Reduced basis methods for optimization of nano-photonic devices

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***Abstract*—Optical 3D simulations in many-query and real time contexts require new solution strategies. We study an adaptive, error controlled reduced basis method for solving parametrized time-harmonic optical scattering problems. Application fields are, among others, design and optimization problems of nano-optical devices as well as inverse problems for parameter reconstructions, as they occur, e. g., in optical metrology. The reduced basis method presented here relies on a finite element modeling of the problem plus parametrization of materials, geometries and sources.**

I. Introduction

The challenge for electromagnetic field solvers is typically efficiency, that is to achieve highly accurate results at low computation times where the numerical error remains below some acceptable threshold. The requirements with respect to computations times become immediately apparent in optimizations tasks and inverse problems. During the optimization of a structure typically a large number of computations with varying parameters has to be performed until the optimal structure is found. The same holds true for inverse problems,where measured data are given and structure details have to be derived. Especially in real time applications, where the measurement data pop up in a quick sequence, new solution strategies for a repeated solution of 3D problems are required. The reduced basis method (RBM) is a method able to cope with such challenges. In the following we consider the application of the reduced basis method to time-harmonic Maxwell equations. The structure discussed here is a FinFET from the semiconductor industry. FinFETs are realized on wafers and measured after manufacturing by optical methods to check the actual geometrical shape. The measurement consists of an illumination of an array of periodically placed FinFETs and a determination of the reflected diffraction orders in dependence of the wavelength and polarization.

II. Reduced Basis Method

The basic concepts of the RBM were described in [1] and first applications to nano-optics have been published in [2], [3]. Figures 1 and 2 give the geometrical structure of the FinFETs discussed in the following. In a previous study [4] we analyzed the same structure, but without application of the RBM. The entire task consists in the determination of geometrical parameters of the FinFETs based on the measured reflected field. In the following we consider the sub-problem of a real-time solution of the forward problem. This is the key prerequisite for any fast reconstruction algorithm.

It is assumed that the solution process can be split into an *online* and an *offline* part.

Offline : The part is computational expensive, but it is done only once as preparation of the online phase. It consists mainly of the computation of so called snapshots, which are full 3D solutions, each with respect to a certain parameter setting. These parameters cover the entire range of parameters such that all characteristic solutions are contained in the set of snapshots. This coverage of the parameter space is done automatically by adaptively controlled Greedy algorithms. The number of snapshots is typically in the order of $10 \dots 100$. Additionally, a number of pre-computations for the online step has to be performed.

Online : The actual computation is done online in real time. Given a point in parameter space, the desired 3D solution is constructed by a superposition of the precomputed snapshots. This superposition, sometimes called Galerkin interpolation, requires the solution of a very small linear system with a dimension in the order of the number of snapshots. Hence, each online computation requires the inversion of a, say, 100×100 matrix, which goes extremely fast in comparison to the solution of the original full system. Moreover, the design goal of reduced basis methods is to have online costs completely independent from the size of the original system used in the offline phase.

III. Results

Fig. 1 shows the FEM-discretized FinFET with its two gates. For a simple graphical representation of results we consider a variation in two parameters only: the radii of curvature of the the Fin and the Gate. The reflected field changes according to the variation of these curvatures.

The reduced basis method is used to construct an online algorithm which returns quickly the reflected field depending

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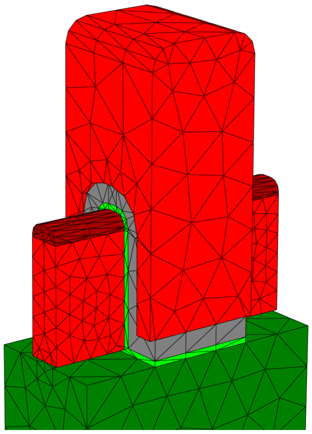

Figure 1. Part of a FinFET, meshed with tetrahedrons, displaying the Fin and the Gate structure. All geometric quantities like widths, heights, curvatures (cf. Fig. 2) may be considered as parameters of a scattering experiment.

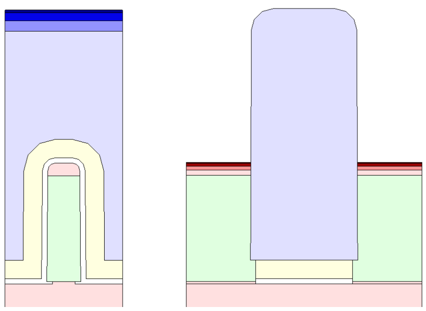

Figure 2. Cross section showing the Fin (left) and the Gate (right) with their curvatures, which are the parameters in the reduced basis study.

on the radii and the given wavelength. Fig. 3 shows the corresponding geometrical representation. What is the numerical effort to compute a single point in the graph of Fig. 3? Conventionally it corresponds to one full 3D simulation. In the reduced bases context it corresponds roughly to the inversion of the reduced matrix with a dimension given by the number of snapshots.

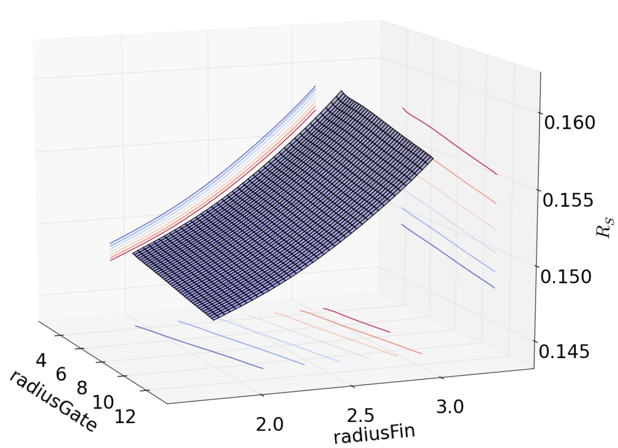

Figure 3. Norm of the reflected field in dependence of the radii of Gate and Fin.

The larger the number of snapshots the better the approximation of the reduced system with respect to the full system. Tab. I shows convergence in the given situation. The use of only five snapshots is not sufficient to cover the entire parameter space, the relative error in the reflected field is about 10%. But already 6 snapshots result in an accuracy acceptable for the application. Increasing the number of snapshots to 20 decreases the maximal error further, finally to about $2 \cdot 10^{-8}$. A more detailed convergence analysis shows an exponential convergence.

Table I
CONVERGENZ OF THE REFLECTED FIELD VS. THE NUMBER OF SNAPSHOTS

number of snapshots	error
5	9.82e-02
6	8.83e-05
20	1.55e-08

IV. CONCLUSIONS

The reduced basis method deals successfully with many-query and real-time simulation tasks. The necessary algorithmic preparations are relatively high: The discrete Maxwell operator has to be parametrized in a way that permits effective offline-online decompositions, here typically discrete empirical interpolation methods come into play [5], the parameter-space has to be covered by snapshots with accepted errors below a pre-defined error threshold, the online phase has to be organized in a way that the independence of the number of unknowns of the full 3D problem is ensured. As a result one gets a very fast, error controlled real time capable procedure successful in situations where a direct application of the direct problem would be not realistic.

ACKNOWLEGMENT

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