Skoltech

Skolkovo Institute of Science and Technology

Jury Member Report – Doctor of Philosophy thesis.

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

Co-advisor: Prof. Athanasios Polimeridis

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

Date of Thesis Defense: 28 November 2019

Name of the Reviewer: Dmitry Dylov

I confirm the absence of any conflict of interest	**Signature:** **Date: 28-10-2019**

The purpose of this report is to obtain an independent review from the members of PhD defense Jury before the thesis defense. The members of PhD defense Jury are asked to submit signed copy of the report at least 30 days prior the thesis defense. The Reviewers are asked to bring a copy of the completed report to the thesis defense and to discuss the contents of each report with each other before the thesis defense.

If the reviewers have any queries about the thesis which they wish to raise in advance, please contact the Chair of the Jury.

Reviewer's Report

Reviewers report should contain the following items:

- Brief evaluation of the thesis quality and overall structure of the dissertation.
- The relevance of the topic of dissertation work to its actual content
- The relevance of the methods used in the dissertation
- The scientific significance of the results obtained and their compliance with the international level and current state of the art
- The relevance of the obtained results to applications (if applicable)
- The quality of publications

The summary of issues to be addressed before/during the thesis defense

The PhD candidate focused her research on the numerical methods for solving the volume integral equation (VIE) for modeling three-dimensional nanophotonic structures. The developed method allows to tackle the problem of reflection generation in the cut off waveguides of conventional photonic wafers for integrated circuitry boards (in optical couplers, ring resonators, etc.). This is accomplished by introducing special absorbing boundary conditions in the computational domain that consider particular spatial geometry of the channel, as well as the finite scatters present in the light propagation pathway.

In this thesis, the PhD candidate describes implementation and characteristics of adiabatic absorbing layers in the volumetric integral equation (VIE) for modeling truncated nanophotonic structures. The applications of this research are important, ranging from basic integrated photonics to quantum beam manipulations that are known to suffer extensively from the very infinitesimal reflections. Interestingly, the reported findings indicate a decrease of reflections with the speed associated with the smoothness of the absorption profile function. This stems from the specifically designed conductivity profile that gradually changes across the boundary.

Possible improvements of the thesis include a more thorough mathematical definition of 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.

This is especially relevant, say, in Section 2.4.1, where the bounds of integration are presented with a lack of formalism and suboptimal rigor. This 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.

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.

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.

It is recommended to create a table of all notation variables used in the text in order to help the reader 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.

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 artefacts that always appear at the sharp interfaces when FFT is used.

The new numerical method for estimating singular integrals over quadrilateral spots that occur when the elements coincide or have a common face or vertex, is noteworthy and follows the publication [3] of the candidate. The Galerkin internal products are well applied to a number of surface-surface integrals over the faces of mesh elements. This part looks polished and can remain unchanged for the thesis.

The effectiveness of the proposed algorithms is demonstrated using numerical experiments on various photonic devices: a rectangular waveguide channel, a waveguide with periodic width corrugations (Bragg grating), and a Y-brunch splitter; and the claims are sufficiently supported.

The questions of SNR and the underlying photons distributions could be added. For example, what is the expectation of the algorithm performance at the very low (Poissonian) distributions?

Last section could be enhanced by giving specific directions about the opportunities for 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.

Provisional Recommendation

☒ *I recommend that the candidate should defend the thesis by means of a formal thesis defense*

☐ *I recommend that the candidate should defend the thesis by means of a formal thesis defense only after appropriate changes would be introduced in candidate's thesis according to the recommendations of the present report*

☐ *The thesis is not acceptable and I recommend that the candidate be exempt from the formal thesis defense*