# *Review of a Doctoral Thesis at FIT BUT*

**Doctoral thesis** (hereinafter referred to as "thesis"), title of the thesis:
LARGE-SCALE ULTRASOUND SIMULATIONS USING ACCELERATED CLUSTERS

**Name of the doctoral student** (hereinafter referred to as "student"), name and surname:

Ing. FILIP VAVERKA

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**Name and institution of the reviewer:**

Dr. Christian Boehm
Institute of Geophysics, Department of Earth Science
ETH Zurich
8092 Zurich
Switzerland


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I. Thesis

Appropriateness and relevance

The past decade has witnessed significant efforts in utilizing digital twins and advanced numerical modelling to assist with applications of medical ultrasound. Going beyond conventional imaging, which relies on a simple ray approximation, several studies have shown the great potential of simulation-based approaches and ultrasound computed tomography, which rely on accurate physical models of the wave equation.

A major obstacle in bringing those methods into clinical practice, however, is their increased computational complexity, which is often prohibitively expensive given the expectations of in-situ imaging and near real time results. Algorithmic improvements and interdisciplinary efforts are thus crucial to amalgamate computer science and scientific computing with medical imaging and biomedical engineering.

This thesis marks an important step in this direction and addresses the above-mentioned challenges for efficient scaling on novel compute architectures and hardware accelerators. The results and algorithmic developments are highly relevant for the design of novel ultrasonic systems, and will benefit researchers in this field.

A summary of the contributions of the thesis

The main contributions of the thesis can be found in Chapters 5 and 6. After a brief motivation introducing possible applications in medical ultrasound, the following three chapters provide background information on different architectures of modern computer hardware and accelerators, numerical methods for solving partial differential equations, and different formulations of the wave equation including linear and non-linear variants.

The key research question addressed in this thesis is the design of efficient and scalable algorithms for simulating the wave equation with k-space pseudo-spectral methods. To this end, Chapter 5 describes different algorithmic approaches for decomposing the computational domain. This is a crucial step in reducing the communication overhead observed in global k-space methods. The implementation of domain decomposition based on the local Fourier basis is detailed in Chapter 6. Extensive tests for strong and weak scaling on various systems show speed-ups of 5 to 8 for realistic problem sizes. The method is particular attractive to multi-node GPU systems, which have proven in other fields to be a key driver of bringing novel imaging methods into clinical practice.

Novelty and significance:

The non-local support of the 3D Fourier transform is the major hurdle for the scalability of global k-space methods on large distributed computer architectures. The thesis mentions that up to 80% of the wall-time might be spent on the communication overhead. This underlines the importance of parallel and scalable algorithms in this field.

The proposed approach based on domain decomposition using local Fourier basis has proven to reduce the communication overhead substantially. I consider this a novel and significant contribution to k-space pseudo-spectral methods, which are widely used to model ultrasonic wave propagation. The extensive tests on various computer hardware and accelerators (including Haswell, Knights Landing, NVIDIA, DGX-2, ...) show the efficacy of the algorithms developed in this thesis.

Evaluation of the formal aspects of the thesis:

The thesis is well-written and structured concisely. The outline is clear and references to other works are in-line with good scientific practice. From a domain-scientist's perspective, it would have been nice to elaborate more on the background of medical ultrasound or to extend the numerical examples with more use cases. I understand, however, that this is not the main scope of this thesis.

Major results are well-documented in charts and figures, and the sketches of the communication patterns of different cluster configurations are helpful. The language level is good, though there is a bit of room for improvement in future work.

Quality of publications

The results of this thesis have been published through different outlets, including peer-reviewed journal articles and conference proceedings. Key aspects of this research have been presented at multiple conferences, resulting in at least four first-author conference proceedings. The proceedings show a good mix of targeting researchers in computational acoustics and high-performance computing, and are highly relevant for their fields.

II. Student's overall achievements

Overall R&D activities evaluation:

The results of the thesis proof a deep technical understanding of the challenges of scaling methods involving 3D Fourier transforms on modern computer architectures. A major pillar of the work is the efficient implementation of the proposed domain decomposition methods and their validation on various

HPC systems. The student successfully ran scaling tests including various architectures and accelerators on supercomputing clusters hosted by IT4Innovations and the Swiss National Supercomputing Cluster (CSCS).

In addition to the publications directly resulting from the thesis, the student co-authored several conference proceedings and extended abstracts, including three submissions to the prestigious Supercomputing conference.

<u>Assessment of other characteristics</u>:

The student excelled in international research collaborations involving scientists from their home faculty and the University College London. Furthermore, the student participated in the Horizon 2020 project PAMMOTH, which is a multi-national initiative on photoacoustic mammoscopy involving 9 institutions from 7 different European countries. In addition to these scientific merits, the student gained experience in industry which is an important aspect for bringing the simulation tools into (clinical) practice.

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III. Conclusion

In summary, the thesis contains innovative and important results to improve the scalability of large-scale simulations for medical ultrasound, and to efficiently utilize modern computer hardware including multi-node GPU clusters. The contributions to k-Wave are of great importance to the scientific community and overcome previous bottlenecks related to the non-local characteristics of 3D Fourier transforms.

In my opinion, the thesis and the student's achievements meet the generally accepted requirements for the award of an academic degree (in accordance with Section 47 of Act No. 111/1998 Coll., on higher education institution). I recommend that the Faculty of Information Technology of Brno University of Technology accepts this document as a doctoral thesis for the purpose of conferral of a doctoral degree.

Zurich, 31.05.2023

Signature of the reviewer: