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Opponent's review of the Doctoral Thesis

Candidate Martin Ladecký

Title of the doctoral thesis Advanced spectral methods for computational homogenization of periodic media

Study Programme Mathematics in Civil Engineering

Tutor doc. RNDr. Ivana Pultarová, Ph.D.

Opponent doc. RNDr. Petr Tichý, Ph.D.

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Topicality of the doctoral thesis theme

Commentary: The thesis is concerned with multiscale material modeling which represents one of the key areas of development for future industries. In particular, the thesis focuses on a deeper understanding and development of spectral methods for computational homogenization of periodic microstructures. Considering periodic microstructures allows, e.g., to exploit acceleration techniques based on fast Fourier transform (FFT) and low-rank tensor approximations, and to solve efficiently large-scale engineering problems.

☒ excellent	☐ above average	☐ average	☐ below average	☐ poor

Fulfilment of the doctoral thesis objectives

Commentary: Three major research objectives (concerning operator preconditioning, analysis of discretization artifacts, and reduction of computational costs) were formulated in Section 1.1. The objectives were achieved, and the results were summarized in five manuscripts, four of them already published in refereed journals.

☒ excellent	☐ above average	☐ average	☐ below average	☐ poor

Research methods and procedures

Commentary: The candidate developed and discussed several new approaches which in combination with methods of modern computational mathematics provide interesting and efficient tools for solving practical homogenization problems.

☒ excellent	☐ above average	☐ average	☐ below average	☐ poor

Results of the doctoral thesis – dissertant's concrete achievements

Commentary: The candidate has presented important results that contribute to theory as well as to the practical use of spectral homogenization methods. He demonstrated broad knowledge of the considered topics and advanced techniques of modern computational mathematics.

Concerning operator preconditioning, bounds on the eigenvalues of the preconditioned operator were developed. The candidate and coauthors use a different approach than Gergelits et al., based on the Courant-Fisher min-max principle. While the approach of Gergelits et al. can provide more accurate estimates of (parts of) the spectra, the approach introduced in the thesis can be applied to more general problems and types of discretization. Such bounds can be very useful, e.g., for predicting convergence behaviour of the conjugate gradient method for solving the resulting systems of linear equations.

In the second part related to the minimization of discretization artifacts, a micromechanical solver is derived in a standard finite element (FE) manner that eliminates ringing artifacts while keeping the efficiency of spectral methods. The candidate and coauthors discuss the problem of discretization artifacts, derive a formulation for the projection operator based on a general gradient stencil, and test several other stencils. They observe that the only FE discretization stencil fully eliminates all ringing artifacts and delivers oscillation-free results.

Finally, the candidate and coauthors introduced the innovative idea of low-rank tensor approximations to accelerate Fourier-Galerkin methods. This approach leads to a significant reduction of memory and computational costs in the solution of the homogenisation problems. The efficiency of the approach discussed in the thesis builds on the incorporation of FFT and low-rank tensor approximation into the iterative linear solvers.

The candidate produced the results in collaboration with coauthors from several institutions. The specific contribution of the candidate is always mentioned at the beginning of each chapter. The candidate has always contributed significantly to the formulation of the theoretical results as well as to the implementation of methods and numerical experiments.

☒ excellent	☐ above average	☐ average	☐ below average	☐ poor

Importance for practice and for development within a branch of science

Commentary: The results of the thesis provide efficient tools for solving practical homogenization problems. The idea of using finite element spaces instead of Fourier while keeping the efficiency of spectral methods, and the idea of accelerating Fourier-Galerkin methods using low-rank tensor approximations seem to be very promising for practical computations and open the door for other research topics mentioned in Section 7.1.

☒ excellent	☐ above average	☐ average	☐ below average	☐ poor

Formal layout of the doctoral thesis and the level of language used

Commentary: The thesis is well structured and presented, with a sufficient level of details in each chapter. The level of language is at a very high level. In the thesis, there are the following typographical errors caused probably by the used LaTeX style. Starting from Chapter 4, the numbers of equations are not displayed. Moreover, when using a reference to an equation in the text, the number of the current section is sometimes displayed instead of the number of an equation; see, e.g., Section 4.4.1. This made it sometimes difficult to read the text and I had to consult the original works.

☐ excellent	☒ above average	☐ average	☐ below average	☐ poor

Statement on compliance with citation ethics

I have no objections.

Remarks

None.

Final assessment of the doctoral thesis
This is an excellent thesis with fundamental contributions to the computational homogenization of periodic media. The candidate has demonstrated that he is capable of producing scientific results at a very high scientific level.

Following a successful defence of the doctoral thesis I recommend the granting of the Ph.D. degree

yes ☒ *no* ☐

Date: 24.08.2022

Opponent's signature: ... .