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Review of Thesis

submitted in partial fulfilment of requirements for promotion to associate professorship

Specialization: Theory of Building Structures and Materials

Applicant: Ing. Anna Kučerová, Ph.D.

Reviewer: Prof. Oberguggenberger Michael

Thesis title: Inverse Problems in Modeling of Random Materials

Importance of topic of thesis

Comments: The thesis subsumes work on three important areas:

(1) Random materials morphology (Chapter 2, 2 papers): The first paper develops a new approach to compressing and reconstructing microstructures using Wang tilings in place of single periodic unit cells, thereby avoiding artificial longe range correlations.
The second paper addresses the same theme in a very broad approach, comparing two statistical descriptors (two-point probability function and lineal path function), especially focussing on the challenging algorithmic implementation of the latter, using parallelization on a GPU device. This algorithm is compared with a standard CPU-based approach in various cases of microstructure compression and reconstruction for both descriptors.

(2) Calibration of random material models (Chapter 3, two papers): Here the first paper addresses heat and moisture transfer in a porous medium, described by a system of nonlinear diffusion equations with random coefficients. The method of choice is building a response surface by combining a Karhunen-Loève expansion with a polynomial chaos basis in a finite element program. The random parameters are log-normally distributed, so that a nonlinear transformation to Gaussian space is required. Based on the numerical model approximation, parameters are finally calibrated by Bayesian updating with the Markov chain Monte Carlo method.
The second paper addresses probabilistic parameter calibration in a lattice discrete particle model (LDPM) for concrete. The model mapping inputs to outputs is extremely expensive with around 300.000 particles. Thus a polynomial chaos (PC) based surrogate model is developed (together with a study of the required size of the PC-expansion). The material parameters are again calibrated by Bayesian updating, using two experimental set-ups (uniaxial compression, three-point bending). A thorough statistical analysis is done, including a sensitivity analysis which can be conveniently derived from the PC expansion. The paper includes verification at synthetic data and validation at laboratory measurements.

(3) Acceleration of model calibration based on surrogates (Chapter 4, two papers): The first paper addresses the capabilities of artificial neural networks (ANNs) with one hidden layer to serve as surrogate for the model response, the inverse relationship for parameter calibration, and the model error. It is applied to cement hydration (with the additional challenge of a time-dependent response). Various archtitectures of the ANN and training strategies are thoroughly analyzed and compared.
The second paper on this theme compares various methods of fitting a PC expansion (regression, collocation, stochastic finite elements), using a case study of a simple frame structure from the literature. This example comes with the difficulty that the statistics of the random parameters are given by histograms, making the transformation to Gaussian space discontinuous. The paper contains a thorough comparative study of different variants of the determination of the PC expansion and the treatment of the parameter distributions.

Chapter 1, the introduction, gives an overview over topic (1), with further applicative examples, especially addressing the involved optimization steps. Topic (2) is also addressed, starting with some principal

considerations on aleatory and epistemic uncertainty and an additional example of parameter calibration based on a cyclic loading test.

All three areas of research are extremely important and topical in engineering modelling. On the one hand, the statistical analysis of microstructures is a central current research direction in material sciences. On the other hand, parameter calibration has been ubiquitous in engineering for a long time, but has undergone a tremendous development in the past years due to the increase of computing power and the development of new numerical methods.

Superior	☒	Good	☐	Average	☐	Poor	☐	Not applicable	☐

Method of solution

Comments: The methods of solution are based on stochastic models and on optimization algorithms. Especially the construction of stochastic surrogate models is a main thrust in current engineering sciences. The applicant proves that she is an expert in these methods at current international level. The methods are sound and appropriate.

Superior	☒	Good	☐	Average	☐	Poor	☐	Not applicable	☐

Quality and correctness of results achieved

Comments: The submitted papers are on the high level of quality to be expected by publications in international journals. The presentation is clear, the mathematics behind the results is difficult and correct, as are the numerical implementations.

