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:

I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict)	**Signature:** **Nikolay Koshev** **Date: 28 October 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

1 General comments

The thesis is devoted to the development of modelling techniques of wave distribution inside the waveguide. The modelling of the wave behavior in silicon waveguides is one of the crucial issues of photonic applications and being highly demanded in a number of areas related to high-speed data communications: long-haul optical transmissions, short-reach communications in datacenters and supercomputers, intra- and inter-chip connections etc. The main objective of the thesis is development of both concepts and numerical algorithms, allowing the accurate reduction of computationally expensive modelling problem in infinite waveguides to the modelling problem in bounded domains with usage of Volume Integral Equation approach. Such reduction demands of research on methods of representation of the boundaries of the finite bounded computational domain; moreover, decrease of dimensionality of the computational problem leads to the singular kernels in the integral equations, obtained using the Maxwell's system. The thesis contains a number of novel contributions to the numerical modelling of nanophotonics, based on the Volume Integral Equation (VIE) approach. Author presents both new concepts for modelling the electromagnetic waves inside the waveguide, and numerical algorithms showing better accuracy and higher performance in comparison with previously developed methods. The proposed concepts, approximations and developed numerical methods allow to make the modelling more effective due to high performance and accuracy. An important contribution of the thesis is the introduction of a new concept of adiabatic absorbers, representing the boundaries of finite computational domain. Conventional modelling of the waves in waveguides needs these absorbers in order to use finite computational domains instead of infinite ones. The adiabatic absorbers are deployed near the domain boundaries in order to make the boundary to reproduce accurately nonlossy infinite medium with all non-physical reflections being minimized. The absorbers are being represented with areas with gradually increasing electric conductivity. These areas are being accurately considered in the thesis both in terms of physics and mathematical 1 modelling. The developed concept allows to produce a VIE formulation in a simple and straightforward manner, without affecting the performance of the VIE algorithm, built with usage of Fast Fourier Transform (FFT). The proposed concepts were applied to a number of modelling problems in order to validate the theory and approximations. The numerical results were accurately presented in the thesis together with complete analysis and comparison with existing other methods of modelling the waves in waveguides. For the comparison purposes, the well-known COMSOL Multiphysics software package has been used for a various waveguide presets. The results of usage of COMSOL package and the proposed algorithm are completely analyzed in terms of relative difference and show good coincidence to each other. Another important contribution relates to a novel fully numerical approach of evaluation of the singular integrals over quadrilateral elements. These singular integrals, represented with the singular kernels, occurring after the reduction of computationally expensive volume-volume 6D integrals to 4D surface-surface integrals. Thesis depicts a method of calculation of three kinds of singular integrals (Coincident self-term integrals, edge adjacent and vertex adjacent integrals). Despite the fact the method was considered with a rough piecewise-constant Galerkin discretization, the proposed method shows better performance and comparable

accuracy in comparison with existing methods. The developed numerical method was accurately and completely analyzed in terms of computational complexity and accuracy. For these purposes, the previously developed DIRECTFN method has been used. The developed approach shows higher accuracy and comparable performance in calculation of singular integrals. Cons and pros of the proposed method were depicted and analyzed, together with possibilities of further improvement of efficiency. The proposed fully-numerical method is called DIRECTFN-quad and supposed to be an extension of previously developed DIRECTFN numerical method based on usage of triangular elements.

2 Specific comments

The objective of this section is to provide several specific comments and recommendations on how to improve the quality of the presentation. The provided comments are not critical and mostly related to some inaccuracies in the thesis appearance.

1. Title. 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.

2. The statement of the problem. 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.

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+.

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.

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.

3 Summary and conclusion

The thesis presents a numerical technique, allowing to use the VIE approach with the infinite scatterers, which becomes possible due to representation of the boundaries with the concept of adiabatic absorbers, introduced by Author. In order to reduce computational complexity, the dimensionality has been decreased and occurred problems of calculation of singular integrals

were accurately managed. The thesis seems to present a novel work, which value for scientific and industrial modelling is doubtless high. The research presented in the thesis is definitely actual and refers to contemporary results in the area. Despite some inaccuracies in the thesis appearance, the research is interesting. Author of the thesis definitely proved her ability to perform a research and to achieve high-rated scientific results. After some minor revision, I definitely recommend the thesis for the presentation with the aim of receiving the Ph.D. degree.

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*