. More precisely, we introduce a quantity of interest (QoI) as

\[
Q(p, r) := \left( q_r, u_r(p) \right)_D,
\]

where \( q_r \in L^2(D) \) and \( L^2(D) \) denotes the space of complex square-integrable functions with inner product \( \langle \cdot, \cdot \rangle_D \).

A finite element approach leads to the linear parametric system

\[
A_{p,r}u_r(p) = f_r,
\]

where

\[
A_{p,r} := \left[ \frac{
abla u_r(p)}{u_r(p)} \right]_{p \in \mathbb{R}^n}
\]
where \( A_{p,r} \) denotes the system matrix. Furthermore, we define the discrete linear QoI by

\[
Q_h(p, r) = q_r \cdot u_r(p).
\]  

(2)

We denote with \( u_{h,\Omega} \) the interpolated discrete finite element solution, without explicitly introducing the underlying polynomial finite element space.

We assume that the uncertainties originate in the manufacturing process which lead to deviations in the design parameters. These uncertainties are often classified as aleatory. The setting could be generalized by interpreting the computed yield to be conditioned on epistemic uncertainties and by further quantifying these uncertainties as outlined for instance in [19][20]. However, since the focus of the present work is on adaptivity and error control in the context of yield estimation, this will not be considered here. The percentage of functioning realizations in mass production is called the yield \( \Pi \). To give a mathematical definition, we model \( p \) as a random design parameter vector, with independent distributed elements \( p_j, j = 1, \ldots, n_p \). Typically the \( p_j \) are assumed to follow a normal distribution, i.e., \( p_j \sim \mathcal{N}(\mu_j, \sigma_j) \) with mean value \( \mu_j \in \mathbb{R} \) and standard deviation \( \sigma_j \in \mathbb{R} \) and probability density function

\[
\text{pdf}_{\mathcal{N}(\mu_j, \sigma_j)} = \frac{1}{\sqrt{2\pi \sigma_j^2}} e^{-\frac{(p_j - \mu_j)^2}{2\sigma_j^2}}.
\]

Then, the uncertain parameter \( p \) follows a multivariate normal distribution, i.e., \( p \sim \mathcal{N}(\mu, \Sigma) \) with mean value \( \mu \in \mathbb{R}^{n_p} \) and a diagonal covariance matrix \( \Sigma \in \mathbb{R}^{n_p \times n_p} \) and probability density function

\[
\text{pdf}_{\mathcal{N}(\mu, \Sigma)} = \frac{1}{(2\pi)^{n_p/2} \sqrt{\det(\Sigma)}} e^{-\frac{1}{2} ((p - \mu)^T \Sigma^{-1} (p - \mu))}.
\]

The normality assumption may be justified by the central limit theorem in the presence of averaging processes or by maximum entropy arguments. Note that, in order to simplify notation, we do not distinguish between a random vector and its realization, whenever there is no confusion in a specific context. Following [1] we further define a range parameter \( r \in T_r = [r_1, r_2] \subset T \) and the performance feature specifications

\[
Q(p, r) \leq c \quad \forall r \in T_r,
\]

where \( c \) is a constant and \( Q \) the QoI introduced above. The safe domain \( \Omega_s \) is the set of all parameters, which fulfill the performance feature specifications, i.e.

\[
\Omega_s := \{ p : Q(p, r) \leq c \quad \forall r \in T_r \}.
\]

Then we can express the yield as

\[
Y(\bar{p}) := E[I_{\Omega_s}(p)] := \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} I_{\Omega_s}(p) \text{pdf}_{\mathcal{N}(\mu, \Sigma)}(p) \, dp,
\]

(3)

where \( E \) denotes the expected value and \( I_{\Omega_s}(p) \) the indicator function defined by

\[
I_{\Omega_s}(p) = \begin{cases} 
1 & p \in \Omega_s, \\
0 & \text{else}.
\end{cases}
\]

Note that \( \bar{p} \) will be a design parameter during optimization, whereas the covariance is fixed, which is taken into account by our notation in (3).

### 3 Yield Estimation

We proceed by describing a numerical method for yield estimation. The starting point will be a brief description of the MC method, followed by an outline of surrogate modeling based on stochastic collocation. The section will conclude with a description of a hybrid Monte Carlo method.

#### 3.1 Monte Carlo

The most straightforward approach in order to estimate the yield, i.e., compute the intergrals of (3), is a Monte Carlo analysis [21][22]. In a Monte Carlo approach, we consider a large number of independent random variables, distributed in the same way as \( p \). The set \( \{p_i\}_{i=1}^{N_{MC}} \), where each \( p_i \) represents a realization of the corresponding random variable, is called a sample and \( N_{MC} \) represents the sample size. At each sample point \( p_i \), we evaluate the high fidelity finite...
element (FE) model and count the sample points, which fulfill our performance feature specifications. Then we obtain a yield estimator as

\[ Y(p) \approx \hat{Y}(p) := \frac{\# \text{ sample points in } \Omega_s}{\text{sample size}}, \]

or equivalently

\[ \hat{Y}(p) = \frac{1}{N_{MC}} \sum_{i=1}^{N_{MC}} I_{\Omega_s}(p_i). \]

MC estimation is based on the law of large numbers, which ensures convergence for \( N_{MC} \to \infty \) under mild regularity assumptions on the integrand. Since in practice, the sample size is always finite, we need to estimate the associated error. To this end, we use an error indicator from [3]. An estimator of the approximated yield variance is derived as follows. Let \( I_{\Omega_s}(P_i) \) denote the Bernoulli random variable associated to the observation \( P_i \). Then, since all observations are independent, we obtain

\[ \text{Var} \left[ \hat{Y}(p) \right] = \frac{1}{N_{MC}^2} \sum_{i=1}^{N_{MC}} \text{Var} \left[ I_{\Omega_s}(P_i) \right] \]

\[ = \frac{1}{N_{MC}^2} N_{MC} Y(p)(1 - Y(p)) \]

\[ = \frac{Y(p)(1 - Y(p))}{N_{MC}}, \]

where the expectation and variance are now defined with respect to the i.i.d. observations. Then, we derive the standard deviation of the yield estimator as

\[ \sigma_Y = \sqrt{\frac{Y(p)(1 - Y(p))}{N_{MC}}} \leq \frac{0.5}{\sqrt{N_{MC}}}. \]

The standard deviation depends on the size of the yield. For a yield of 50% it is maximum and so we obtain the upper bound for the standard deviation given in (5). Since, the Monte Carlo estimator is unbiased, the variance is equal to the mean-square error. In view of (5), this approach guarantees a high accuracy for a large sample size, but it converges slowly with \( O \left( \frac{1}{\sqrt{N_{MC}}} \right) \). In many cases this is unaffordable due to the large number of expensive function evaluations required [3].