Superior	☒	Good	☐	Average	☐	Poor	☐	Not applicable	☐

Originality of results achieved

Comments: The main merit of the submitted thesis is the thorough understanding of the methods, the challenging numerical implementation, and the comparative studies, to be highly appreciated by workers in the fields and their applications. The algorithmic implementations are original.
Except for the first paper in Chapter 2, the approaches have been around in the literature, although one should say that a number of the algorithms, such as GRADE, have been originally developed by the applicant in earlier research.

Superior	☒	Good	☐	Average	☐	Poor	☐	Not applicable	☐

Publication rate of results achieved

Comments: In my view, the publication rate is excellent. As can be seen from the second example of the introduction, the author has worked on classified projects, e.g., with the European Space Agency. Nevertheless, she succeeded in publishing her scientific results continuously in international journals.

Superior	☒	Good	☐	Average	☐	Poor	☐	Not applicable	☐

Response to results and citation rate

Comments: The applicant and her work is internationally well-known in the stochastic mechanics community and the computational engineering community. Both her results on stochastic surrogate modelling and her earlier work on genetic algorithms is widely appreachiated.
Formally, I found 29 of her publications in the Web of Science Core Collection, with more than 250 citations and an h-index of 8. Google Scholar returns 91 item, with a citation number of 916 and an h-index of 15. In my view, this is impressive in the field.

Superior	☒	Good	☐	Average	☐	Poor	☐	Not applicable	☐

Applicability of results to development in the field and for further research

Comments: As already said, the results are at the core of current research in stochastic methods in engineering, in optimization, and in the analysis of microstructures.
At this stage of develpment, there is a broad opportunity for extensions, for example, PC-expansions with non-Gaussian variables or extension to other descriptors in microstructures. Apart from that, the applicant's broad expertise will allow her to open up new applications in other technical fields.

Superior	Good	Average	Poor	Not applicable
☒	☐	☐	☐	☐

Applicability of results to technical practice

Comments: Both the resrach on microstructures and parameter calibration is of high interest in practical engineering applications.
The stochastics part is also important in reliability analysis, a branch of engineering currently moving to the center of engineering design.

Superior	Good	Average	Poor	Not applicable
☒	☐	☐	☐	☐

Compliance with requirements on thesis – quality of thesis

Comments: There is no doubt that the applicant has proven with this thesis that she is able to perform new and significant research and to promote research directions on her own.
The thesis is of an excellent quality and meets all international requirements of a habilitation in the engineering sciences.

Superior	Good	Average	Poor	Not applicable
☒	☐	☐	☐	☐

Comments

As far as I know from her CV and various encounters at international conferences, the applicant has also engaged in international activities, having spend years abroad at ENS Cachan and the University of Braunschweig. In addition, she has been principal investigator in a number of research projects in uncertainty quantification, reliability analysis and computational modelling.

She is an internationally recognized expert in uncertainty quantification, and she has a broad expertise in this field as well as in mechanical engineering, material sciences, and scientific computing. One of her important contributions with significant international impact has been the development of the optimization software GRADE and CERAF, a genetic algorithm with probabilistic restart, which has been successfully used by many research groups, including my own group and other engineering groups in Innsbruck. She is also a recognized expert in stochastic simulation methods, both in polynomial chaos expansions and Bayesian algorithms, in design of experiments and in parameter identification.

The applicant has also guided younger students to reach international research level.

This emphasizes that she has a lot of important qualifications going beyond the submitted thesis.

Overall evaluation of thesis
As follows from my assessment above, this is an excellent thesis that definitely places the applicant in the high upper range of current international research in her fields. My overal essessment is "superior". Additional comments on the thesis and the author: Judging the applicant not only from the thesis, but also her previous original research contributions and her engagement in research projects, as well as her ability to initiate and promote independent research, I recommend that she will be promoted to "associate professor".

Promotion to associate professorship recommended	*yes* ☒	*no* ☐

Date: Innsbruck, March 19, 2020

Reviewer's signature: