Uncertainty Quantification Using Reduced-Order Maxwell's Equations

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Summary. We compare stochastic collocation and Monte Carlo simulation by applying them to the reduced-order time-harmonic Maxwell's equations.

1 Motivation

During the design process of new semiconductor structures, simulation is very important due to the expensive production of prototypes. The simulation of integrated circuits involves the solution of discretized Maxwell's equations in thousands up to some millions of degrees of freedom. Therefore, the evaluation is often only feasible using reduced order models (ROMs).
Another important aspect is that the material parameters as well as the geometry of circuits and devices are subject to small variations. To handle these uncertain variations, the concerned quantities are replaced by random variables (RVs). The distributions of these RVs are assumed to be given for the moment - in practice, it is a non-trivial task to obtain this information.
We are now interested in the influence of the uncertainties on the solution of the considered system. This influence can be analyzed with the help of Uncertainty Quantification (UQ) [5, 7]. We assume that in our approaches the discretization of the underlying structure is fixed. This is a requirement which comes from industrial applications where the discretization is provided by external (black box) tools. Therefore, we need to work with non-intrusive UQ methods, which do not enter the level of discretization. Non-intrusive UQ methods are sampling methods that require repeated evaluations of the system. Therefore, it is even more important that we use ROMs in our computations.

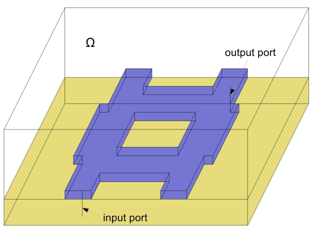

Fig. 1. Branchline Coupler, see [6].

Owing to the uncertain parameters in our system, we need a parametric model order reduction (PMOR) method that can be applied to Maxwell's equations and preserves the uncertain parameters. Therefore, we use a new parametrized version of the adaptive-order rational Arnoldi-type (AORA) methods described in [1, 2], later called pAORA. It was developed in cooperation with the authors of the original paper.
Figure 1 shows a branchline coupler which serves as a benchmark and for which we show some numerical results in the talk.

2 Parametric Model Order Reduction for Maxwell's Equations

Throughout the talk, we will work with the discretized second-order Maxwell's equations, i.e.

$$\begin{aligned} A_{\mu_0}(\mu_r)\mathbf{e} + A(\sigma)\dot{\mathbf{e}} + A_{\varepsilon_0}(\varepsilon_r)\ddot{\mathbf{e}} &= Bu, \\ y &= C\mathbf{e}, \end{aligned} \tag{1}$$

with the electric field intensity $\mathbf{e}$, the input u, and the output y. The material parameters are the relative permeability μ_r, the electric conductivity σ, and the relative permittivity ε_r. Besides that, we use the magnetic constant $\mu_0 = 4\pi \cdot 10^{-7}\, Vs/Am$ and the electric constant $\varepsilon_0 = (\mu_0 c^2)^{-1}$, with $c = 299792458\, m/s$ the speed of light in vacuum.
For simplicity, we assume that the system matrices $A_{\mu_0}(\mu_r), A(\sigma), A_{\varepsilon_0}(\varepsilon_r) \in \mathbb{R}^{n_f \times n_f}$, n_f large, are affine with respect to the parameters μ_r, σ, and ε_r. In our numerical example, see Section 4, we have $\sigma \equiv 0$. Therefore, the second term on the left-hand side vanishes. Thanks to this property, we can apply the pAORA method described below.

