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Reduced basis method for the optimization of nano-phonic devices

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Reduced basis method for the 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 occurring e. g. in optical metrology. The reduced basis method presented here relies on a finite element modeling of the scattering problem with parametrization of materials, geometries and sources.

1 Introduction

Electromagnetic field solvers must be efficient to be of use for optimization tasks of 3D structures where computation times are of importance as typically a large number of computations with varying parameters have to be performed until the optimal structure is found. The same holds true for inverse problems where measured data is given and structural details are sought after. Hence there is a demand for highly accurate, error controlled results at low computation times. Especially for real time applications new solution strategies for a repeated solution of 3D problems are required.

The reduced basis method (RBM) is such a strategy. Here we consider application of the RBM to time-harmonic Maxwell's equations based on a finite element (FEM) discretization. The setup discussed here is light scattering off a fin field-effect transistor (FinFET)(analyzed previously without the RBM[3]). FinFETs are realized on wafers and measured after manufacturing by optical methods to control the actual geometrical shape. The measurement consists of an illumination of an array of periodically placed FinFETs and a determination of the reflectance in dependence of the wavelength and polarization.

2 Reduced basis method

The reduced basis method [8, 9] allows to construct error controlled approximations to the relationship of an input, a specific configuration of parameters $\mu \in \mathbb{R}^d$, to an output quantity $s(\mu) = s(\mathbf{E}(\mu))$ derived from a solution \mathbf{E} of the parameter dependent Maxwell's equations. Here we consider electromagnetic scattering problems where a parameter μ may describe geometry and/or properties of the illumination or materials. In the following we describe the method only briefly and refer to [5, 6] for details.

Essential for the RBM is the splitting of the solution process into two phases: a computationally expensive *offline phase* and an inexpensive, fast *online phase*. The discrete Maxwell operator thus must be parametrized in a way that permits an effective offline-online decomposition. As it is generally not affine in μ it has to be approximated by the Empirical Interpolation Method (EIM)[1].

During the *offline* construction of the reduced basis the underlying, high-dimensional FEM model is solved multiple times for certain parameter configurations to compute so-called snapshots. Subsequently solutions of the reduced problem are sought in the linear space spanned by these snapshots by a Galerkin projection. As the number of snapshots is typically in the order of 10 to 100, the reduced problem stated on the reduced basis requires only a low dimensional linear system to be solved. This operation can be done real time and for many parameters *online* if the assembly of the reduced system remains independent of the FEM dimension and only depends on the reduced basis dimension N . This is guaranteed by EIM.

The selection of snapshots spanning the reduced basis can be carried out self-adaptively through a Greedy strategy by selecting the worst resolved parameter configuration contained within a finite dimension training set $\mathcal{D}_{train} \subset \mathcal{D}$ of the parameter domain. An efficient and cheap a posteriori error estimator for the reduced basis approximation error is crucial for this selection[7].

3 Results

Optical model The investigated structure is a periodic array of FinFETs (at the 22 nm technology node). These complex 3D architectures have become a crucial driver for down-scaling of structures on integrated circuits [2].

The device geometry is depicted schematically in two side views together with FEM meshes in Figure 1. The device dimensions and optical parameters are taken from [2] and [4]. The pitches of fin and gate are 44 nm and 88 nm respectively. The fin is 12.7 nm wide and 40 nm high with an undercut of 2.1 nm and a side-wall angle of 89.5 deg. The gate is 40 nm wide and 95 nm high with an undercut of 2 nm. A SiN layer (dark red) of 5 nm, a high-k layer (green) of 2 nm and a TiN layer (grey) of 7 nm complete the structure sitting on top a 200 nm thick substrate. Additionally a rounding of the fin and gate top edges is used. The FinFET is discretized with a parametrized tetrahedral mesh which accurately resolves the undercuts and corner roundings.

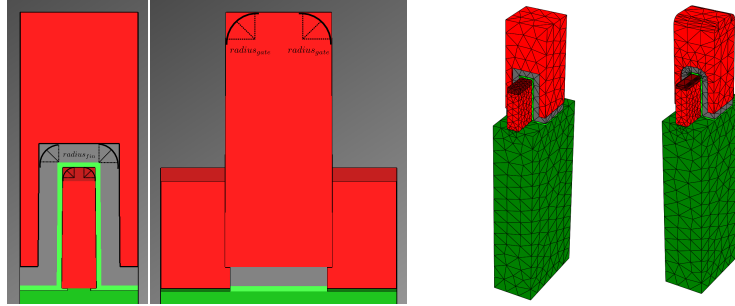


Figure 1: Left: Schematic side views of the FinFET geometry and varied parameters. Right: FEM-meshes of the unit cell without and with corner rounding of gate and fin.

