Stochastic Collocation Methods and Model Reduction for Maxwell's Equations

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Summary. We use a Stroud-based collocation method to analyze the parameter behavior of the time-harmonic Maxwell equations and reduce the computational costs by applying model order reduction to the system matrices.

1 Motivation

During the design process of semiconductor structures, simulations of new micro and nano scale systems are essential due to, e. g., the expensive production of prototypes. An important aspect is the ongoing miniaturization of the structures on the one hand and the increase in the working frequencies on the other hand. The high density of electric conductors induces parasitic effects, e. g., crosstalk, which have to be considered already in the design stage. Therefore, the exact knowledge of the semiconductor structures and the surrounding electromagnetic (EM) field is necessary.
Another effect, which plays a no longer negligible role, is the variation of the feature structure size caused by inaccuracies of the resolution during the lithography. To consider these variations in the simulation, models with parametric uncertainties are required. A variational analysis of the effect of these uncertainties on the EM field requires methods for uncertainty quantification (UQ) [4, 6]. For this purpose, we will employ non-intrusive approaches as they allow the use of EM field solvers for deterministic problems without accessing the source code. Possible choices are Monte Carlo and stochastic collocation. Here we will employ the latter due to their faster convergence. Still, UQ via stochastic collocation requires numerous full-order EM field solves which can be a time-consuming task for complicated 3D geometries. It is thus our goal to combine this approach with model order reduction methods (MOR) for the Maxwell equations to reduce the computational cost, where the reduced-order model needs to preserve the statistical properties of the full-order model. All these problems are addressed within the research network *Model Reduction for Fast Simulation of New Semiconductor Structures for Nanotechnology and Microsystems Technology (MoreSim4Nano)*, see [5]. Figure 1 shows a coplanar waveguide which serves as a benchmark within MoreSim4Nano and for which we show some numerical results in Section 4.

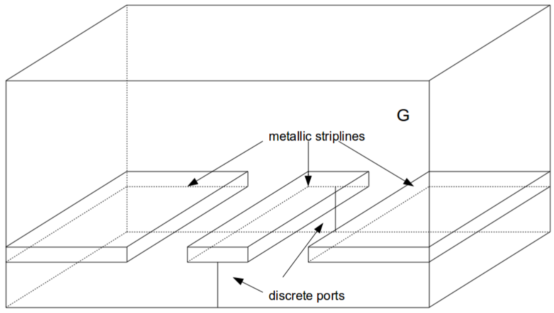

Fig. 1. Coplanar waveguide.

2 Stochastic Collocation for EM Field Computations

The system of equations describing the EM field are Maxwell's equations

$$\begin{aligned}\partial_t(\varepsilon \boldsymbol{E}) &= \nabla\times\boldsymbol{H} - \sigma\boldsymbol{E} - \boldsymbol{J}\\ \partial_t(\mu\boldsymbol{H}) &= -\nabla\times\boldsymbol{E}\\ \nabla\cdot(\varepsilon\boldsymbol{E}) &= \rho\\ \nabla\cdot(\mu\boldsymbol{H}) &= 0,\end{aligned}$$

with the electric field intensity $\boldsymbol{E}$, the magnetic field intensity $\boldsymbol{H}$, the charge density ρ, the impressed current source $\boldsymbol{J}$, and material parameters $\varepsilon = \varepsilon_r\cdot\varepsilon_0$ (permittivity), $\mu = \mu_r\cdot\mu_0$ (permeability), σ (electrical conductivity). For simplification, we work with the time-harmonic form

$$\nabla\times(\mu^{-1}\nabla\times\boldsymbol{E}) + i\,\omega\,\sigma\boldsymbol{E} - \omega^2\,\varepsilon\boldsymbol{E} = i\,\omega\boldsymbol{J}, \qquad (1)$$

on the space $X = \{\boldsymbol{E}\in H^0_{curl}|\nabla\cdot(\varepsilon\boldsymbol{E}) = \rho\}$.
Up to now, we consider the material parameters ε_r, μ_r, and σ as uncertain. For the examination of their influence on the statistical behavior of the solution $\boldsymbol{E}$ we use stochastic collocation [1] with Stroud interpolation points [2].

