Ao.Univ.Prof. DI Dr. Martin Kozek
Institute for Mechanics and Mechatronics
Div. for Control and Process-Automation
Getreidemarkt 9 / 325 - 6
1060 Vienna, Austria
Tel.: 58801 325512
Email: kozek@impa.tuwien.ac.at

TECHNISCHE
UNIVERSITÄT
WIEN
Vienna University of Technology

Professor Lukas Sekanina
Head of Department of Computer Systems
Faculty of Information Technology
Brno University of Technology
Bozetechova 2
CZ-612 66 Brno, Czech Republic

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Review on the Doctoral Thesis of Gabriela Nečasová titled

„Parallel numeric solution of differential equations "

1. *Overview*

The thesis of Gabriela Nečasová is written as a monography treating the application of a variable order Taylor-series method to partial differential equations. It is structured in an Introduction where the motivation for the specific research is given, the research objectives are stated, and a thesis outline is presented. Dedicated Chapters of the main work deal with the numerical solution of differential equations, the numerical treatment of partial differential equations (PDEs), the specific Modern Taylor Series Method (MTSM), a section on parallel and distributed computing, an extensive results Section, and a short Conclusion.

The work mainly written as an overview on existing methods and publications, a substantial part of which have been authored or co-authored by the defendant of the thesis.

2. *Appraisal of the Thesis*

Appropriateness and relevance:
The thesis primarily addresses topics which form the fundamental backbone of simulation methods – the numeric solution of initial-value problems of ordinary differential equations, so the addressed topics are highly relevant for many areas of science. This core part is extended to the solution of PDEs, using the Method of Lines to achieve spatial discretization and consecutive application of the MTSM to the resulting set of ordinary differential equations. An important contribution of the thesis

is the linkage of the presented mathematical methods with parallel computation schemes, which is especially important from the implementation perspective. The thesis therefore not only addresses relevant problems, but also provides a hands-on guideline for practical implementation. It is a compact and well-structured work to instruct researchers on the specifics of Taylor Series integration both from a fundamental and a practical perspective.

Summary of the contributions of the thesis:
The goal of the thesis is to develop, apply and demonstrate extensions to the Modern Taylor Series Method (MTSM) for the time-domain simulation of linear system dynamics, with a focus on partial difference equations and a beneficial parallel computing implementation. Several research questions detail this goal and are elaborated within the thesis respectively in the comprehensive portfolio of publications of the defendant.
The thesis is clearly organized into an Introduction (Ch. 1), where the research objectives are explicitly stated, a Chapter on the numerical solution of ODEs (Ch. 2) comprising all classical methods and MTSM, a large part on the application to PDEs where also stability of the numerical algorithms is covered (Ch. 3), followed by a Chapter on the MTSM with higher-order implementations (Ch. 4) accompanied by again a selection of different problems and their solution via MTSM. An additional Chapter is focusing on the practically important part of parallel and distributed computing implementations of the proposed MTSM method (Ch. 5). Chapter 6 contains an extensive listing of results for PDE solutions of different physical domain problems (heat equation, wave equation, and telegraph equation). In particular, the thesis builds up on the previously existing MTSM and adds several contributions. A large portion of Chapters 2, 3, and 5 compiles state of the art results and serves as a foundation for understanding MTSM and its applications.

The core or main contribution of the defendant's work lies in the proposed range of extensions to the MTSM (outlined in Ch. 3, 4 and 5): An approach and its assessment of modeling transformations to get the PDE problem into a form suitable for the MTSM, applying automatic differentiation and transformation techniques, optimizing/minimizing the number of terms in the pre-processed ODE representation, and providing optimized representations for parallel computation of the solution. Especially for the method of lines the workflow was constructed in a complete and detailed way, so that a reader might be able to set up his own problem based only on the information contained in the thesis.
The second contribution is that of providing an extensive reference of example problems and benchmarks to illustrate the MTSM application itself, as well as the methodology to combine MTSM with the Method of Lines to model and solve PDEs in a numerically efficient way.
Finally, a contribution also lies in presenting the performance of MTSM applied to PDEs in parallel computation implementations. In the last topic a wide range of important variables have been varied, and the effects of those variations are clearly presented.
The thesis satisfactorily achieves the set research goals as defined by the given research objectives in Chapter 1. The student's own contributions can be clearly identified from the literature list and directly address the above-mentioned core contributions of the thesis.

Novelty and significance:
Although the thesis contains a wide overview on existing methods for the numerical solution of ODEs it combines original and novel contributions in the field of high-accuracy solutions of PDEs. Moreover, it adds a valuable part of how to implement such approaches in a parallel computing environment, and addresses the effects of the most important parameters for such a parallel implementation. In the reviewer's opinion, the broad overview contained in the thesis is not a weak point, but it adds significantly to understanding the novelty of the proposed solution to PDEs and how it is linked to existing numerical methods.
The significance for the scientific area of numerical solutions of PDEs is definitely given, as for such problems always alternative and especially high-accuracy solvers are sought for. There is also room

for substantiating the method: It would be beneficial to obtain theoretical formulas relating the performance of MTSM with some benchmark integration algorithm. This could lead to a quantitative criterion telling the user when to switch from one algorithm to the other in order to obtain the best results in a minimum of time.

As MTSM is a versatile computational method with high potential, it is desirable to deepen the sound theoretical understanding of the method. A systematic truncation error analysis and a deeper analysis of the stability region associated with the variable order nature of the MTSM would be a strong theoretical backing. Also, the solution of PDEs is currently addressed only for the Method of Lines.
As follow-up research, it seems necessary to investigate ways to compute a fixed, limited number of operations and guarantee a limited approximation error. This is not yet available and would increase usability for most applications. To summarize, the topic is extremely relevant and interesting as the computational solution of ODEs and PDEs is at the heart of scientific computing. The work provides insights into and new results with respect to many relevant extensions for the MTSM to open up its use in the simulation of linear dynamical systems, and provides many concrete examples. It also exemplary presents selected MTSM applications for PDEs. The thesis also points the way for relevant future work on this topic to further increase the applicability of MTSM in PDE application areas.

Evaluation of the formal aspects of the thesis:
The level of English language is appropriate and high. The extensive thesis text is carefully written, proofread, and practically free of typos. I like the easily understandable yet fluent style of the thesis. The work is carefully elaborated and typeset, including correct mathematical expressions and many illustrative figures, and only passages remain vague and do not specifically pinpoint the meaning of the text. The thesis is overall a scientific work of generally high technical quality and clarity.

Quality of publications:
The student's publication record shows a large number of related conference publications (25, from 2015 to 2022) as well as 3 journal articles (2018 in a Q3 journal, 2019 in a Q3 journal, and 2021 in a Q2 journal). This scientific output is consistent with the thesis structure and content. The thesis contains many application examples and a broad spectrum of applications, but does not provide deep theoretical results or proofs. The results shown in the thesis, the research topic itself and the specific field of Taylor series methods have completely been published in peer-reviewed publications. Considering the research objectives and the research questions, the portfolio and wide field of publications is highly satisfactory. Although the defendant is not first author of any of the journal publications, the numerous conference papers with first authorship and 80% participation are proof to the high international scientific standard.

3. *Student's overall achievements*

Overall R&D activities evaluation:
The student has written an extensive, well-readable doctoral thesis with a broad range of remarkable and relevant results. The large number of conference publications indicate that the student realizes a high level of scientific dissemination and engages in scientific outreach and networking. The task of putting the MTSM context into a control perspective could mostly be achieved by the student, which also adds an inter-disciplinary aspect to his research work. Combined with the student's journal publications, the scientific standing fulfills the typical international requirements for a doctoral degree. The listed research activities indicate that the student is capable of scientific high-quality work and show the structural skills and abilities demanded from scientists.
Moreover, the defendant has shown broad engagement in many extracurricular activities. She is permanently involved in faculty programs to organize and develop teaching structures, curricula and

support students. She also actively participated in international study exchange programs (Aktion Czech-Austria) with the partner research group at TU Wien. Being consistently active in these fields is a high-valued quality in any researcher, and this generates benefits for the community, the national education system, and for international partnerships alike.

4. *III. Conclusion*

I find this dissertation a sound scientific piece of work, and together with the student's prolific publication activity, to be commendable. I recommend the thesis for defense, and upon successful defense, I recommend granting the Ph.D. degree. (in accordance with Section 47 of Act No. 111/1998 Coll., on higher education institution).

Best regards,

Martin Kozek