The structure is illuminated by a plane wave at 390 nm and tilted 30 deg along the gate direction. Using 4th order ansatz functions and 190 089 degrees of freedom the FEM problem is solved in ≈ 270 s of cpu time.

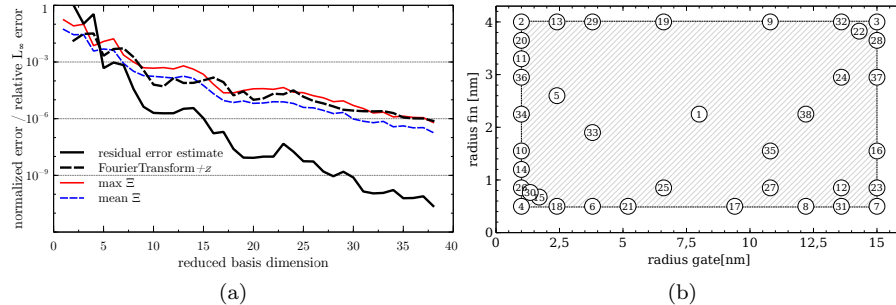


Figure 2: (a): Error estimates with increasing reduced basis dimension in a semi-logarithmic plot. The residual error estimate (black solid line) is normalized with the estimate for $N = 1$. The error estimate for the Fourier transform (black dashed line) estimates the relative error in the L_∞ norm. (b): Snapshot positions in parameter space are marked as circles and the number indicates the sequence of snapshot selection.

Reduced basis construction We build a reduced basis for the corner rounding radii $radius_{gate}$ and $radius_{fin}$ in the parameter domain $\mathcal{D} = [1 \text{ nm}, 15 \text{ nm}] \times [0.5 \text{ nm}, 4 \text{ nm}]$. The reduced model is constructed for the Fourier transform of the electromagnetic field which is used to compute the reflectance of the structure.

The training set \mathcal{D}_{train} used for the Greedy searches is adaptively refined from a fine initial mesh of 11 by 11 equidistant values. The EIM approximation uses 13 snapshots for the system matrix leading to an estimated approxima-

tion error of $5.3 \cdot 10^{-7}$ over the training set. A single snapshot is sufficient to approximate the right-hand side.

In the offline phase 38 truth solutions are computed to construct the reduced basis. Figure 2 (b) depicts the snapshot order and location in the parameter domain \mathfrak{D} (numbered circles). The first snapshot is chosen in the centre and the subsequent snapshots cover the corner of \mathfrak{D} first. Generally the snapshot locations follow the boundaries of \mathfrak{D} with a slight clustering at the corners.

The Greedy algorithm chooses in each iteration the worst resolved parameter in the training set as the new snapshot location. Thus the error estimate generally decreases with increasing reduced basis dimension N . In Figure 2 the residual error estimate (solid black line) with increasing N is shown in a semi-logarithmic plot. The estimate is normalized with the first estimate. The normalized estimate converges exponentially with N up to an estimated error of less than $2.5 \cdot 10^{-11}$. The adaptive refinement of the training set leads to the non-monotonic convergence as new values are included.

The estimated error in the output quantity (dashed black line, Fourier transform in the z direction) shows a similar decrease although with a different rate due to different norms employed (relative L_∞ norm and $H(\mathbf{curl}, \Omega)$ norm). The error estimate converges up to an estimated error of less than $1 \cdot 10^{-6}$.

Online evaluation of the reduced basis In the online phase we evaluated the reduced system on 21 by 21 equidistant points evenly spread over the whole parameter space \mathfrak{D} . Each evaluation takes ≈ 200 ms. The contour plots in Figure 3 (center column) show the computed reflectance of P and S polarization respectively. The plots beside the contourplots show the horizontal and vertical (left and right) cross-sections through the center of the parameter space supplemented by reference solutions (blue dots) and in the outermost plots the linear trend of the reference data is removed to highlight deviations. We observe a much stronger dependence on the corner rounding radius of the gate than of the fin in both polarizations. In both polarizations the deviations to reference is in the order of $1 \cdot 10^{-5}$.

Error analysis In the following we investigate these different errors by comparing the reduced basis approximations to reference solutions for a randomly selected set Ξ of 100 parameter values. For $\mu \in \Xi$ we solve the truth approximation including the EIM approximation and compare the results.

In Figure 2 the relative errors in the Fourier transform are shown in addition to the error estimate on the left. The mean relative error over Ξ is depicted by the blue dashed line whereas the maximum is shown in red. Both lines follow the error estimate very closely. The errors are reduced from about $1 \cdot 10^{-1}$ to $1 \cdot 10^{-6}$ with increasing reduced basis dimension.