Moment Matching Methods

The application of the pAORA method to the time-harmonic Maxwell's equations associated to (1) with $\sigma \equiv 0$ requires the transfer function of the system

$$G(s,p) = C\left(s^2 A_{\varepsilon_0}(\varepsilon_r) + A_{\mu_0}(\mu_r)\right)^{-1} B,$$

with the parameter vector $p = (\varepsilon_r, \mu_r)^T$ and $s \in \mathbb{C}$ and yields an orthonormal matrix $V \in \mathbb{R}^{n_f \times n_r}$ for the Galerkin projection $\Pi = VV^T$. Hence, we can compute a ROM of size $2n_r \ll n_f$

$$\begin{aligned} \tilde{A}_{\mu_0}(\mu_r)\tilde{\mathbf{e}} + \tilde{A}_{\varepsilon_0}(\varepsilon_r)\ddot{\tilde{\mathbf{e}}} &= \tilde{B}u, \\ \tilde{y} &= \tilde{C}\tilde{\mathbf{e}}, \end{aligned}$$

such that the input-output behavior of the original system is preserved. The size of the reduced system is $2n_r$ to ensure that the reduced matrices are real.
Using this ROM for the UQ methods described in Section 3 saves computation time.

3 Uncertainty Quantification

Uncertainty propagation is the quantification of variations in the system outputs spread from uncertain inputs. The methods can be divided in so-called intrusive and non-intrusive ones. The most popular non-intrusive method is the Monte Carlo (MC) simulation, see e.g. [4]. The idea behind MC is the law of large numbers which describes the result of running the same experiment a large number of times for realizations of the RVs obeying their probability distribution. We will also discuss stochastic collocation. Like MC it is sampling based, only the choice of sample points and weights is different. We will discuss Stroud-based and sparse-grid-based collocation as in [9].

3.1 Monte Carlo Simulation

As mentioned before, MC is well known and easy to implement. It uses equally weighted random points for the sampling. Hence, it is independent of the number of parameters in the system. The only drawback is that the convergence is proportional to $1/\sqrt{n}$, where n is the number of sample points. Therefore, we need a very high number of sample points to guarantee accuracy. We use an MC simulation of the full order model (FOM) with 10^6 sampling points as reference solution for the error computation.

3.2 Stochastic Collocation

For collocation methods, the number of used sample points depends on the number of parameters. The idea is to use less points than MC but to choose them more carefully. There are several possibilities for the choice of collocation points. The easiest but also most expensive choice would be a full tensor grid. With that, we would not gain much compared to MC. In the following, we will use two other sets of sample points. On the one hand, we apply the so-called Stroud-3 rule [8] to compute the collocation points. On the other hand, we use a Hermite Genz-Keister [3] sparse grid of level 1 and 2 (HGK 1, HGK 2). Both sets yield normally distributed sample points and weights in the quadrature rule.

Model \ Method	Stroud-3	HGK 1	HGK 2
FOM (27679 dofs)	$1.18 \cdot 10^{-5}$	$1.17 \cdot 10^{-5}$	$1.18 \cdot 10^{-5}$
ROM (40 dofs)	$4.49 \cdot 10^{-3}$	$4.49 \cdot 10^{-3}$	$4.49 \cdot 10^{-3}$

Table 1. Relative errors for the output y of the branchline coupler with $\omega = 10\,GHz$.

4 Numerical Example

We apply the described approaches to the branchline coupler shown in Figure 1 which consists of four strip line ports, coupled by two transversal bridges with each other. The branchline coupler is placed on a substrate. The rest of the simulation domain is filled with air. The metallic ground plate of the device is represented by the electric boundary condition. The magnetic boundary condition is considered for the other sides of the structures. We have three uncertain parameters, the relative permittivity in substrate and air, ε_r^s and ε_r^a, and the relative permeability μ_r in the whole domain. The electric conductivity $\sigma \equiv 0$ in the whole domain. The discrete port 1 imposes 1 Ampere current as the input u of the system. The voltage along the coupled port 2 is measured as output y. Therefore the discretized time-harmonic system we work with reads

$$A_{\mu_0}(\mu_r)\mathbf{e} - \omega^2(A^s_{\varepsilon_0}(\varepsilon_r^s) + A^a_{\varepsilon_0}(\varepsilon_r^a))\mathbf{e} = -i\omega B u,$$
$$y = C\mathbf{e}.$$

In Table 1 we show the relative errors for the output y at a frequency of $\omega = 10\,GHz$. More results will be shown in the talk.

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