Skoltech
Skolkovo Institute of Science and Technology

Thesis Changes Log

Name of Candidate: Alexandra Tambova

PhD Program: Computational and Data Science and Engineering

Title of Thesis: The numerical modeling of nanophotonics by means of well-conditioned volume integral equation methods.

Supervisor: Prof. Maxim Fedorov

Chair of PhD defense Jury: Prof. Ivan Oseledets ***Email***: *I.Oseledets@skoltech.ru*

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The thesis document includes the following changes in answer to the external review process.

Dear Reviewers,

I would like to thank you for the useful comments which were invaluable in improving the thesis. I also consider all the comments in my future research. Below please find the responses.

Yours sincerely,
Alexandra Tambova

Reviewer: Prof. Nikolay Koshev

Comment 1: "*The title of the thesis is "The numerical modeling of nanophotonics by means of well-conditioned volume integral equation methods". Despite the fact the title is related to the general topic of the thesis, it does not depict the fact that the thesis is devoted to the development of novel concepts and numerical algorithms. Author may be interested in changing the title to make it more related to the proposed concepts and methods.*"

Response: We agree that the title is too general. Unfortunately, we are not allowed to change the title at this stage.

Comment 2 : *“The computational problem is becoming clear not from start of reading the thesis. In reviewer’s opinion, the computational problem should be described mathematically clearer from the start, maybe, with adding the section accurately explaining the input data for the algorithms (conductivities, permeabilities etc), and the data which should be obtained using the modelling.“*

Response: We have added the Problem Statement section (Section 2.1) at the beginning of Chapter 2. There we have established the general scattering problem and explicitly indicated the input and output data. Next, we have added Section 2.8 (Field Computation), where we have explained how the electric and magnetic fields are computed from the equivalent currents obtained from the solution of the linear system. Moreover, at the end of the chapter, we have added Section 2.9 (Summary of the Algorithm), summarizing all the stages of the proposed method. Also, we have renamed Chapter 2 from “Numerical Methods” to “Numerical Simulation Method” to emphasize that it present the complete algorithm.

Comment 3: *“Inaccurate figures references. The text of the thesis contains sometimes a big number of references to the figures. The references, however, are not accurate and sometimes not clear. For example, the section 2.5 contains mostly references to figure 2.5, while the corresponding figures should be 2.16+.”*

Response: Thank you for your careful reading. We have fixed all the issues with the figures’ references. Also, please see the response to Comment 5 of Prof. Francesca Vipiana.

Comment 4: *"Comparison with COMSOL Multiphysics. The comparison is made in accurate way; however, the comparison on the base of errors is not evident. In reviewer's opinion, it is better to use not the absolute differences or errors, scaled by their maximum values, but just relative errors. Otherwise, it is not evident if comparison depicts good or bad result for the proposed method (figures 4-14, 4-15 etc). Also, the text references to the figures also should be fixed."*

Response: We agree that the comparison of the absolute values is quite unuseful, therefore we have removed Figure 4-14 and left the one containing the relative difference of the solutions. (Now it's Fig. 4-14). We would like to note, that the scaling by the maximum values was made for the electromagnetic fields themselves, not for the errors/ discrepancies of the solutions. This scaling is unavoidable since it's complicated to make the magnitude of the fields equal due to different source implementation in COMSOL and the proposed algorithm. Also, Fig. 4-15 intentionally contains the absolute difference, not the relative difference. The explanation of this is given in the text.

Comment 5: *"Numerical aspects. The numerical aspects section (section 4.4) presents the reasoning on the theme of implementation of the computational algorithm. In reviewer's opinion, this section should be placed earlier, before the presentation of the numerical results. "*

Response: We have renamed this section to "Preconditioning", since this name describes the section's content more specifically, and placed it into the Numerical Simulation Method Chapter. Now it is Section 2.7.

Reviewer: **Prof. Dmitry Dylov**

Comment 1: *"Possible improvements of the thesis include a more thorough mathematical definition practical/experimental constraints one could encounter in real life. Namely, the material limitation and the sampling geometry, in which continuously changing fields and material properties are represented by the piecewise constant functions, should be described as a strict mathematical set of allowed values."*

Response: We agree, that there is a lack of explicit definition of the allowed set of the material parameters and the geometries. Therefore, we have created a new Problem Statement section, where we emphasize that we consider the scattering on the inhomogeneous isotropic dielectric object in a homogeneous background, occupying the bounded or unbounded domain (infinite or semi-infinite waveguide). We further state that the object is characterized by its relative permittivity and permeability, which can be in general complex numbers.

Moreover, we have noted in Section 1.3, that most of nanophotonic devices consist of homogeneous or piecewise homogeneous regions since they are man-made structures. Hence, in the context of this thesis, the only regions where continuously varying material properties may take place are the artificial adiabatic absorbers. However, we will demonstrate via numerical experiments, that the asymptotic estimates of the reflections from the continuous absorption profiles hold for the reflections from discontinuous ones. We conclude, that the piecewise constant functions, firstly, fairly represent the materials inside the real structures of interest, and secondly, do not bother the wave attenuation in artificial absorbers.

In addition, we have created a new Discussion section, where we discuss the limitations of uniform discretization in the representation of some geometries. We have also mentioned, that discretization of the right-angled structures such as strip and grated waveguides, using the voxels leads to a substantially fewer number of unknowns than the discretization with tetrahedra.

Comment 2: *"This is especially relevant, say, in Section 2.4.1., where the bonds of integration are presented with a lack of formalism and suboptimal rigor. The reviewer suggests to define 2D integration/ validity sets in the Edge vicinity and to show clearly which domain each particular variable belongs to. After completing the constraint definitions, the step-by-step details of the integration can be placed into the appendix. Detailed derivations obscure the final deliverables.*

Response: We have added Figure 2-1, introducing the rectangular parametric space for transformation the original arbitrary quadrilateral to a square. Further, we depict more explicitly the upper limit of integration of variable ρ, denoted as ρ_L, in the ST and EA cases (Figs. 2.3 and 2.5). We would like to note that all the integration bonds are given by explicit expressions as well as depicted schematically.

Next, it's difficult to separate the bonds of integration and the details of the derivation since each step contains its own change of variables and, correspondingly, own limits of integration. While in principle it is possible to left only the final formulas, containing the sums of the smooth integrals, and move all the derivation in the Appendix, we believe this is unjustified, since these derivations are the core of the novel method and should be presented in the main part of the thesis. However, to make the thesis more coherent, we moved the part of the numerical results, related to applications of DIRECTFN-quad that go beyond its use in the described JM-VIE method, to Appendix.

Comment 3: *"It would also benefit the reader if the formulae of conceptual parts were moved into a single sub-section; whereas the numerical tests section would be left with nothing but the algorithmic part of the particular finite difference or the details on the grid scheme."*

Response: We would like to note that the Numerical Results of Absorbers section is mostly devoted to studying the adiabatic absorber performance, to one of the numerical solver itself. Nonetheless, the Numerical Aspects section (Now it is called "Preconditioning") was moved to Chapter 2, devoted to the VIE method. Further, in this section we have provided the typical times of operator assembly, constructing the preconditioner and the iterative solution of the linear system.

Comment 4: *"Introduction of magnetic conductivity in Section 4.1.3. is seemingly taken out of its place as well. Perhaps a generically combined introduction of electric and magnetic conductivities should precede; and only then one would consider adding the magnetic one back in the numerical scheme."*

Response: We have specified that the imaginary part of magnetic permeability stands for the presence of magnetic conductivity in a new Problem Statement section at the beginning of Chapter 2. We hope that after reorganizing the thesis structure we've done, it has become more coherent.

Comment 5: *"It is recommended to create a table of all notation variables used in the text in order to help the reader to follow the derivation. Otherwise, the VIE background (Maxwell, etc.) overwhelm the variables that are actually left over for the main part containing the description of the absorbing boundary conditions."*

Response: We have already made such a table containing almost all of the used symbols, except the intermediate variables of the singular integrals part (List of symbols, pp. 19-20). However, we have added all the missed variables, which are mainly from the "Absorbers and Reflections" part, to have the list complete.

Comment 6: "*Imperfections of the algorithm of discretization that had accelerated the method by means of a fast Fourier transform (FFT), and, in addition, preserved the acceleration speed, should be discussed in detail. It is not clear, for example, at which extent of FFT the minor reflections would reappear just due to the finite size of the Fourier decomposition and the standard artifacts that always appear at the sharp interfaces when FFT is used.*

Response: As far as we know, the edge artifacts originate when the Discrete Fourier Transform is applied to a non-periodic image, which is assumed to be periodic. However, there is a completely different story in our algorithm, since we use the FFT only to accelerate the multiplication of a vector by a circulant matrix. So there are no unjustified assumptions about the periodicity. Nonetheless, we have changed the phrases "acceleration via FFT", where they took place, to "acceleration the matrix-vector product associated with the iterative solver", to avoid misunderstanding. Moreover, we have added Section 2.6 dedicated to details of FFT-based matrix-vector product acceleration.

Comment 7: *"The questions of SNR and the underlying photons distributions can be added. For example, what is the expectation of the algorithm performance at the very low (Poissonian) distributions."*

Response: We have added Section 4.4, where we introduce SNR as practically a more convenient and comprehensive measure of the absorber performance. There we have presented some results of measuring the SNR dependence on the absorber parameters.

Comment 8: *"Last section could be enhanced by giving specific directions about the opportunities for the improvement and optimization that the future work would comprise. The reviewer suspects that the final chapter was supposed to be edited a little more. Potential direction of future work is to try application of Machine Learning and Image analytics techniques. Another interesting angle is to use Reinforcement Learning to suppress the reflections in the interface (like those in the Y-splitter). The candidate could add more speculations on these subjects.*

Response: Thank you for your suggestions. We have pointed on the possibility of exploiting machine learning techniques in multi-parametric optimization, required for using the absorbers in practical modeling tasks, in the new Discussion section. In addition, in this section, we present the other possible improvements of the proposed method, which can be considered as directions for future research.

Reviewer: Prof. Francesca Vipiana

Comment 1: *"page 39, line 6 correct "To avoid this compications, we use the dimensionality reduction method"with "To avoid this complications, we use the dimensionality reduction method".*

Response: Thank you for careful reading. Done. We've also corrected another typo "this" to "these".

Comment 2: *"page 74, last line, in "Figs. 2.5–2.5 show different components of interior electric field along the x, y"figures' numbers seem wrong."*

Response: Fixed.

Comment 3: *"page 75, last line, in "Finally, the convergence rate of the interior fields calculated for the spheres of conductivities from 0 S to 104 S is examined in Fig. 2.5 by showing numerical errors"figure number seems wrong."*

Response: Corrected.

Comment 4: *"-page 92, line 5, in "From Figs. 4.1–4.1"figures' labels seem wrong. "*

Response: Corrected.

Comment 5: "*I would suggest to checkin all the Thesis the figures' citation numbers because most of them seem wrong or not updated.*"

Response: Thank you again for your careful reading. It was a common problem for those figures, where we placed LaTex command "\label" at the wrong place. Now we have checked them all and fixed these issues.

Reviewer: Prof. Vladimir Okhmatovski

Comment 1: *"Lack of discussion on pros and cons of the proposed VIE formulation and alternative hybrid surface IE + VIE alternatives. Considered nanophotonics structures are homogeneous except for relatively small regions of adiabatic absorbers. As a result, surface integral equation formulations could be utilized for analysis of the bulk of the structures, while VIE could be used only for the absorber regions. Such formulation could be significantly more efficient.*"

Response: Thank you for this suggestion. We have added the Discussion section, where the pros and cons of the presented method are discussed, as well as the advantages of coupling with SIE. Moreover, we have mentioned the possibility of implementation of the domain decomposition method based on VSIE, which allows fast modeling of large complex systems.

<u>Comment 2:</u> *Lack of breadth in the literature review. References on use of MLFMA accelerated surface integral equation formulations for solution on nanophotonics problems should be added (e.g works of O. Ergul) as well as overview of new integral equations formulations such as, for example, de-coupled potential integral equations (works by L. Greengard and W.C. Chew).*

<u>Response:</u> Thank you for this comment. We have extended the list of the references for the accelerated integral equation methods (Section 1.2, p. 26), including the MLFMA-based and FFT-based techniques. Moreover, we have added an overview of the volume-potential IE formulation in Section 1.3. We would like to note also, that in the literature review we are mostly focused on *volume* IE formulations, since we initially consider inhomogeneous objects, therefore we believe it is not necessary to consider the particular *surface* IE formulations.

<u>Reviewer:</u> Prof. Ivan Oseledets

<u>Comment 1:</u> Page 104, Figure 4-9: It quotes «theoretical convergence rates», which, as I can see, are empirical estimates, which are not strictly speaking theory in mathematical sense (i.e. there are no theorems).

<u>Response:</u> We have removed the word "theoretical" from where we are talking about estimations of the field decay rate or round-trip reflection since there are indeed the empirical estimations. However, the evaluation of the transition reflection is based on the exact results, obtained using the coupled-mode theory and adiabatic theorem. so, in this case, the word "theoretical" is justified. Note that we cite the corresponding works where the detailed derivations can be found.

<u>Comment 2:</u> A close question: some comments about theoretical justification of the proposed methods are needed.

Response: We would like to note, that we already have some comments about the theoretical justification of the proposed methods. First, when briefly describing the particular choice of VIE formulation in Section 1.3, we note that using the Galerkin method of moments with the square-integrable functions guarantees the convergence of the solution in norm. Nonetheless, we have additionally pointed out in Section 2.2-2.3, that the testing functions used in the discretization of the original system of IE should span the dual space of the associated operator in order to guarantee the convergence of the solution in norm, and that this condition is satisfied, if the IE is discretized using the Galerkin MoM with the identical square-integrable basis and testing functions, such as piece-wise constant ones, which we are using in this thesis. Moreover, we have added an explicit justification of the block-Toeplitz structure of system matrices into Section 2.4

Comment 3: The algorithms proposed are not summarized as formal algorithms, see, for example, 2.9

Response: We would like to note that Section 2.9 contains not only the algorithm but also the summary of all the stages between the initial scattering problem formulation and constructing the final linear system to solve, together with recalling to some features of the method. Therefore we renamed this section to "Summary of the Numerical Method". Nonetheless, we have provided pseudocode for constructing the block-Toeplitz operators and pseudocode for the whole VIE solver.

Comment 4: Section 2.10 (Fig 2-12, 2-14)./ The mesh refinement is presented as convergence when mesh size goes to zero. This is good, but estimate of the order of convergence is needed, which is achieved by plotting the error of the approximation, between, say, linear interpolates of these quantities. Also, typically, the mesh is refined like lam/2, lam/4, ... and then the order of the convergence is recovered.

Response: We have added the plot of the maximum relative error between the numerical and Mie analytical solution versus the mesh size (Fig. 2-16).