OPPINION

By: Prof. DSc Svetoslav Marinov Markov, Institute of Mathematics and Informatics, BAS

Subject: dissertation on "Composite numerical methods and scalable block algorithms" by Dimitar Georgiev Slavchev, in connection with the procedure for obtaining the educational and scientific degree "Doctor" at the Institute of Information and Communication Technologies of BAS (IICT-BAS)

1. General information on the procedure. Pursuant to Art. 4, para. 2 of the Law on the Development of Academic Staff in the Republic of Bulgaria and Decision of the Scientific Council of the Institute of Information and Communication Technologies of BAS (IICT-BAS), Protocol № 1/ 26.01.2022, in connection with the procedure for acquiring educational and scientific degree "Doctor" in professional field 4.5. Mathematics, doctoral program "Computational Mathematics", by Dimitar Georgiev Slavchev with a dissertation on " Composite numerical methods and scalable block algorithms", as a member of the scientific jury for the defense of the dissertation I present this opinion.

2. Brief information about the author. Dimitar Slavchev has a master's degree from the Technical University of Sofia - Applied Mathematics - 2013. Slavchev is a full-time PhD student at IICT from 2017 to 2020, and from 2020 to 2022 he is an assistant. Scientific adviser is Cor. Mem. Svetozar Margenov. The dissertation is discussed and admitted to the defense at an extended meeting of the section "Scientific Computations with Laboratory of 3D Digitization and microstructure Analysis" of IICT-BAS, held on 11.01.2022. Presented: dissertation, abstract, list of publications on the dissertation, approbation of the results, appendix and bibliography.

3. Brief data on the dissertation. The dissertation is structured in: introduction, presentation of four chapters and conclusion. The dissertation consists of 140 pages, 47 figures and 7 tables, 90 cited literature sources and 2 appendices.

4. Relevance of the topic. Numerical solving of large-scale problems requiring the use of high-performance computing systems is a topical issue. It requires specialized hardware and software - graphics cards, accelerators, high-speed communication between system servers, software standards and packages for communication between processor cores and servers, software packages implementing efficient numerical methods and many others. When discretizing the differential equation with the boundary element method, as well as when applying the finite element method for nonlocal problems (for example, the anomalous (fractional diffusion) studied in this dissertation), the obtained stiffness matrix is dense. One possible approach to reducing the computational complexity of the solution of systems with such matrices is the hierarchical compression introduced by Hackbusch. It uses the structure of the output matrix. The goal is both to reduce memory usage and to improve computational efficiency. Here, the structure of a dense matrix means the presence of an approximation of the output matrix with a low rank of the off-diagonal blocks. This property allows the representation of off-diagonal blocks as a product of smaller matrices. There are different variants of hierarchical matrices, incl. H, H2 or (Hierarchically Semi-Separable) HSS matrices. Supercomputer simulations are crucial for development in a number of high-tech fields. Examples are *in silico* molecular biology and drug design, turbulent flow analysis, non-destructive testing, 3D image processing, fluid dynamics, and many others. After appropriate discretization, mathematical models are usually reduced to problems of linear algebra, among which the role of solving systems of linear algebraic equations is decisive. For this purpose, specialized software tools are being developed. In the general case, variants of the Gaussian method are used to solve systems of linear algebraic equations with dense matrices, which use sequential ellimination of the unknowns. The dense matrix is homogeneous by default, since it is not assumed that there are zero elements. The Gaussian

method has computational complexity $O(n^3)$. In the present dissertation an alternative approach based on hierarchical compression is investigated. The goal is to reduce computational complexity. Here, the structure of a dense matrix means the presence of low-rank off-diagonal blocks. An essential part of the dissertation is dedicated to the numerical solution of fractional diffusion problems. Fractional diffusion (also called anomalous diffusion) describes non-local processes that occur in different physical and social environments. Unlike ordinary (local) diffusion, anomalous diffusion includes the so-called fast transport (jumps) or tunnel effects. Various examples of mathematical models of processes and phenomena have been published in the literature, which are described by fractional diffusion. Such examples are: flows in highly inhomogeneous porous media, superconductivity, diffusion of polymers in supercold media; electrodiffusion of ions in nerve cells and diagnostics using photon diffusion; image processing and machine learning, the spread of viral diseases, computer viruses and crime. The *fractional* Laplace operator describes anomalous diffusion in space. There are different definitions of *fractional* Laplacian. It is important to note that they are not equivalent. For example, in [13] the difference between integral and spectral definitions is analyzed (see also the papers in the list of references).

5. The main objectives of the dissertation are: 1. Comparative analysis of the speed and parallel performance of commonly used software packages applying direct Gaussian elimination to solve systems of linear algebraic equations with dense matrix using CPUs and accelerators (MIC). 2. Analysis of the speed, parallel speedup and accuracy of an approximate method for solving systems of linear algebraic equations based on hierarchical semi-separable compression (HSS) from the STRUMPACK software package for systems with appropriate matrix structure. 3. Development of algorithms for reordering of the unknowns in problems arising afrer discretization of fractional diffusion problems by finite element method in order to improve the efficiency of the hierarchical semi-separable compression of the thus computed stiffness matrix. 4. Numerical solution of elliptic and parabolic problems in the field of anomalous diffusion described by the integral formulation of fractional Laplacian and discretized in space by the finite element method.

