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Title:	Intermediate Report on Models and algorithms for quantification of uncertainties in materials, geometry and boundaries of devices
Authors(s):	Herbert De Gersem, Sebastian Schöps, Ulrich Römer
Affiliation(s):	KUL, TUDA
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1 Introduction

Appropriate methods for treating uncertainties coming from undesired variabilities and imperfections in the manufacturing process are needed. Uncertain parameters may be material properties, geometrical parameters and environmental parameters, such as, e.g., the temperature at the device boundaries. Task T2.1 improves on methods for characterizing given uncertainties in volumetric discretization of the Maxwell equations and on techniques for propagating uncertainties through the field simulation. A special emphasis is on field-circuit coupled models and electromagnetic-thermal coupled models.

2 Models

From the numerous types of possible model input parameters, we focus on uncertainties in the material properties and the geometry. In general, in a stochastic setting, uncertain inputs are modeled by means of (infinite-dimensional) random fields and hence, for computer simulations the task of discretization needs to be accomplished. Several techniques have been proposed to this end. We refer to the Karhunen-Loève expansion, the generalized Polynomial Chaos technique, as well as model specific grid based, or analytic representations. Moreover, as the dimensionality of the discrete representation is directly related to the computational cost, efficient low-rank representations are highly desirable and efforts should be devoted to their construction. In this context controlling the respective (modeling) error in the stochastic solution is of importance.

2.1 Materials

Material uncertainties can be found in, e.g., the (nonlinear) material constitutive law [1]. It has been observed that in several applications this is the most influential source of uncertainty [2]. The stochastic modeling is complicated by the fact that the nonlinear material relation and hence the random field is subject to shape constraints. In particular the monotonicity and the smoothness need to be preserved. We investigate how this can be achieved by means of the Karhunen-Loève expansion and flexible spline representations of the constitutive law. In particular relations for the input discretization errors and for accomplishing the shape constraints are derived.

2.2 Geometry

Uncertainties in the geometry may refer to both an interface between two different materials and the boundaries of the computational domain. A major difficulty arises as the equations are formulated on different domains due to the uncertainty. Also shape perturbations have to be modeled appropriately and re-meshing efforts should be kept minimal. Here, spline representations are used to model shape deformations. Moreover, in the context of sensitivity analysis we employ the velocity method [3], a well established technique from shape optimization. A transformation $\mathcal{T}_s = x_s$ can be defined by means of the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}s} x_s = \mathcal{V}, s \geq 0, \tag{1}$$

endowed with suitable initial conditions, where V is referred to as velocity field, see also Figure 1.

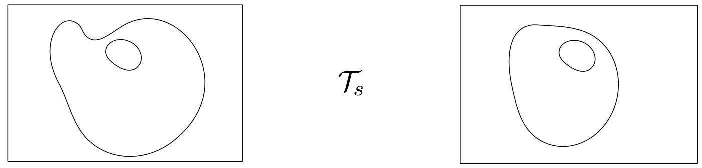

Figure 1: Velocity Method: family of transformed interfaces/domains by means of $\mathcal{T}_s$.

Considering uncertainties of geometrical parameters is particularly challenging. A straightforward procedure consists of changing the geometry, remeshing and recalculating. This approach is, however, unfeasible because the numerical noise due to a possible change of the mesh topology may exceed the variations due to the uncertainty [4]. It is absolutely necessary to define geometrical uncertainties by a continuous mapping from a reference geometry [5]. The intended developments go in that direction.

3 Algorithms

Once a finite representation of the stochastic inputs is at hand, uncertainties need to be propagated efficiently through the model. To this end various deterministic techniques, such as spectral methods [6, 7] and moment based perturbations methods [8], have been found to be superior to classical Monte Carlo sampling in several circumstances. This is true in particular for low-rank input representations and an analytical input-output dependence of the model.

3.1 Stochastic Collocation

The stochastic collocation method has received considerable attention due to the ease of handling nonlinear problems and its non-intrusive character [9, 10]. For a quantity of interest F, depending on an input random field Y, approximations of statistical moments are obtained by

$$\begin{aligned}\mathbb{E}\big[F(Y)\big] &\approx \sum_{k=1,\ldots,N} w_k\, F(Y^{(k)}),\\ \operatorname{var}\big[F(Y)\big] &\approx \sum_{k=1,\ldots,N} w_k\, \big(F(Y^{(k)}) - \mathbb{E}\big[F(Y)\big]\big)^2.\end{aligned}$$

Here, $Y^{(k)}$ and w_k represent the collocation points and weights, respectively. See also Figure 2 for a popular sparse grid construction as opposed to stochastic Monte Carlo sampling. They are chosen according to the underlying probability distribution of Y, giving rise to spectral convergence rates of the methods in many situations. However, most of the results have been established for linear model problems with uncertainties in the coefficients and additional efforts with regard to the application to complex engineering applications, with non-linearities are needed.

3.2 Perturbation

Perturbation methods are among the most efficient methods for uncertainty propagation, though limited to small input variations. The input random field is represented in the form $Y_s = \overline{Y} + s\tilde{Y}$, possibly infinite-dimensional. By means of a stochastic Taylor expansion

$$F(Y_s) = F(\overline{Y}) + s\,\underbrace{dF(\overline{Y};\tilde{Y})}_{:=dF_{\tilde{Y}}} + \mathcal{O}(s^2) \tag{2}$$

Figure 2: Smolyak sparse grid on the left and Monte Carlo sampling of the two-dimensional random vector on the right.

approximations of the first two statistical moments are given by

$$\mathbb{E}[F] = F(\overline{Y}) + \mathcal{O}(s^2), \tag{3}$$

$$\mathrm{var}[F] = s^2 \mathbb{E}[dF_{\overline{Y}}^2] + \mathcal{O}(s^3). \tag{4}$$

With the gradient at hand, the computation of $\mathbb{E}[dF_{\overline{Y}}^2]$ now only involves the evaluation of high-dimensional integrals by means of sparse-grid or Monte-Carlo techniques. The asymptotic expressions (4) are numerically justified [11], whereas the efficient estimation of the remainder terms, indispensable for the method's reliability is still work in progress.

The computation of gradients with respect to geometry, i.e., shape calculus, is rather involved. Recently, based on the velocity method, shape calculus has been embedded in a differential form setting [12]. This approach is not only well suited for electromagnetics but also typically simplifies manipulations. This work further contributes to the application of shape calculus to electromagnetics with special emphasis on shape derivatives of fields. This is particularly important for the propagation of uncertainties given by low-rank representations of stochastic geometries.

4 Outlook

Further work on Task 2.1 will focus on uncertainty quantification for field-circuit coupled and electromagnetic-thermal coupled models of nano-electronic components. The specific structure of these models will be exploited to improve the algorithms.

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