In Figure 4 the max and mean of of the approximation error over Ξ in the $H(\mathbf{curl}, \Omega)$ norm are shown as well as a scatter plot relating the estimated error and the true error in the $H(\mathbf{curl}, \Omega)$ norm. The maximum as well as the mean error exhibit identical convergence trends to the estimated error. With

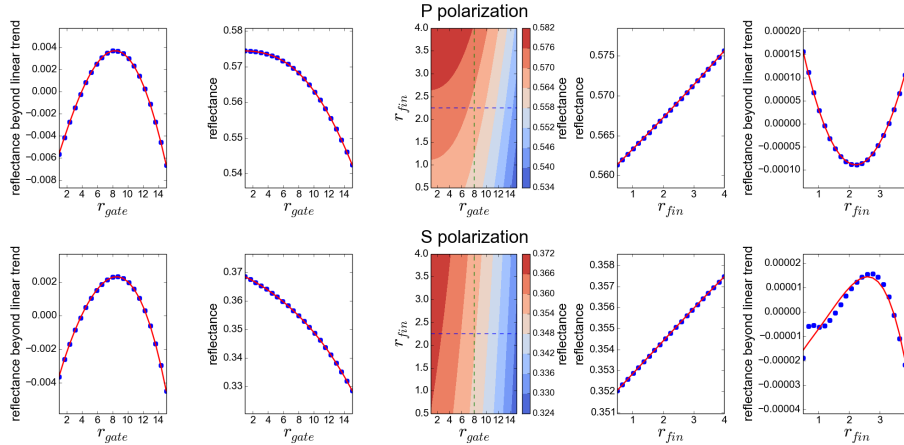


Figure 3: Reflectance for the P (top row) and S polarization (bottom row) over radii as contour plots (central column), as cross-sections through the parameter domain (left and right from center columns) and with removed linear trend (outermost columns).

increasing N the error decreases exponentially from $1 \cdot 10^{-2}$ to $1.2 \cdot 10^{-12}$ at most with the mean being an order of magnitude smaller. The scatter plot demonstrates the good performance of the error estimator. The error and the estimate are highly correlated over more than 9 orders of magnitude.

4 Conclusions

The reduced basis method is well suited for many-query and real-time simulation tasks. We have demonstrated its application to optical scattering simulations of a parameterized FinFET where it allows to compute online solutions with three orders of magnitude speedup. The errors in both the field solution and the output are satisfyingly controlled. As a result we have an efficient, error controlled, real-time capable procedure for situations where the application of the direct problem would be not realistic.

The results were obtained at the Berlin Joint Lab for Optical Simulations for Energy Research (BerOSE) of Helmholtz-Zentrum Berlin für Materialien und Energie, Zuse Institute Berlin and Freie Universität Berlin. This research was carried out in the framework of MATHEON supported by Einstein Foundation Berlin through ECMath within subprojects SE6 and OT5.

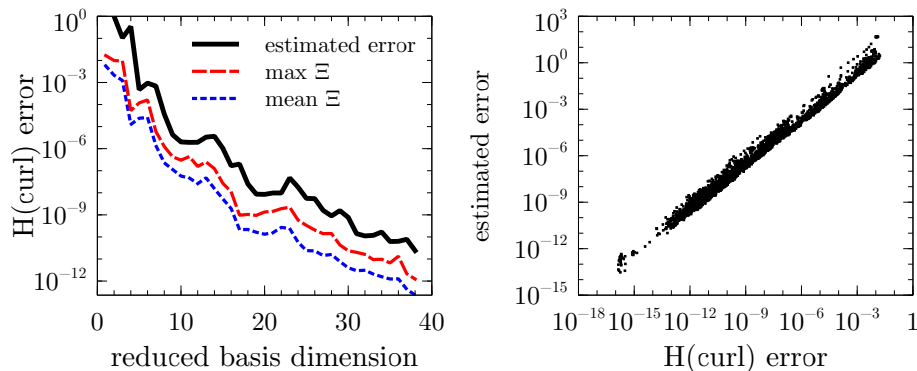


Figure 4: Maximum and mean error of $\Xi \subset \mathfrak{D}_{train}^N$ in $H(\mathbf{curl}, \Omega)$ norm over the reduced basis dimension (left) and estimated reduced basis error over the error in $H(\mathbf{curl}, \Omega)$ norm (right). The maximal and mean error decrease with increased reduced basis dimension. The estimated and actual error are highly correlated.

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