### 3.2 Stochastic Collocation and Error Estimation

To reduce the computational complexity of sampling the underlying FE solver, surrogate models can be employed. Based on the assumption that the map \( Q_h : \mathbb{R}^{n_p} \times T_r \to \mathbb{C} \) is well-defined and sufficiently smooth, we approximate the QoI as

\[ \hat{Q}_h(p, r) = \sum_{i=0}^{N} \alpha_i(r) \Phi_i(p), \]

where \( \Phi_i : \mathbb{R}^{n_p} \to \mathbb{R} \) are multivariate global polynomial basis functions with respect to \( p \) and \( \alpha_i : T_r \to \mathbb{C} \) denote the corresponding coefficients. Such a construction is appealing, as spectral convergence with respect to the polynomial degree can be expected [22]. In this work, we compute such approximations based on the stochastic collocation method [23, 17]. In particular, the surrogate model is obtained by evaluating (1) for a set of multivariate interpolation nodes \( \{p^{(i)}\}_{i=0}^{N} \) and enforcing the corresponding collocation conditions on the surrogate model. The choice of the multivariate nodes \( p^{(i)} \) is crucial for the efficiency of stochastic collocation. To this end, we first consider the tensor grid of univariate interpolation nodes \( \{p_i^{(i)}\} \times \{p_2^{(i)}\} \times \ldots \times \{p_M^{(i)}\} \). Employing all points of the grid is computationally intractable for many parameters. Sparse-grids [24] are a viable alternative, where a subset of points, which do not significantly contribute to the approximation accuracy is neglected. In this work, we use an algorithm proposed in [25, Algorithm 2], which constructs the sparse-grid adaptively. For convenience of the reader, we recall the main ideas in the following.
The algorithm is based on weighted Leja nodes \([26]\) which are defined recursively by an optimization problem, i.e. univariate weighted Leja nodes \(\{p_m^{(i)}\}_i \subset \mathbb{R}\) are obtained as

\[
p_m^{(i)} = \arg \max_{p \in \mathbb{R}} \sqrt{w(p_m)} \prod_{i=0}^{m-1} |p_m - p_m^{(i)}|,
\]

where the weight function \(w(p_m)\) is typically chosen as the probability distribution of the corresponding input parameter, i.e., \(w(p_m) = \text{pdf}_{\mathcal{N}(\mu_m, \sigma_m)}\), and for the first node we set \(p_m^{(0)} = 0\). Leja nodes are well suited for adaptive approximations in higher dimensions, since they are, by construction, nested and allow for a granular refinement \([26]\).

To steer the adaptive selection of the corresponding multivariate nodes, an adjoint error indicator \([27][28]\) is employed. To this end, we introduce the dual problem to (1), which is given by

\[
\text{univariate weighted Leja nodes} \{\tilde{u}_m\}
\]

where

\[
\tilde{u}_m = \arg \max_{p \in \mathbb{R}} \sqrt{w(p_m)} \prod_{i=0}^{m-1} |p_m - p_m^{(i)}|,
\]

Adjoint techniques can further be used to estimate the finite element error following \([30][31]\). However, in this case, it can then be used as an inexpensive substitute of (2) for an extensive MC analysis \((4)\).

Once an accurate surrogate model is available, approximations until a given computational budget is reached and the algorithm terminates. For further details on the employed adaptive sparse-grid interpolation scheme, we refer to \([25]\). A computable expression can only be obtained if the adjoint is replaced with a finite element approximation. However, contrary to the surrogate error \((8)\), a discussion of this finding can be found in \([27]\). Hence, we approximate the error, as the solution of the high fidelity adjoint problem. Hence, following \([29]\), we employ the error indicator

\[
\hat{\epsilon}_{sc}(p, r) := \tilde{z}_r(p) \cdot (\tilde{f}_r - A_{p,r} \tilde{u}_r(p)) \tag{7}
\]

The evaluation of (7) would always require the computation of \(z\), i.e. the solution of the high fidelity adjoint problem. Hence, following \([29]\), we employ the error indicator

\[
\hat{\epsilon}_{sc}(p, r) := \tilde{z}_r(p) \cdot (\tilde{f}_r - A_{p,r} \tilde{u}_r(p)) \tag{8}
\]

It should be noted that, under mild assumptions, cf. \([27][25]\), the error occurring when \(z\) is replaced with \(\tilde{z}\) is of higher order. The error indicator is then used to select interpolation nodes which are admissible for refinement of the approximations until a given computational budget is reached and the algorithm terminates. For further details on the employed adaptive sparse-grid interpolation scheme, we refer to \([25]\). Once an accurate surrogate model is available, it can then be used as an inexpensive substitute of \([2]\) for an extensive MC analysis \([4]\).

Adjoint techniques can further be used to estimated the finite element error following \([30][31]\). However, in this case, the continuous adjoint equation is required, which reads

\[
L_{p,r}^* z_r(p) = q_r \quad \text{on } D,
\]

where \(L_{p,r}^*\) denotes the adjoint operator with respect to the inner product \((\cdot, \cdot)_D\). With this notation at hand, we derive the following identity for the FE-error

\[
\epsilon_{fe}(p, r) = (q_r, u_r(p) - u_{h,r}(p))_D = (L_{p,r}^* z_r(p), u_r(p) - u_{h,r}(p))_D = (z_r(p), L_{p,r}^*(u_r(p) - u_{h,r}(p)))_D \approx (z_r(p), g_r - L_{p,r} u_{h,r}(p))_D.
\]

A computable expression can only be obtained if the adjoint is replaced with a finite element approximation. However, we cannot simply employ \(z_{h,r}\) as it is orthogonal to the residual. Hence, a higher order adjoint is required for the FE error, contrary to the surrogate error \((8)\). A discussion of this finding can be found in \([27]\). Hence, we approximate the adjoint solution on a refined grid, but other options, such as higher polynomial degrees or recovery techniques \([32]\), are equally applicable.

Finally, an error identity comprising both SC and FE-contribution is obtained as

\[
Q(p, r) - \tilde{Q}_h(p, r) = Q(p, r) - Q_h(p, r) + Q_h(p, r) - \tilde{Q}_h(p, r) \approx (z_h/2; r)(g_r - L_{p,r} u_{h,r}(p))_D + \tilde{z}_r(p) \cdot (\tilde{f}_r - A_{p,r} \tilde{u}_r(p)) \tag{9}
\]

Building surrogate models for both contributions, we obtain expressions which can be easily evaluated for all \(p\). We note, that the combined estimation of deterministic and stochastic discretization errors, has for example also been considered in \([28]\), in the context of the stochastic Galerkin method for time-dependent forward and inverse problems.
3.3 Hybrid approach

The number of collocation points $N$, for which the high fidelity FE model needs to be solved, depends on the number of uncertain parameters and the polynomial degree the surrogate model is supposed to have. This number grows rapidly with the number of parameters ("curse of dimensionality") [33]. For adaptive sparse grids the required FE solver calls can be reduced significantly. However, we know from [14] that yield estimation may produce erroneous results even though the surrogate model may be highly accurate.

The aim of the hybrid approach is to restore the accuracy of the MC method while relying on surrogate modeling as much as possible to enhance the numerical efficiency. We propose a particular hybrid approach, which is an extension of the one presented in [14]. The main difference lies in the selection of sample points which have to be re-evaluated with the high fidelity model. These points are referred to as critical sample points in the following. In [14] a tube around the boundary of the failure domain is defined, where the tube size is either fixed in advance, or determined iteratively by an algorithm which adds critical samples points until some error bound is satisfied. In comparison to [14] the method we propose is using stochastic collocation with Leja nodes as surrogate model (see Section 3.2). Also, in addition to the surrogate model error (SC error), we also consider the finite element error (FE error) in order to determine the critical sample points. Both error contributions are estimated by the adjoint error indicator, according to [9].

![Figure 1: Scheme of the hybrid approach.](image-url)

Our procedure is summarized in Figure 1. The first step is to build a surrogate model and to carry out a MC analysis with it. Then, we use an adjoint error indicator to quantify both the FE and surrogate error as

$$\hat{\epsilon}_{sc}(p_i, r_j), \hat{\epsilon}_{fe}(p_i, r_j) \forall i = 1, \ldots, N_{MC}, \forall j = 1, \ldots, |T_d|,$$

where $T_d$ is a discrete subset of $T_r$. We then verify whether the approximated QoI value, taking into account the aforementioned errors, meets the requirements. To this end, we define the interval

$$Q^1_{sc}(p_i, r_j) = \left[ \left| \hat{Q}_h(p_i, r_j) \right| - s \left( |\hat{\epsilon}_{sc}(p_i, r_j)| + |\hat{\epsilon}_{fe}(p_i, r_j)| \right), \left| \hat{Q}_h(p_i, r_j) \right| + s \left( |\hat{\epsilon}_{sc}(p_i, r_j)| + |\hat{\epsilon}_{fe}(p_i, r_j)| \right) \right],$$

where $s \geq 1$ indicates a safety factor. If the performance feature specifications are fulfilled (or not fulfilled) for the whole interval $Q^1_{sc}$, we can classify the sample point $p_i$ as accepted (or not accepted). If the performance feature specifications are fulfilled only for a subset of the interval $Q^1_{sc}$, we classify the sample point as critical.

