Review

by Assoc. Prof. Dr. Kiril Shterev, Institute of Mechanics - BAS

for the thesis of Dimitar Georgiev Slavchev

"COMPOSITE NUMERICAL METHODS AND SCALABLE TILE ALGORITHMS"

presented for awarding the educational and scientific degree "Ph.D."

in professional area 4.5 "Mathematics"

The performance of modern computational algorithms is closely related to their parallel efficiency due to the parallel architecture of modern processors. Parallelism in modern computers is on many levels. The direction of their development comes from the fundamental limitations of the maximum frequency at which a processor can run. Therefore, increasing the performance of modern processors is possible through parallelization. One core can execute several instructions per clock cycle, and each processor has several cores. Such parallelization is available in all processors at the moment. By comparison, widely available processors from the recent past had a single core that performed a single operation on several clock cycles. Algorithms and programs have been developed for old processers with the idea of the fastest serial execution. However, in the general case, the best serial algorithms and programs are challenging to parallelize, and their acceleration is limited. "Parallel-friendly" algorithms are usually slower than serial algorithms in serial execution, so they have not been of interest to most researchers in the recent past. An algorithm and a code must correspond to parallel processor architecture to use their potential, i.e., the need to have good parallel efficiency. That is why I find the work in this direction very relevant.

Formally, according to the Rules for the Implementation of the Law on the Development of the Academic Staff in the Republic of Bulgaria on July 6, 2018, a Ph.D. candidate in 4.5 "Mathematics" is expected to meet the minimum requirements of 50 points for indicator A (presentation of doctoral thesis) and to have minimally at least 30 points in the "Г" - group of indicators. Dimitar Georgiev Slavchev presents a list of 5 scientific articles in which he is the first coauthor and two articles he is the only author. The articles were published in the period 2017 -2021 in connection with the results of the dissertation; all of them are indexed by Scopus, with one paper in Scopus Q2 quartile. The points

collected from the publishing activity (220) exceed the requirements of a minimum threshold for the indicators group "Г" in the case of the Ph.D. dissertation defense. With this, the formal conditions for satisfying the national criteria are fulfilled, and it is possible to start reviewing and defending the presented dissertation.

The major goals of the thesis are: comparative analysis of the performance and parallel speed-up of frequently used software packages applying direct Gaussian elimination for solving systems of linear algebraic equations with dense matrix on CPUs and accelerators (MICs); analysis of the performance, parallel speed-up and accuracy of an approximate method for solving systems of linear algebraic equations based on hierarchical semi-separable compression from the software package STRUMPACK for systems with suitable structure; development of reordering algorithms for the unknowns for systems of linear algebraic equations arising from discretization with finite element method of fractional diffusion. The reordering is aimed at improving the effectiveness of hierarchical semi-separable compression when applied on the stiffness matrix; numerical solution of elliptic and parabolic problems in the field of fractional diffusion, modeled with the integral formulation of the fractional Laplacian and discretized with finite elements.

A dissertation contains 140 pages, which is organized into an introduction, four chapters, and a conclusion. Some 90 references are cited. The thesis is illustrated with 47 figures and contains 7 tables. A glossary of terms and abbreviations is included.

Content and contributions of the thesis

The introduction to the thesis presents the importance of the theme of the thesis. It starts from the motivation for computer modeling of processes, the guidelines for modern hardware development are considered, and current tasks are presented, which are described by the equations calculated in the dissertation. An overview of the methods and packages for solving systems of linear algebraic equations with dense matrices was made. The goals and tasks of the dissertation, the research methodology, and the specifications of the used high-performance computing systems are presented.

Chapter 1 presents methods for solving systems of linear equations with dense matrices. A description of the block methods analyzed in the dissertation for

solving systems of linear algebraic equations with dense matrices is given, and basic estimates of their computational complexity. Special attention is paid to the hierarchical semi-separable (HSS) compression of dense matrices and its implementation in the software package with free access STRUMPACK.

