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Opponent's review of the Doctoral Thesis

Candidate: Martin Doškář

Title of the doctoral thesis: Wang tiling for modelling of heterogeneous materials

Branch of study: Physical and Materials Engineering

Tutor: Jan Novák, Ph.D. and Jan Zeman, Ph.D.

Opponent: Dr. Felix Fritzen

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Topicality of the doctoral thesis theme				
Commentary: The topics under consideration is at the same time interesting, challenging and useful. They form a well-balanced blend of state of the art challenges in modern computational mechanics of materials and structures, microstructure generation/modeling and advanced numerics. The Wang tile concept is a refreshing enrichment.				
☑ excellent	☐ above average	☐ average	☐ below average	☐ poor

Fulfilment of the doctoral thesis objectives				
Commentary: The objectives of the doctoral thesis are fulfilled: The candidate has exceptionally well proven that he is capable to work in challenging scientific fields, to find solutions using interdisciplinary methodologies, to promote his topic and results in the international and European community with success and to develop ideas for current and future research topics.				
☑ excellent	☐ above average	☐ average	☐ below average	☐ poor

Research methods and procedures				
Commentary: The candidate has used methods from the fields of microstructural characterization and modeling (in particular Wang tile generation & their application in stochastic material modeling). The level that he attained in the different disciplines is on par with leading researchers in the field or at least matching the current state-of-the-art.				
☑ excellent	☐ above average	☐ average	☐ below average	☐ poor

Results of the doctoral thesis – dissertant's concrete achievements				
Commentary: Establishing the Wang tile concept despite some initial criticism from the community is a big achievement. The application in homogenization and structural simulations where separation of scales is not granted and by using model reduction techniques are key achievements.The ambition of the candidate to go beyond provided paths & expectations is exceptional.				
☑ excellent	☐ above average	☐ average	☐ below average	☐ poor

Importance for practice and for development within a branch of science				
Commentary: The methods investigated are mostly academic although applications in engineering practice are available. The usability for academia is manifold, e.g., structural synthesis and optimization using Wang tiles for parameterization are one interesting challenge. In particular, they can leverage modern metamaterials for acoustics, structural damping, ...				
☑ excellent	☐ above average	☐ average	☐ below average	☐ poor

Formal layout of the doctoral thesis and the level of language used				
Commentary: The thesis is prepared by using parts that were either published in high-ranked international journals or that are submitted. This is complemented by an introduction and discussion of appropriate size. All the data is prepared with a high level of accuracy and many (useful) graphical representations. English language skills are on a very good level, too.				
☑ excellent	☐ above average	☐ average	☐ below average	☐ poor

Remarks
Questions are attached in a separate file. They are provided in order of significance. Some questions are rather comments which I would still like to provide to the candidate before the defence. Besides the scientific judgement on the manuscript I would like to express that the interactions with the candidate during conferences, workshops and when discussing research topics were of outstanding quality and responsiveness, thereby underlining the maturity, modesty and open-minded character of the candidate.

Final assessment of the doctoral thesis
The thesis condenses a large number of individual results evolving around the Wang tile concept. The generation of a variety of microstructures, the generation of the tile sets, the determination of the size of the RVE, the use in simulations lacking separation of length scale, etc. highlighten the broad spectrum covered. The representation is pleasant, well-organized and technically matching the state of the art. In summary I conclude that the thesis is the well-deserved end of a significant scientific episode for the candidate who certainly deserves a Phd degree for his work. Additionally, if given the option I will support the label "with distinction" given the defence matches the quality of the monography.

Following a successful defence of the doctoral thesis I recommend the granting of the Ph.D. degree		
	yes ☑	*no* ☐

Date: Nov 29, 2019

Opponent's signature: .....

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Opponent questions for Ing. Martin Doškář

Opponent
Dr. Felix Fritzen
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Q1 Can you elaborate on the quantitative randomization of the Wang tile-based UC, i.e.: How small (tile-wise) can (and/or should) you go with the tiling concept in order to generate greater variability of the tiles? Are constrained on the tile ensemble necessary and possible in order to enforce (despite great local variability) certain microstructural characterstics? How accessible is the cardinality of the ensemble of all tilings for a given tile set (with/without constraints)? How could a different lattice layout influence the variability qualitatively (triangular, hexagonal, ...)?

Q2 Can you think about Wang tiling being a way to leverage machine learned algorithms? For instance, can you image Wang tiles to be merged into convolutional deep learning and what benefits and drawbacks do you see?

Q3 Visionary question: Can you imagine the use of the Wang tile concept for the modeling of stochastic time dependent processes by letting the time another coordinate to consider? What modification would be needed in order to achieve this objective? Do you consider this a viable path for future research?

Q4 The variability of the two point correlation is restricted by the tiles. Is there a bound on the variability of the 1 point statistics (i.e. volume fractions) and 2 point statistics (i.e. autocorrelation for two phase materials to keep it *simple*)? In particular, how does the tile size and in-tile variability translate to the variability of the n-PCF of synthesized microstructures of given size? What implications can be drawn from this consideration regarding the tile size and optimized target system size? Is the use of a larger tile set (possibly smaller tiles though) favorable compared to a small tile set with high variability?

Q5 In Section 3.3.1 a series of constraints is introduced that can provide different distributions of particles. Regarding the stochastic nature of the process, is there some understanding how the posterior information (i.e. the information about all previously placed particles) impacts the placement of the future particles and, thereby, predefines the overall statistical properties? I.e. can, based on the data at m particles it be concluded that a certain statistical property can be reached or not? Which tools from statistical microstructure analysis lend themselves to this problem?

Q6 Regarding the level-set approach, it seems that the order in which the particles are placed in the tiles can heavily influence the statistics. For instance, filling one tile until the stopping criterion is met will pre-define many other tiles—it will lead to a (heavily) constrained distribution. If particles are placed unordered in various tiles until all tiles have stopped, then the statistical impact seems different. Is there some evidence on how (qualitatively and quantitatively) the order does influence the overall statistics of the tile ensemble? What are the implications on tilings (i.e. on synthesized microstructures)? If I understand correctly, then seeing tile I as *central tile* in Modification 1, p. 32, implies that after a placement of particle therein, each *possibly connected* tile from the database sees a particle addition, as well (what if no particles were added? is the local particle adding repeated until one is found or the tile is complete?). *[This question is related to the previous one.]*

Q7 For the level-set method how does the performance deteriorates if the particle morphology gets oblate/prolate [i.e. whisker/fiber like particles]? This would be interesting for potential applications to fibrous materials where the generation of artificial structures is a big struggle. Could it be possible to have tiles even for rather unidirectional particles in order to genereate variable high volume fraction UC of fibrous materials?

Q8 *(comment-style question)* Is the vertex based tiling the dual to the edge based tiling, i.e. can an edge based tile set be directly transformed into a (possibly differently sized) vertex tile set? It would be very interesting to investigate such primal/dual spaces and the advantages of using the one or the other (estpecially using them simultaneously for the respective optimal purpose).