For all critical sample points the high fidelity FE model will be evaluated, hence, we obtain $Q_h(p_i, r_j)$. For these points, the surrogate error is zero, however, the FE error remains unchanged. The new interval we have to examine is given by

$$Q^2_{sc}(p_i, r_j) = \left[ |Q_h(p_i, r_j)| - s \left( 0 + |\hat{\epsilon}_{fe}(p_i, r_j)| \right), |Q_h(p_i, r_j)| + s \left( 0 + |\hat{\epsilon}_{fe}(p_i, r_j)| \right) \right].$$
to be carried out for the remaining range parameter points as well. However, if \( p \) fails to fulfill the requirements for a specific range parameter point, it is immediately classified as not accepted. Thereby, we can avoid the computational effort of evaluating the remaining range parameter points. This strategy is also applied for the standard MC method and the stochastic collocation surrogate-based MC method. In the hybrid method we can further benefit from the fact, that we can use the stochastic collocation results to sort the order of the range parameter points. Then, we start examining the range parameter point satisfying

\[
\arg \max_{r_j \in T_d} Q_h(p_i, r_j).
\]

In total, three different errors have to be considered within the yield estimation process: the MC error, the FE error and the error of the surrogate model, in our case the SC error. The hybrid approach proposed in this paper takes into account the surrogate and FE error. The FE error depends on the refinement of the mesh. Instead of evaluating the entire MC sample (or all critical sample points in a hybrid approach) with the finest mesh, we start with a coarse

---

**Algorithm 1 Hybrid decision**

1: **Input:** sample point \( p_i \), range parameter point \( r_j \)
2: Evaluate surrogate model and set
   \[
   Q = \left| Q_h(p_i, r_j) \right|
   \]
   \[
   \epsilon = |\bar{\epsilon}_e(p_i, r_j)| + |\bar{\epsilon}_c(p_i, r_j)|
   \]
3: **while** max. refinement not reached **do**
4:   **if** \( Q - s \epsilon > c \) **then**
5:     classify \( p_i \) as not accepted, i.e. \( p_i \notin \Omega_s \) (middle picture in Fig. 1)
6:       continue with next sample point \( p_{i+1} \)
7:   **else if** \( Q + s \epsilon \leq c \) **then**
8:     sample point \( p_i \) accepted for this range parameter point \( r_j \)
9:       **if** all \( r_j \) checked **then**
10:      classify \( p_i \) as accepted i.e. \( p_i \in \Omega_s \) (left picture in Fig. 1)
11:         continue with next sample point \( p_{i+1} \)
12:   **else**
13:     check next range parameter point \( r_{j+1} \)
14: **end if**
15: **if** first loop **then**
16:   Evaluate FE model and set
   \[
   Q = |Q_h(p_i, r_j)|
   \]
   \[
   \epsilon = |\bar{\epsilon}_e(p_i, r_j)|
   \]
17: **else**
18:   Refine the mesh with \( h = h/2 \)
   Evaluate FE model and set
   \[
   Q = |Q_h(p_i, r_j)|
   \]
   \[
   \epsilon = |\bar{\epsilon}_e(p_i, r_j)|
   \]
19: **end if**
20: **end if**
21: **end while**
22: **if** sample point \( p_i \) still critical with last refinement **then**
23:   classify \( p_i \) according to \( Q \) with the finest mesh into accepted or not accepted
24: **end if**
mesh, calculate the error indicator and refine the mesh if necessary. Thereby, the FE error is controlled and reduced if required and unnecessary computational effort avoided. The SC error is controlled by calculating an adjoint error indicator after building the surrogate model. If the sum of both indicators is too large, a sample point may be classified as critical. In this case, we evaluate the FE model and the associated SC error vanishes. In order to control the MC error, we define a target accuracy by a maximum value of the standard deviation $\sigma_Y$ and determine the minimum sample size needed by $\text{(5)}$.

4 Yield Optimization

4.1 General Newton approach

The idea of yield optimization is to change the mean value of the uncertain parameter, i.e. $\mathbf{p}$, in order to maximize the yield. We can formulate the optimization problem as follows

$$\max_{\mathbf{p}} Y(\mathbf{p}) = \max_{\mathbf{p}} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} I_{\Omega_{\mathbf{p},\Sigma}}(\mathbf{p}) \, \text{pdf}_{\mathcal{N}(\mathbf{p},\Sigma)}(\mathbf{p}) \, d\mathbf{p}.$$ 

Let the uncertain parameter $\mathbf{p}$ be modeled as a normally distributed random variable. Then, since only the probability density function of the uncertain parameter $\mathbf{p}$ depends on the optimization variable $\mathbf{p}$, from (3) we can derive the gradient and the Hessian of the yield according to [1]. Therefore, we first introduce the distribution of the subset of MC sample points belonging to the safe domain $\Omega_{\mathbf{p}}$. Its probability density function is given by

$$\text{pdf}_{\Omega_{\mathbf{p}}}(\mathbf{p}) = \frac{1}{Y(\mathbf{p})} I_{\Omega_{\mathbf{p}}}(\mathbf{p}) \, \text{pdf}_{\mathcal{N}(\mathbf{p},\Sigma)}(\mathbf{p}).$$

The mean and covariance of this distribution are given by

$$\mathbf{p}_{\Omega_{\mathbf{p}}} = E_{\text{pdf}_{\Omega_{\mathbf{p}}}}[\mathbf{p}] = \frac{1}{Y(\mathbf{p})} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \mathbf{p} I_{\Omega_{\mathbf{p}}}(\mathbf{p}) \, \text{pdf}_{\mathcal{N}(\mathbf{p},\Sigma)}(\mathbf{p}) \, d\mathbf{p},$$

$$\Sigma_{\Omega_{\mathbf{p}}} = E_{\text{pdf}_{\Omega_{\mathbf{p}}}}[(\mathbf{p} - \mathbf{p}_{\Omega_{\mathbf{p}}})(\mathbf{p} - \mathbf{p}_{\Omega_{\mathbf{p}}})^T]$$

$$= \frac{1}{Y(\mathbf{p})} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} (\mathbf{p} - \mathbf{p}_{\Omega_{\mathbf{p}}})(\mathbf{p} - \mathbf{p}_{\Omega_{\mathbf{p}}})^T I_{\Omega_{\mathbf{p}}}(\mathbf{p}) \, \text{pdf}_{\mathcal{N}(\mathbf{p},\Sigma)}(\mathbf{p}) \, d\mathbf{p}$$

and can be estimated by

$$\mathbf{p}_{\Omega_{\mathbf{p}}} = \frac{1}{N_{\text{in}}} \sum_{i=1}^{N_{\text{MC}}} I_{\Omega_{\mathbf{p}}}(\mathbf{p}_i) \, \mathbf{p}_i,$$

$$\Sigma_{\Omega_{\mathbf{p}}} = \frac{1}{N_{\text{in}} - 1} \sum_{i=1}^{N_{\text{MC}}} I_{\Omega_{\mathbf{p}}}(\mathbf{p}_i) \, (\mathbf{p}_i - \mathbf{p}_{\Omega_{\mathbf{p}}}) (\mathbf{p}_i - \mathbf{p}_{\Omega_{\mathbf{p}}})^T,$$