2.1 Stochastic Collocation

Collocation methods rely on interpolation. The idea is to approximate high-dimensional integrals, e. g., the expectation value of our solution $\boldsymbol{E}$, by an (efficient) quadrature rule

$$\mathbb{E}(\boldsymbol{E}) = \int_{\Gamma} \boldsymbol{E}(\xi) f(\xi) d\xi \approx \sum_{i=1}^{n} \boldsymbol{E}(\xi_i) w_i.$$

Here Γ is the image of the probability space under the probability measure, f is the unknown probability density function of $\boldsymbol{E}$, ξ_i are the n interpolation points and w_i are the associated weights.

2.2 Stroud Integration

The interpolation formula used in our algorithm was introduced in 1957 by A. H. Stroud [7] and yields either beta or normal distributed interpolation points which are weighted by $1/n$, where n is the number of interpolation points as in Sec. 2.1. Though we need $\varepsilon_r, \mu_r > 0$ and $\sigma \geq 0$, we suppose them to be lognormal distributed and use the exponential of the normal distributed Stroud points as interpolation points.

3 Model Order Reduction

The discretization of (1) leads to the following system

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

where $\boldsymbol{e}$ is the discretized electric field, $A_{\mu_0}, A_{\varepsilon_0}$ and A are the parameter independent system matrices in $\mathbb{R}^{N \times N}$, u, y define the inputs/ outputs, and B, C specify the input/ output behavior. Here N is the number of grid points in G and large. This system is then reduced, e. g., by means of rational interpolation methods as in [3] and we achieve a reduced system of the form

$$\begin{aligned} \mu_r \hat{A}_{\mu_0} \hat{\boldsymbol{e}} + \varepsilon_r \hat{A}_{\varepsilon_0} \ddot{\hat{\boldsymbol{e}}} + \sigma \hat{A} \dot{\hat{\boldsymbol{e}}} &= \hat{B}u, \\ \hat{y} &= \hat{C}\hat{\boldsymbol{e}}, \end{aligned}$$

where $\hat{A}_{\mu_0}, \hat{A}_{\varepsilon_0}, \hat{A} \in \mathbb{R}^{r \times r}$ with $r \ll N$ and $||y - \hat{y}||$ small.

4 Numerical Results Concerning the Stochastic Collocation Approach

As a benchmark we consider a coplanar waveguide with dielectric overlay, see Figure 1. The model consists of three perfectly conducting striplines situated at a height of $10mm$ in a shielded box with perfect electric conductor (PEC) boundary. The system is excited at one of the discrete ports and the output is taken at the other one.
Below a height of $15mm$ there is a substrate with $\varepsilon_r^1 \approx 4.4$ and $\sigma^1 \approx 0.02S/m$, above there is air with $\varepsilon_r^2 \approx 1.07$ and $\sigma^2 \approx 0.01S/m$, while $\mu_r \approx 1$ within the whole box. The variance of each parameter is approximately 1% of the expected value.
The system is treated as a system with 5 uncertain parameters, which leads to the affine discretized form

$$\begin{aligned} \mu_r A_{\mu_0} \boldsymbol{e} + (\varepsilon_r^1 A_{\varepsilon_0}^1 + \varepsilon_r^2 A_{\varepsilon_0}^2) \ddot{\boldsymbol{e}} + (\sigma^1 A^1 + \sigma^2 A^2) \dot{\boldsymbol{e}} &= Bu, \\ y &= C\boldsymbol{e}. \end{aligned}$$

The discretization is done in FEniCS by use of Nédélec finite elements and the Stroud-based collocation is implemented in MATLAB®. Since the used discretization has only 18755 degrees of freedom, there is no model order reduction used up to now.
The Stroud-based collocation uses only 10 supporting points and the computation requires less than a minute. To verify the accuracy, the results are compared with a Monte Carlo simulation which operates on 10000 interpolation points. This takes several hours. Using the frequency $\omega = 0.6 \cdot 10^9$ we achieve the following relative errors for the expected value of $\boldsymbol{e}$ and y

$$err_{rel,\mathbb{E}(\boldsymbol{e})} = 0.0038\% \quad \text{and} \quad err_{rel,\mathbb{E}(y)} = 0.0042\%.$$

Considering the fact that we use only 10 Stroud points the results are satisfactory. To achieve more accuracy one could use, e. g., a lot more sparse grid points, which would be much more expensive. For this reason and for systems of higher dimension we need MOR.

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