Chapter 2 discusses the boundary element method for calculation of flow past Zhukovsky's airfoils. The test task is the flow past five Zhukovsky's airfoils located vertically. The numerical results for the velocity field and strealines are presented. A detailed analysis of the parallel efficiency of the used software packages and computer architectures is made. It is concluded that the accuracy and computational efficiency of HSS compression depend on the thresholds of relative and absolute error, and the structure of the matrix is decisive for the quality of hierarchical compression. The matrix structure is suitable for the considered problem, i.e., allows the effective application of HSS compression.

Chapter 3 discusses the finite element method for the numerical solution of a two-dimensional stationary fractional diffusion problem. The subject of research in this chapter is a two-dimensional boundary value problem for anomalous diffusion. Anomalous diffusion is described by a Laplace operator defined in integral form using the Ritz potential. The finite element method is applied. Five methods for rearranging the unknowns are presented: rearrangement along the "Y" coordinate - "top"; along horizontal lines - "stripes"; in a spiral around the center - "snake"; nested dissection and recursive bisection. Numerical experiments on computer systems with shared memory are considered. It is concluded that the matrix structure obtained by sampling the fractional diffusion problem is less suitable for HSS compression compared to the problem of wrapping the wing profiles discussed in Chapter 2.

Chapter 4 discusses the finite element method for solving a two-dimensional parabolic fractional diffusion problem. This chapter discusses a non-stationary problem. An implicit Euler method with a constant time step was applied for time sampling. The problem is reduced to solving a series of systems of linear algebraic equations with the same transition matrix and changing the right parts at every time step. This allows factoring to be done once. The accelerations of the parallel program and the error of the HSS-based solver are analyzed. The results show that the parallel times for solving the parabolic problem using the solver from the STRUMPACK software package are significantly better compared to the times when using block LU factorization from the MKL package.

Discussion

I accept the scientific and applied contributions of the author in the dissertation as declared in the dissertation. The Ph.D. student has been seriously involved in the subject for about 4 years, which is a very good achievement. The analysis is done on different hardware architectures using different software packages. It is possible to expand the software to solve three-dimensional tasks, which will lead to considerable increases in the number of mesh nodes and improve its parallel efficiency.

The thesis text is concise and specific, appropriately organized with a clear division into chapters and topics, a reader-friendly presentation sequence, a sufficient level of detail, and well-illustrated with figures and tables. The specific terminology for the formulation of the tasks and the presentation of the results for the flow past Zhukovsky's airfoils is correctly used. Including a list of author's publications after each chapter is helpful because it helps to understand where the results are presented. The Abstract correctly reflects the content of the dissertation

I want to make the following remarks: in each of the considered problems, the speed-up is presented depending on the number of mesh nodes, but no information is given about the sufficient number of mesh nodes to obtain a sufficiently accurate numerical solution and the corresponding spatial steps. This information is essential to get a clear idea of the speed-up of the parallel program in the calculation of problems with certain requirements for the accuracy of the solution for the considered sizes of the computational domain. When solving real problems, the size of the computational domain is usually much larger than the test tasks, and the number of mesh nodes to obtain a sufficiently accurate solution is also much larger than that of the test tasks.

Conclusion

The Law on the Development of the Academic Staff in the Republic of Bulgaria requires any Ph.D. thesis to contain scientific or applied results which represent an original contribution to the respective scientific discipline. The thesis should show that the candidate possesses deep theoretical knowledge in the corresponding scientific field and abilities for doing independent research. These requirements are fully met in the case of Dimitar Slavchev's dissertation and the scientific publications where the thesis results are presented.

On these grounds, I will vote positively to award the degree, and I propose with conviction to the honorable Scientific Committee to award Dimitar Slavchev the educational and scientific degree "doctor" (Ph.D.) in 4.5 "Mathematics".

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