where $\mathbf{p}_i, i = 1, \ldots, N_{\text{MC}}$ are independent observations of the random variable $\mathbf{p}$ and $N_{\text{in}}$ indicates the number of sample points within the safe domain. Using these formulations, the gradient and the Hessian of the yield with respect to $\mathbf{p}$ can be written as

$$\nabla_{\mathbf{p}} Y(\mathbf{p}) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} I_{\Omega_{\mathbf{p}}}(\mathbf{p}) \nabla_{\mathbf{p}} \text{pdf}_{\mathcal{N}(\mathbf{p},\Sigma)}(\mathbf{p}) \, d\mathbf{p} \approx Y(\mathbf{p}) \Sigma^{-1}(\mathbf{p}_{\Omega_{\mathbf{p}}} - \mathbf{p})$$

$$\nabla^2_{\mathbf{p}} Y(\mathbf{p}) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} I_{\Omega_{\mathbf{p}}}(\mathbf{p}) \nabla^2_{\mathbf{p}} \text{pdf}_{\mathcal{N}(\mathbf{p},\Sigma)}(\mathbf{p}) \, d\mathbf{p}$$

$$\approx Y(\mathbf{p}) \Sigma^{-1} \left( \Sigma_{\Omega_{\mathbf{p}}} + (\mathbf{p}_{\Omega_{\mathbf{p}}} - \mathbf{p})(\mathbf{p}_{\Omega_{\mathbf{p}}} - \mathbf{p})^T - \Sigma \right) \Sigma^{-1}.$$ 

A detailed derivation can be found in [1]. It should be mentioned that we first differentiate and then discretize. Hence, this gradient does not necessarily coincide with the gradient obtained by differentiating after discretization.

The fact that we have given the gradient and the Hessian in analytical form allows us to use a gradient based optimization algorithm, such as the globalized Newton method [16] as proposed in [1]. A pseudo code is given in Algorithm 2. The associated parameters have been set as follows

$$\beta = \frac{1}{2}, \gamma = \frac{1}{100}, \alpha_1 = \alpha_2 = 10^{-6}, \, \theta = \frac{1}{10}.$$
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Algorithm 2 Globalized Newton method

1: Input: Starting point $\mathbf{p}_0 \in \mathbb{R}^d$, $\beta \in (0, 1)$, $\gamma \in (0, 1)$, $\alpha_1, \alpha_2 > 0$, $q > 0$
2: Output: Optimal solution $\mathbf{p}^*$
3: while $\nabla Y(\mathbf{p}^k) \neq 0$ and $\|\mathbf{p}^k - \mathbf{p}^{k-1}\| > 0$ do
4: Calculate $d^k$ by solving the Newton’s equation $\nabla^2 Y(\mathbf{p}^k) \mathbf{d}^k = -\nabla Y(\mathbf{p}^k)$.
5: if "Calculation of $d^k$ possible" and $-\nabla Y(\mathbf{p}^k) d^k \geq \min (\alpha_1, \alpha_2 \|d^k\|^q) \|d^k\|^q$ then
6: Set search direction $s^k = d^k$.
7: else
8: Set search direction $s^k = -\nabla Y(\mathbf{p}^k)$.
9: end if
10: Determine step size with Armijo rule, i.e. search for largest $\sigma^k \in \{\beta^0, \beta^1, \beta^2, ...\}$
11: such that: $Y(\mathbf{p}^k + \sigma^k s^k) - Y(\mathbf{p}^k) \leq \sigma^k Y(\mathbf{p}^k)^T s^k$.
12: Set $\mathbf{p}^{k+1} = \mathbf{p}^k + \sigma^k s^k$ and $k = k + 1$.
13: end while

In this paper we assume that all uncertain parameters are optimization variables and vice versa. Little modifications in the algorithm also cover other cases. If additional optimization variables without uncertainty are present, we simply set their standard deviation to zero, i.e. $\sigma = 0$. In order to calculate the gradient, we need the inverse of the covariance matrix $\Sigma$, which would be singular in this case. As a remedy, we define a reduced covariance matrix containing only the uncertain parameters, calculate their inverse and insert zero rows and columns at the positions where we eliminated the optimization parameters. If, instead, there are uncertain parameters $\mathbf{u}$, which are not optimization variables, they have to be considered during yield estimation, which can be achieved by setting $\mathbf{p}' = [\mathbf{p}, \mathbf{u}]^T$. Nevertheless, during optimization we only use $\mathbf{p}$, e.g. to calculate $\Sigma$, $\mathbf{p}_{1\mathbf{u}}$, $\Sigma_{1\mathbf{u}}$, etc.

4.2 Adaptive Newton-MC

The size of the MC sample is crucial, not only for accuracy but also for the efficiency of the algorithm. According to [5], for yield estimation we can use the MC error indicator to determine the sample size depending on the desired accuracy. For yield optimization, the situation is more involved. The accuracy of yield estimators at intermediate steps of the Newton algorithm is not essential to obtain a satisfying final result. In each individual iteration, it is sufficient to obtain a gradient that indicates the right direction. The stochastic gradient approach also deals with approximated or inexact gradients, used during the optimization process, see [34] for example. However, our approach uses more sample points than usual in the stochastic gradient approach, but we also calculate the objective function with the reduced sample. Only towards the termination of the algorithm, a very accurate gradient may be decisive to accurately determine the optimal solution. Our algorithmic construction ensures that the high, pre-defined, accuracy requirements at the final stages of the algorithm are fulfilled. More precisely, we propose the following adaptive Newton-MC approach. The optimization method is based on a globalized Newton method, as described in Algorithm 2. We start with a very small sample size and proceed with a few fast initial Newton iterations. If no further yield improvement is observed during the iteration process, the globalized Newton method described in Algorithm 2 would stop. Here, instead, we increase the number of MC observations until an improved yield is observed or a target accuracy is reached, then we start the next Newton iteration. Only when the target accuracy has been reached and the yield is not improving anymore, the algorithm terminates.

A pseudo code for the adaptive Newton-MC is given in Algorithm 3. First, we need to define a target accuracy in form of a maximal standard deviation $\sigma_Y$ for our terminal solution. Furthermore, we have to define the size of the initial MC sample $N_{\text{MC}}^{\text{start}}$ and an incremental factor inc $> 0$ such that

$$N_{\text{MC}}^{\text{new}} = N_{\text{MC}}^{\text{old}} + \text{inc} \cdot N_{\text{MC}}^{\text{start}}.$$  

The sample size is increased until the target accuracy is reached (see line 14 in Algorithm 3), and the standard globalized Newton method terminates because no further yield improvement can be obtained, i.e., the difference between $\mathbf{p}^k$ and $\mathbf{p}^{k-1}$ tends to zero (see line 3). In line 15 we can see the rules for a sample size increment. This loop is activated, if the two previous mentioned conditions are fulfilled. Then, we increase the sample size stepwise (see line 16), re-evaluate the yield with the new size $Y'(\mathbf{p}^k)$, and its new standard deviation $\sigma_Y'$ (see line 17). Note that in order to estimate $Y'(\mathbf{p}^k)$ it is not necessary to evaluate $N_{\text{MC}}^{\text{new}}$ new sample points. Only the inc $N_{\text{MC}}^{\text{start}}$ additional points have to be evaluated and can then be fused with the $N_{\text{MC}}^{\text{old}}$ old points to obtain the new yield estimator. This procedure is repeated until the new standard deviation $\sigma_Y'$ reaches the target accuracy (i.e. $\sigma_Y' \leq \sigma_Y$) or the improvement of the
dispersive complex magnetic permeability and ε the dispersive complex electric permittivity, with

$$\nabla \times (\mu^{-1} \nabla \times \mathbf{E}_\omega) - \omega^2 \varepsilon \mathbf{E}_\omega = 0 \quad \text{on } D$$

(12)

to be solved for the electric field phasor $\mathbf{E}_\omega$, where $\omega$ denotes the angular frequency, $\mu = \mu_r \mu_0 \in L^\infty(D)$ the dispersive complex magnetic permeability and $\varepsilon = \varepsilon_r \varepsilon_0 \in L^\infty(D)$ the dispersive complex electric permittivity, with

yield is large enough (i.e. the difference between the actual yield $Y(\mathbf{p}^k)$ and the yield with the increased sampling $Y'(\mathbf{p}^k)$ is larger than the target accuracy $\hat{\sigma}_Y$). In that case we start a new iteration of the Newton algorithm, with updated yield and sample size (see line 19). If the target accuracy is fulfilled after a regular Newton procedure (after line 13), the algorithm terminates (see line 23).

