ČESKÉ VYSOKÉ UČENÍ TECHNICKÉ V PRAZE
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KATEDRA MATEMATIKY

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Supervisor's report of doctoral thesis

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Thesis: Data Structures and Parallel Algorithms for Numerical Solvers in Computational Fluid Dynamics

The doctoral thesis under review focuses on the development of parallel methods for the numerical solution of partial differential equations, with an interdisciplinary approach that spans high-performance computing (HPC) and numerical mathematics, specifically computational fluid dynamics (CFD). This work provides a detailed exploration of these topics, with a structure that is derived from this intersection.

The first chapter provides a comprehensive overview of the main software tools for parallel programming of multicore CPUs and graphics processing units (GPUs). The author explores a range of frameworks and libraries, including OpenMP, OpenACC, OpenCL, CUDA, ROCm, and MPI, as well as higher-level libraries like Thrust, Kokkos, and Template Numerical Library (TNL). The latter is an ongoing development effort at the Department of Mathematics, with Jakub Klinkovský serving as the main developer during his doctoral studies [3]. In this chapter, the author showcases the implementation of the *axpy* operation (i.e. vector operation $\vec{y} = a\vec{x}+\vec{y}$) across the mentioned libraries and frameworks, highlighting the strengths and weaknesses of each of them.

The second chapter is dedicated to two data structures commonly used in numerical simulations. The first is a multidimensional array, which is later used to represent the lattice in the lattice Boltzmann method. The implementation of this structure is highly flexible, leveraging templates in the C++ language. Additionally, the author explores a distributed version of this data structure, which is designed to support parallel architectures with distributed memory. The second data structure is an efficient representation for unstructured numerical meshes [2]. Its key feature is the ability to be fine-tuned during compile-time for specific numerical methods, resulting in highly efficient computations. Even when working with architectures that have distributed memory, computations are possible. In this chapter, the author presents benchmark results for several basic operations on unstructured meshes, comparing the implementation in TNL with the MOAB library. While the MOAB library is more general and supports adaptive meshes, the TNL implementation is highly optimized, with performance approximately two orders of magnitude faster in some cases.

The third chapter explores the solution of large sparse linear systems. The author provides an overview of the state-of-the-art of iterative methods and preconditioning for the solution of these systems. He presents a comprehensive list of small libraries and large numerical frameworks that deal with linear systems, including TNL, in which the author implemented several solvers and support of distributed matrices.

The fourth chapter is about the mixed-hybrid finite element method (MHFEM) [4], specifically the numerical scheme referred to as NumDwarf. This method can be used to solve second-order parabolic partial differential equations with general coefficients. The author describes the derivation of the numerical scheme in detail, and summarize it in the form of a pseudo-algorithm. Additionally, the author showcases the application of this scheme to problems in two-phase flow in porous media. As a benchmark problem, the generalized McWorther-Sunada problem is solved, and the author presents an experimental order of convergence, as an analytical solution is known for this problem. From the computational point of view, the limiting factor for performance is the solution of resulting sparse linear systems. In this chapter, the author compares solvers from TNL with the Hypre library, a popular library with distributed solvers of sparse linear systems, and shows scalability up to 336 CPU cores. Efficiency drops to approximately 0.6 in this case, which shows the potential for using more efficient preconditioners based on domain decomposition methods in the future.

The fifth chapter of the doctoral thesis focuses on the lattice Boltzmann method (LBM), a modern and widely used numerical technique, particularly for computational fluid dynamics, that is well-suited for GPUs. The author explains the fundamentals of the LBM and specifically addresses various streaming patterns that can be applied to the method. Some of these mogifications of streaming offer reductions in memory requirements, which are a weakness of the LBM. Furthermore, the author discusses implementation details, referring to an LBM solver being developed at the Department of Mathematics at FNSPE [5, 6]. It should be noted that the author significantly contributed to the development of this software package.

The sixth chapter explores the coupling of the MHFEM and LBM methods mentioned previously [1]. The reason for this coupling is that the LBM is efficient in simulating turbulent flow, whereas the MHFEM method is better suited for advection-diffusion problems. This novel approach combines the advantages of both methods and was fully derived by the author, representing one of the main achievements of their doctoral study.

In chapter seven, the author demonstrates the application of the coupled LBM-MHFEM method for mathematical modeling of vapor transport in turbulent airflow [1]. This problem was solved in collaboration with the Center for Experimental Study of Subsurface Environmental Processes (CESEP) at the Colorado School of Mines and the US Army Engineer Research and Development Center (ERDC), both institutions located in the USA. Originally, the aim was to investigate coupled soil-plant-atmosphere processes, including airflow, heat, mass, and moisture transfer. In the experimental facility at CESEP, the plants are replaced with limestone blocks since experiments show that they behave similarly. The author presents the results of numerical simulations and compares them with experimental data obtained through experiments conducted at CESEP. Remarkably, a high level of agreement was achieved between the numerical simulations and experimental data.

The work on the thesis was conducted as part of several research projects, including one OP RDE project, projects by the Ministry of Education, Youth, and Sports, the Ministry of Health of the Czech Republic, projects by the Czech Science Foundation, and projects by the Grant Agency of the Czech Technical University. During his studies, the candidate visited several research centers, including the Center for Experimental Study of Subsurface Environmental Processes (CESEP) at Colorado School of Mines in Colorado, USA, the US Army Engineer Research and Development Center (ERDC) at Vicksburg in Mississippi, USA, and the Computational center CINECA in Bologna in Italy.

He has also actively attended 18 international conferences and is a co-author of 11 scientific papers listed on the Web of Science. The candidate has also assisted in the education of students by guiding exercises and teaching lectures in calculus and programming. He has supervised two master students at the Faculty of Information Technology at CTU in Prague and bachelor students at FNSPE. Additionally, he has done a lot of work as an administrator of a small cluster equipped with GPUs installed at the Department of Mathematics at FNSPE.

The candidate has demonstrated excellent skills in programming languages like C++ and

Python. He also has very good knowledge of hardware architectures, including multicore CPUs, GPUs, and distributed clusters. He has significantly contributed to the development of the TNL library and an in-house code for LBM, which is being developed at the Department of Mathematics at FNSPE. His thesis clearly shows that advanced programming techniques available in modern programming languages can significantly aid the development of advanced and highly optimized numerical solvers. Furthermore, the author made good use of his deep knowledge of numerical mathematics when he developed the coupled LBM-MHFEM method.

Jakub Klinkovský is a very systematic person, which helps him write code of excellent quality. He pays attention to small details, which are often very important, not only in programming but also in scientific papers and his research work. He is also able to act as an excellent team researcher willing to help others especially, but not only, in code development.

The thesis fulfills all the requirements for a Ph.D. thesis. Therefore, I strongly recommend the candidate to the committee for doctoral theses to award him the title of Doctor of Philosophy.

Prague, April 1, 2023

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