The parameters are chosen as for Algorithm 2 additionally we set the maximal standard deviation, the starting sample size and the incremental factor as follows

$$\hat{\sigma}_Y = 0.01, \quad N_{\text{start}} = 100, \quad \text{inc} = 1.$$

Another difference in comparison to Algorithm 2 is, that we bound the number of Armijo backward steps. If the inequality in line 10 is not fulfilled after three steps, we set $\sigma^k = \beta^3$ and proceed with the next iteration.

5 Numerical results

We apply the methods for yield estimation and optimization discussed in the previous sections to a benchmark problem in the context of electromagnetic field simulation. In particular, we employ the model of a rectangular waveguide with a dielectric insert, similarly to the one used in [35]. This model is well suited for validation purposes, as a closed-form solution is available [36]. In the following, we first introduce the problem setting before numerical results for yield estimation as well as yield optimization are presented.

5.1 Problem setting

Starting from the time-harmonic Maxwell’s equation on a computational domain $D \subset \mathbb{R}^3$, one can derive the curl-curl equation

$$\nabla \times (\mu^{-1} \nabla \times \mathbf{E}_\omega) - \omega^2 \varepsilon \mathbf{E}_\omega = 0 \quad \text{on } D$$

(12)

to be solved for the electric field phasor $\mathbf{E}_\omega$, where $\omega$ denotes the angular frequency, $\mu = \mu_r \mu_0 \in L^\infty(D)$ the dispersive complex magnetic permeability and $\varepsilon = \varepsilon_r \varepsilon_0 \in L^\infty(D)$ the dispersive complex electric permittivity, with
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Figure 2: Finite element model of a rectangular waveguide with dielectric inset of length $p_1$. The waveguide is excited at the port $\Gamma_{p1}$ (red color) by an incident TE$_{10}$ wave.

The vacuum permeability $\mu_0$ and the relative permeability $\mu_r$, respectively vacuum and relative permittivity $\epsilon_0$ and $\epsilon_r$. Further we have assumed absence of charges and source currents.

The boundary of the domain $D$ is split into three parts, i.e. $\partial D = \Gamma_{\text{PEC}} \cup \Gamma_{p1} \cup \Gamma_{p2}$, since we consider the model of an electric waveguide with two ports $\Gamma_{p1}, \Gamma_{p2}$ and assume [perfect electric conductor (PEC)] boundary conditions at the waveguide walls, i.e.

$$\mathbf{n} \times \mathbf{E}_\omega = 0 \quad \text{on } \Gamma_{\text{PEC}}.$$

(13)

At the waveguide ports $\Gamma_{p1}, \Gamma_{p2}$ we impose lowest order waveguide boundary conditions [37, Chapter 8.5]

$$\mathbf{n} \times (\nabla \times \mathbf{E}_\omega) - j k_{z10} (\mathbf{n} \times \mathbf{E}_\omega) \times \mathbf{n} = -2 j k_{z10} \mathbf{E}^{\text{inc}}$$

on $\Gamma_{p1}$,

$$\mathbf{n} \times (\nabla \times \mathbf{E}_\omega) - j k_{z10} (\mathbf{n} \times \mathbf{E}_\omega) \times \mathbf{n} = 0$$

on $\Gamma_{p2}$,

where $\mathbf{n}$ denotes the outer unit normal vector. The propagation constant $k_{z10}$ is given by $k_{z10} = \sqrt{\omega^2 \mu_0 \epsilon_0 - \frac{\pi^2}{a^2}}$, where, in turn, $a$ denotes the width of the waveguide, as depicted in Fig. 2. According to [38], the boundary conditions (14) can be derived based on the assumption, that the rectangular waveguide is excited at $\Gamma_{p1}$ by an incident TE$_{10}$ wave

$$\mathbf{E}^{\text{inc}} = E_0 \mathbf{E}^{\text{TE}}_{10} e^{-j k_{z10} z} \quad \text{with } \mathbf{E}^{\text{TE}}_{10} := \sin \left( \frac{\pi x}{a} \right) \mathbf{e}_y,$$

where $E_0$ refers to the amplitude of the incident wave and $\mathbf{e}_y$ denotes the unit vector in $y$-direction. Additionally it is assumed that the waveguide dimensions are chosen s.t. only the TE$_{10}$ mode is propagating without attenuation, that the ports are placed sufficiently far from any obstacles in the waveguide which might excite higher-order modes and that the homogeneous material at the ports $\Gamma_{p1} \cup \Gamma_{p2}$ fulfills $\epsilon_r = \mu_r = 1$. For further details on waveguide boundary conditions, we refer to [37].

As QoI we consider the fundamental scattering parameter (S-parameter) of the TE$_{10}$-mode on $\Gamma_{p1}$

$$S := \frac{2}{E_{0}ab} (\mathbf{E}_\omega - \mathbf{E}^{\text{inc}}_{\omega}, \mathbf{E}^{\text{TE}}_{10})_{\Gamma_{p1}},$$

(15)

where we assumed $z = 0$ on $\Gamma_{p1}$ for simplicity (without loss of generality). Note that the QoI (15) is, in this case, an affine-linear functional of $\mathbf{E}_\omega$.

5.2 Weak formulation and discretization

In order to solve the boundary value problem (12)-(14) numerically by the FEM we devise the corresponding weak formulation. Therefore, we build the inner products of (12) with test functions $\mathbf{E}' \in V$, where $V$ is to be determined, and integrate by parts

$$\left( \mu_r^{-1} \nabla \times \mathbf{E}_\omega, \nabla \times \mathbf{E}' \right)_D - \omega^2 \mu_0 (\varepsilon \mathbf{E}_\omega, \mathbf{E}')_D + \left( \pi_1 \mu_r^{-1} \nabla \times \mathbf{E}_\omega, \pi_T \mathbf{E}' \right)_{\partial D} = 0.$$

(16)

Note that we introduced the trace operators

$$\pi_1 [\mathbf{u}] := \mathbf{n} \times \mathbf{u}|_{\partial D},$$

$$\pi_T [\mathbf{u}] := (\mathbf{n} \times \mathbf{u}|_{\partial D}) \times \mathbf{n}.$$
for brevity of notation. The boundary integral in (16) vanishes on \( \Gamma_{\text{PEC}} \), since we impose \( \text{PEC} \) boundary conditions \([13]\) for the test functions \( E' \) as well. On \( \Gamma_{p1} \cup \Gamma_{p2} \) we employ the boundary conditions \([14]\) and obtain the weak formulation: find \( E \in V \) s.t.

\[
(\mu_r^{-1} \nabla \times E_\omega, \nabla \times E')_D - \omega^2 \mu_0 (\varepsilon E_\omega, E')_D + j k_{z10} (\pi_T[E_\omega], \pi_T[E'])_{\Gamma_{p1} \cup \Gamma_{p2}} = 2 j k_{z10} (E^{\text{inc}}_\omega, \pi_T[E'])_{\Gamma_{p1}} \quad \forall E' \in V.
\]

(17)

The appropriate function space \( V \) is a subspace of

\[
H(\text{curl}, D) := \left\{ u \in (L^2(D))^3 : (\nabla \times u, \nabla \times u)_D < \infty \right\},
\]

where, in turn, \( (L^2(D))^3 \) denotes the complex vector function space of square integrable functions, i.e.

\[
(L^2(D))^3 := \left\{ u : (u, u)_D < \infty \right\},
\]

cf. \( [39] \). To account for the \( \text{PEC} \) boundary conditions \([13]\) and obtain a well-defined boundary integral in \( (17) \), \( V \) is chosen as

\[
V := \left\{ u \in H(\text{curl}, D) : \pi_T[u]|_{\Gamma_{p1}} \in (L^2(\Gamma_{p1}))^3 \quad \land \quad \pi_T[u]|_{\Gamma_{p2}} \in (L^2(\Gamma_{p2}))^3 \quad \land \quad \pi_i[u]|_{\Gamma_{\text{PEC}}} = 0 \right\}.
\]

In order to solve \( (17) \) with \( \text{FEM} \) we introduce a finite-dimensional function space \( V_h \subset V \) and express the electric field as

\[
E_{\omega, h} = \sum_{j=1}^{n_{\text{DoF}}} e_{\omega,j} N_j,
\]

where \( e_{\omega,j} \in \mathbb{C} \) are the degrees of freedom (DoFs), \( n_{\text{DoF}} \) is the number of DoFs and \( N_j \in V_h \) denotes second order, first kind Nédélec basis functions defined on a tetrahedral mesh of the domain \( D \). For further details on the curl-conforming discretization, we refer to \([40]\). The discrete solution \( e_\omega = [e_{\omega,1}, \ldots, e_{\omega,n_{\text{DoF}}}]^T \) is then obtained by solving the linear system

\[
\begin{pmatrix}
K - \omega^2 M' + j k_{z10} M^{\text{port}} \\
A_{\omega}
\end{pmatrix}
\begin{pmatrix}
e_{\omega} \\
e_{\omega}^{\text{inc}}
\end{pmatrix} = \begin{pmatrix} f_{\omega} \\
f_{\omega}^{\text{inc}}
\end{pmatrix},
\]

where \( A_{\omega} \in \mathbb{C}^{n_{\text{DoF}} \times n_{\text{DoF}}} \) is the system matrix and \( f_{\omega} \in \mathbb{C}^{n_{\text{DoF}}} \) is the discretized right-hand side. The stiffness matrix \( K \), the mass-matrix \( M' \), the matrix \( M^{\text{port}} \) and the right-hand side \( f_{\omega} \) in the above expression are given by

\[
\begin{align*}
K_{ij} &= (\mu_r^{-1} \nabla \times N_j, \nabla \times N_i)_D, \\
M'_{ij} &= \mu_0 (\varepsilon N_j, N_i)_D, \\
M^{\text{port}}_{ij} &= (\pi_T[N_j], \pi_T[N_i])_{\Gamma_{p1} \cup \Gamma_{p2}}, \\
[f_{\omega}]_i &= 2 j k_{z10} (E^{\text{inc}}_\omega, \pi_T[N_i])_{\Gamma_{p1}}.
\end{align*}
\]

The S-parameter can then be obtained from the discrete counterpart of \( (15) \)

\[
S_h(\omega) = q_\omega \cdot (e_\omega - e_\omega^{\text{inc}}).
\]

As discussed in the previous sections, we then introduce a parameter vector \( p \in \Xi \subset \mathbb{R}^M \) to account for variations in the design parameters, which, in this case, might resemble changes in the domain \( D \) or in the material parameters \( \varepsilon, \mu \). Hence, we obtain the parametrized discrete system

\[
\begin{align*}
A_{\omega}(p) e_\omega(p) &= f_{\omega}, \\
S_h(p, \omega) &= q_\omega \cdot e_\omega(p).
\end{align*}
\]

(18)

We proceed with a few details on the implementation of the numerical model. To assemble the linear system \( (18) \), we employ the \( \text{FEniCS} \) library \( \text{FEniCS} \) \([41]\). As \( \text{FEniCS} \) 2017.2.0 does not support complex numbers, we assemble real and imaginary parts of the matrices separately. We then use \( \text{NUMPY} \) to impose the \( \text{PEC} \) boundary condition \([13]\) and \( \text{SCIPY} \) to solve the resulting linear system of equations with a sparse-LU decomposition. Employing the readily available LU decomposition, the corresponding dual solution \( z_\omega(p) \) can then also be obtained with negligible costs, since the dual problem

\[
A_{\omega}^*(p) z_\omega(p) = q_\omega,
\]

can again be solved by forward-backward substitution.
5.3 Numerical results

We consider twelve uncertain parameters

$$\mathbf{p} = [p_1, \ldots, p_{12}]^T.$$  

Two of them are geometrical parameters given in mm (length of the dielectrical inlay $p_1$ and length of the vacuum offset $p_2$) and ten are material parameters with effect on the relative permittivity $\epsilon_r|_{\Omega_2}$ and permeability $\mu_r|_{\Omega_2}$ on the dielectrical inlay

$$\epsilon_r|_{\Omega_2} = p_5 + (p_3 - p_5) \left(1 + j\omega p_6 \tau\right)^{-1} + (p_4 - p_5) \left(1 + j\omega p_7 \tau\right)^{-1},$$

$$\mu_r|_{\Omega_2} = p_{10} + (p_8 - p_{10}) \left(1 + j\omega p_{11} \tau\right)^{-1} + (p_9 - p_{10}) \left(1 + j\omega p_{12} \tau\right)^{-1},$$

where

$$\omega = 2\pi f,$$

$$\omega_0 = 2\pi \left(20 \cdot 10^9\right) \text{Hz},$$

$$\tau = \frac{1}{\omega_0}.$$  

with frequency $f$ (in Hertz). In order to consider the influence of the number of uncertain parameters, tests with four uncertain parameters are also performed. For this purpose we consider a modified parameter vector

$$\mathbf{p}^{(4)} = [p_1, p_2, p_{13}, p_{14}]^T,$$

where $p_1$ and $p_2$ are the geometrical parameters from above, and $p_{13}$ and $p_{14}$ are material parameters with the following effect on relative permeability and permittivity

$$\epsilon_r^{(4)}|_{\Omega_2} = 1 + p_{13} + (1 - p_{13}) \left(1 + j\omega \left(2\pi5 \cdot 10^9\right)^{-1}\right)^{-1},$$

$$\mu_r^{(4)}|_{\Omega_2} = 1 + p_{14} + (2 - p_{14}) \left(1 + j\omega \left(1.1 \cdot 2\pi20 \cdot 10^9\right)^{-1}\right)^{-1}.$$  

For yield optimization we set the starting point $\mathbf{p}_0$ for twelve parameters to

$$\mathbf{p}_0 = [9, 5, 2, 0.5, 1, 1.1, 2.5, 1, 1, 1, 2]^T.$$  

The estimation tests are done for a reference value $\mathbf{p}_e$ close to one optimal solution

$$\mathbf{p}_e = [8, 6, 3.8, 2, 0.5, 0.7, 0.6, 1.4, 2.8, 1.7, 0.8, 0.3, 1.4]^T.$$  

For the tests with four parameters we set the starting points to

$$\mathbf{p}_0^{(4)} = [8, 5, 1, 1]^T,$$

$$\mathbf{p}_e^{(4)} = [10.36, 4.76, 0.58, 0.64]^T.$$  

The standard deviation is set to $\sigma = 0.7^2$ mm for geometrical, and $\sigma = 0.3^2$ for material parameters. In order to avoid unphysical values, instead of a normal distribution we use a truncated normal distribution for the MC sample generation. We truncate with an offset $t$ of $\pm 3$ mm and $\pm 0.3$ for the geometrical and material parameters, respectively. The performance feature specifications are

$$|S(p, \omega)| \leq -24 \text{ dB} \quad \forall \omega \in T_\omega = [2\pi f_1, 2\pi f_2] = [2\pi6.5, 2\pi7.5] \text{ in GHz}.$$  

We consider eleven equidistant frequency points $\omega_j \in T_\omega$ in the frequency range. The reference solution for yield estimation is

$$Y_{\text{Ref}}(\mathbf{p}) = 74.60\%,$$

calculated with a closed form solution of the E-field formulation and standard MC method with $N_{\text{MC}} = 2,500$, which is the smallest sample size fulfilling $\sigma_Y = 0.01$ for all sizes of the yield, according to [5].
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Figure 3: Comparision of the gradients $\nabla_p Y_G$ and $\nabla_p Y_{DQ}$ for $N_{MC} = 10^6$ and finite difference step size $h = 10^{-3}$ for truncated normal distribution.

Figure 4: Convergence of the gradients $\nabla_p Y_G$ and $\nabla_p Y_{DQ}$ for increasing $N_{MC}$. Calculated in $p = 10.8685$ mm and with finite difference step size $h = 10^{-3}$.

5.3.1 Quality of the gradient

As mentioned in section 4 there is a difference between differentiating or discretizing first. Furthermore, for the sample generation we use a truncated normal distribution instead of a normal distribution. Thus, the gradient we use for optimization deviates from the exact gradient, which can be thought of as an inexact Newton method [42], with approximations in the root-finding problem itself, i.e., here the gradient (10), and the Jacobian which is in our case the Hessian (11).

To ensure that the yield is optimal at the end and no further improvement is possible, an extension can be added to the optimization algorithm. At the optimal solution, the gradient can be calculated with a finite difference quotient $\nabla_p Y_{DQ}$. The gradient from (10) will be denoted $\nabla_p Y_G$, to avoid any confusion. We consider the difference between the two gradients and expect it to be smaller than a constant $z$

$$\left|\nabla_p Y_{DQ}(\hat{p}) - \nabla_p Y_G(\hat{p})\right| \leq z.$$  \hspace{1cm} (19)

Figure 3 compares the two gradients $\nabla_p Y_G$ and $\nabla_p Y_{DQ}$ for the waveguide example where the only uncertain design parameter is the length of the inlay $p$. On the left, we see the yield over the parameter $p$, on the right we see the graphs of the gradients over the parameter $p$. For this calculation we set the sample size to $N_{MC} = 10^6$ and the step size in the difference quotient to $h = 10^{-3}$. The two gradients show a similar behaviour, especially near the optimum the gradients agree well. Figure 4 shows how the two gradients approach each other for large $N_{MC}$. Thus, if (19) is not fulfilled the number of sample points to calculate the gradients can be increased until (19) is fulfilled or an upper bound for $N_{MC}$ is reached. In the former case, the applied gradient $\nabla_p Y_G$ is accurate and the optimal solution reliable. In the latter case, a further improvement of the yield would still be possible due to the limited gradient accuracy. In this case the yield optimization could be continued with the gradient $\nabla_p Y_{DQ}$. However, this would require additional computational effort, especially for a large number of uncertain parameters. The optimal solution can also be used as a starting point for an alternative optimization procedure.
Table 1: Comparison of different yield estimation approaches for twelve uncertain parameters.

| approach | # Leja | # HF<sub>h</sub> surr. | # HF<sub>h</sub> MC | # HF<sub>h/2</sub> MC | # HF<sub>h/4</sub> MC | eff | err (%) |
|----------|--------|------------------------|---------------------|-----------------------|-----------------------|-----|--------|
| MC<sub>fine</sub> | -      | 0                      | 0                   | 0                     | 22,705                | 363,280 | 0.0000 |
| MC<sub>refine</sub> | -      | 0                      | 22,705              | 25                    | 6                     | 22,901  | 0.0000 |
| H        | 90     | 990                    | 4,812               | 25                    | 6                     | 5,998   | 0.0000 |
| SC       | 90     | 990                    | 0                   | 0                     | 0                     | 990     | 6.2235 |
| SC       | 1,600  | 17,600                 | 0                   | 0                     | 0                     | 17,600  | 0.4290 |

Different methods: MC, SC and hybrid (H). # Leja indicates the number of Leja nodes for one frequency point ω<sub>j</sub>, # HF the number of high fidelity evaluations to build the surrogate model (surr.), to evaluate (critical) MC samples (MC) with indicated refinement, eff the measurement for computational effort according to (21) and err the relative error according to (20).

5.3.2 Yield estimation

We proceed by comparing the proposed hybrid approach with standard MC and a surrogate-based Monte Carlo approach without hybridization. The surrogate model is constructed based on sparse-grid interpolation as explained in Section 3.2. In order to achieve a high accuracy in the L<sup>∞</sup>-norm, we employ, in this work, uniform weight functions w<sub>m</sub> in the ranges given by the nominal parameter values p ± truncation offset t. The comparison is based on both the computational effort and the accuracy. For the accuracy we use the relative error between the reference solution and the solution of the considered method, i.e. for the hybrid approach

\[
\text{err}_H = \frac{|Y_{\text{Ref}} - Y_H|}{Y_{\text{Ref}}}, \quad (20)
\]

err<sub>SC</sub>, err<sub>MC</sub> for SC and MC respectively. We measure the computational effort with the number of high fidelity (HF) evaluations (i.e. matrix factorizations in FEM). Here we have different levels of HF evaluations due to mesh refinement within the proposed hybrid approach. We start with a mesh size h, and if necessary divide it by two. The difference in the computational effort for each refinement level depends on the model structure and the solver used. Assuming an optimal solver with an effort which is linear in the number of degrees of freedom, the effort increases by a factor of four in the case of a 2D problem and by a factor of eight in the case of a 3D problem. Since in our case the E-field is constant in y-direction, the grid is only refined in x- and z-direction. Thus, the computational effort of a method is measured through

\[
\text{eff} = \#HF_h + 4 \#HF_{h/2} + 16 \#HF_{h/4} \quad (21)
\]

which adds up the number of HF evaluations on the different levels, each multiplied by the factors mentioned above.

The standard approach to carry out yield estimation, with the same accuracy as with the proposed hybrid approach, would be a MC analysis with the finest mesh used within the hybrid approach, referred to as MC<sub>fine</sub>. If the mesh refinement strategy is additionally applied, the method is denoted as MC<sub>refine</sub>. In order to build the surrogate model both for SC and for the hybrid approach, we use the first grid with mesh size h without further refinement to evaluate the model at the Leja nodes. In Table 1 we see the results of the comparison. We consider two versions of SC, each with different accuracy (number of Leja nodes). The surrogate model used for the hybrid approach is the same as for SC with 90 Leja nodes. For each approach we use the same MC sample as for the reference solution. With the hybrid approach and MC we achieve the same result as with the closed form reference solution. Out of these three, the hybrid method requires the least computational effort. Compared to MC<sub>refine</sub>, we can save 73 % computing time, compared to MC<sub>fine</sub> even 98 %. Comparing the hybrid and MC<sub>refine</sub> approach, we observe that most of the MC sample points are evaluated on the coarsest grid. Only for a few points, a refinement of the grid to h/2 (25 sample points) or h/4 (6 sample points) is necessary. Using the same surrogate model as for the hybrid approach, pure SC has much less computational effort with eff = 900, but the error is larger than 6 %. Increasing the number of Leja nodes to 1,600 results in three times higher computational effort compared to the hybrid approach, with an error still larger than 0.4 %. Table 2 shows the results for the same waveguide with only four uncertain parameters. The statement remains unchanged. However, the influence of the number of parameters can be seen. With four uncertain parameters also with SC we can reduce the error to zero, with only about two and a half times the computational effort compared to the hybrid method. The higher the number of uncertain parameters, the more gain can be expected from the hybrid approach compared to a SC method. Compared to MC<sub>refine</sub>, with the hybrid approach, we can save almost 98 % computing time, compared to MC<sub>fine</sub> even 99.8 %. This means that the advantage of the hybrid approach over MC increases as the number of parameters decreases. Nevertheless, we know by construction, that even for high numbers of uncertain parameters, the hybrid method can never become worse than MC excluding the computational effort to build the surrogate model (which could scale poorly for a high-dimensional problem) and evaluate the error indicator.
Table 2: Comparison of different yield estimation approaches for four uncertain parameters.

| approach     | # Leja | # HFₜₜ surr. | # HFₜₜ MC | # HFₜₜ/₂ MC | # HFₜₜ/₄ MC | eff      | err (%) |
|--------------|-------|--------------|-----------|-------------|-------------|---------|--------|
| MCfine       | -     | 0            | 0         | 0           | 26,360      | 421,760 | 0.0000 |
| MC refine    | -     | 0            | 26,360    | 5           | 1           | 26,396  | 0.0000 |
| H            | 30    | 330          | 165       | 5           | 1           | 531     | 0.0000 |
| SC           | 30    | 330          | 0         | 0           | 0           | 330     | 0.1257 |
| SC           | 120   | 1,320        | 0         | 0           | 0           | 1,320   | 0.0000 |

Different methods: MC, SC and hybrid (H). # Leja indicates the number of Leja nodes for one frequency point ωₖ, # HF the number of high fidelity evaluations to build the surrogate model (surr.), to evaluate (critical) MC samples (MC) with indicated refinement, eff the measurement for computational effort according to (21) and err the relative error according to (20).

Table 3: Comparison of adaptive and nonadaptive Newton’s method for yield optimization.

| estimation | # Leja | # param. | optimization   | # It | # YE | eff      | Y* (%) |
|------------|-------|----------|----------------|-----|-----|---------|--------|
| H          | 90    | 12       | adapt. Newton-MC | 33  | 86  | 376,073 | 74.84  |
| H          | 90    | 12       | Newton          | 37  | 42  | 682,745 | 78.20  |
| H          | 30    | 4        | adapt. Newton-MC | 12  | 27  | 13,716  | 95.44  |
| H          | 30    | 4        | Newton          | 30  | 34  | 138,158 | 97.92  |

Comparison of adaptive and nonadaptive Newton’s method with twelve and four uncertain parameters. # Leja indicates the number of Leja nodes for one frequency point ωₖ, # param. the number of uncertain parameters, optimization the method used, # It the number of iterations, # YE the number of yield estimations, eff the computational effort and Y* the optimal yield value.

5.3.3 Yield optimization

We compare the proposed adaptive Newton-MC from Algorithm 3 with the standard Newton method from Algorithm 2, both with the same limited number of Armijo backsteps and the presented hybrid approach for the yield estimation. In both cases we set the target accuracy to $\delta_Y = 0.01$. The adaptive approach starts with 100 sample points and increases this number adaptively until optimality and a target accuracy are achieved. In the non-adaptive approach, we specify a fixed sample size so that the target accuracy is guaranteed at all times during the optimization process. This fixed sample size is $N_{MC} = 2,500$. In Table 3 we see the results for tests with twelve or four uncertain parameters. The number of iterations of single yield estimations within the optimization process, the computational effort (eff) and the optimal yield value ($Y^*$) are given. Note that, during the optimization process the surrogate model is only built once, for the starting point. Accepting higher computational effort, the surrogate model can also be recalculated in each iteration step for the current solution, or built at the beginning in a larger interval than $p_0 \pm t$.

With twelve uncertain parameters, we started with a yield of 15%. The adaptive and the non-adaptive approach lead to different local optima with similar yield values. Both take a bit more than 30 iterations. On average, two and a half yield estimations are performed per iteration using the adaptive approach. This is due to multiple evaluations by Armijo backsteps. The non-adaptive approach has only 1.2 estimations per iteration. This can be explained by the fact that the adaptive approach performs several Newton optimizations with different sample sizes one after the other. Shortly before a Newton procedure is terminated, there is usually no further improvement, which is why Armijo backsteps increase and so does the number of yield estimations. This is the case every time before the sample size is increased in the adaptive algorithm. In the non-adaptive approach, this behaviour occurs only once at the end. Potential for improvement in the adaptive approach lies in further reducing the number of yield evaluations through smoother transitions from one sample size to the other. Nevertheless, the adaptive approach reduces the computational effort by a factor of two compared to standard Newton, see column eff in Table 3. In tests with only four uncertain parameters, the computing effort was even reduced to 10%. In this case, the adaptive approach resulted in significantly fewer iterations. The ratio between iterations and yield estimations remains unchanged.

For the case with four uncertain parameters we also draw a comparison to standard procedures. Standard procedure means in this case, combining a standard Monte Carlo analysis for the yield estimation with a standard Newton method for the optimization. On the coarsest grid ($h$), 816, 816 evaluations with FEM were necessary to optimize the yield, i.e. eff = 816, 816. Thus, with the proposed adaptive Newton-MC, a saving of 98.3% in computing effort could already be achieved compared to the standard procedure mentioned above. However, in order to achieve the same accuracy as with the proposed method, the finest grid ($h/4$) has to be used for all sample points. We assume that the number of
Table 4: Progress of yield optimization with adaptive Newton-MC.

| iteration | \(N_{MC}\) |
|-----------|-------------|
| 0-12      | 100         |
| 13-14     | 200         |
| 15-18     | 300         |
| 19        | 500         |
| 20-22     | 600         |
| 23        | 900         |
| 24-30     | 1,000       |
| 31        | 1,800       |
| 32-33     | 1,900       |

Progress of yield optimization with adaptive Newton-MC for twelve uncertain parameters. Number of MC samples for each iteration of the optimization algorithm.

Function evaluations do not change significantly due to the grid refinement. This can be motivated by the fact, that a similar number of iterations, yield estimations and function evaluations were needed for calculation with the closed from solution as for the FE model with coarser grid. Under this assumption we got an effort factor of \(\text{eff} \approx 13 \cdot 10^6\). Thus the saving of computational effort is even 99.9\%.

For twelve uncertain parameters, in Table 4 we see how many MC samples have been used in which iteration. For most of the iterations a low number of MC samples is sufficient, only in the last iterations we need to expend more computational effort in order to guarantee the pre-defined target accuracy.

6 Conclusion

In this paper we proposed a fully error controlled method for yield estimation and optimization. For yield estimation we developed a hybrid approach combining reliability and accuracy of a high fidelity Monte Carlo (MC) analysis and the efficiency of surrogate based techniques such as stochastic collocation (SC). In case the accuracy of the surrogate model is not sufficient, sample points are re-evaluated employing the high fidelity finite element (FE) model. Mesh refinement is applied if the accuracy of the FE model itself is too low. This guarantees error control while only a very small subset of the MC sample is evaluated based on expensive high fidelity evaluations. Adjoint error indicators were applied to estimate the errors of the surrogate model and the FE model. For yield optimization we proposed an adaptive Newton-MC method, based on a globalized Newton method. During the optimization process, numerous yield estimations are performed. In order to control the MC error and at the same time save computational effort, we adaptively increase the number of MC sample points used during the optimization. Thus, the adaptive Newton-MC in combination with the hybrid approach allows us to control the FE error, the MC error and the surrogate error. At the same time it is much more efficient than conventional MC approaches with a standard Newton method. Numerical tests on a dielectrical waveguide confirm the benefits of the presented method. Future research will deal with the transitions in the adaptive Newton-MC when the MC sample size is increased. Furthermore, although we already use a hierarchical model for Monte Carlo analysis within the optimization, we plan to explore a combination of this with a multilevel Monte Carlo approach [3].

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