6. Short content. The Introduction describes the methods used and the tasks solved. Chapter 1 introduces the block methods used to solve dense systems of linear equations, and estimates of their computational complexity; the method of Gaussian elimination and the LU-factorization based on it is described. Section 1.4 discusses hierarchical methods for solving systems of linear equations developed for solving systems with structured matrices (dense and sparse). The advantages of the method based on HSS compression are described - lower estimate of the computational complexity for problems with appropriate matrix structure. Chapter 2 presents numerical results for the flow around Zhukovsky's wing profiles. The resulting system with dense matrix is used as a benchmark in the comparative analysis of the used block algorithms. Chapter 3 discusses the problem of two-dimensional fractional diffusion modeled with the fractional Laplace operator. The finite element method is used for discretization in space. Chapter 4 discusses the parabolic problem of two-dimensional fractional diffusion in space. The Conclusion presents the main scientific and applied scientific contributions. A list of published articles and reports presented at scientific forums on which the dissertation is based is given. Chapter 2 discusses a numerical method for computer simulation of laminar flow around Zhukovsky's wing profiles. In the dissertation the method described in [23] is applied, as a software implementation for a flow of ideal fluid around a cascade of wing profiles has been developed. The method is based on collocation of splines with pisewise linear interpolation. After discretization of the integral equations by the method of boundary elements, a system of linear equations with a dense matrix is obtained. The results of the application of the methods and algorithms studied in the dissertation are compared with the results obtained by the method of sequential ellimination

(Gaussian method) realized in several popular software packages. On CPU processors, Intel Math Kernel Library (MKL) and Parallel Linear Algebra for Scalable Multi-core Architectures (PLASMA) are used in the performance comparative analysis, while for Intel Xeon Phi coprocessors (short MIC for the Many Integrated Core architecture), MKL performance is also compared to Matrix Algebra on GPU and Multicore Architectures (MAGMA) for MIC architecture (called MAGMA MIC for short). Central to the results presented in Chapter 2 is the study of the method of hierarchical semi-separable compression (HSS compression). The experimental comparative analysis is based on its implementation in the STRUMPACK software package. It shows better performance than direct Gaussian solvers using block LU factorization. At the same time, the obtained parallel speedups with STRUMPACK are smaller, which is due to the more complex hierarchical structure of the algorithm. The accuracy and computational efficiency of the HSS compression depend on the relative and absolute error thresholds. These are parameters that are selected by the user. The presented analysis shows how to get the best efficiency at a given accuracy. Chapter 3 is devoted to fractional elliptic operators in space of degree $\alpha \in (0,1)$ describing fractional diffusion processes. The boundary value problems associated with them are non-local and, in the general case, the numerical solution of such problems is a computationally expensive process. This type of non-local models is used, for example, in image processing, financial mathematics, electro-magnetostatics, peridynamics, modeling of flows in porous media and many others. Several software packages implementing Gaussian elimination methods have been analyzed. Chapter 3 uses only the most effective of these: the Intel's Math kernel Library (MKL). The performance of the algorithm based on hierarchical semi-separable (HSS) compression implemented in the STRUctured Matrix PACKage package (STRUMPACK) is analyzed. Several methods for reordering the unknowns have been investigated aimed at improving the efficiency of the HSS compression. The experimental comparative analysis is based on the implementation of the HSS compression and ULV-like factorization in the STRUMPACK software package. The analysis shows good performance of the sequential algorithm compared to the direct Gaussian solver using block LU factorization. At the same time, the obtained parallel performance and speedup when using the STRUMPACK package are smaller, which is explained by the more complex hierarchical and recursive structure of the compression. The accuracy and computational efficiency of the HSS compression significantly depend on the thresholds of relative error ε_{rel} and absolute error ε_{abs}, as well as on the availability of a suitable matrix structure. In the experiments, a relative error Rrelative of the numerical solution close to ε_{rel} was observed. To improve the structure of the matrix, five ways to reorder the unknowns have been proposed, which significantly increase the compression efficiency. The presented analysis shows that in most experiments the efficiency of the HSS compression is best when reordering with recursive bisection. The proposed reorderings of the unknowns significantly improve the efficiency. Chapter 4 analyzes numerical experiments on shared memory computer systems. A leading topic in the presented results is the analysis of the computational efficiency of the method based on hierarchical semi-separable compression and ULV-like factorization and its parallel implementation in the STRUMPACK software package.

7. Overview. The dissertation analyzes the computational efficiency of block numerical methods and algorithms for solving systems of linear algebraic equations with dense matrices. This study is motivated by applications related to the numerical solution of elliptic and parabolic partial differential equations. Two such problems were used in the presented comparative analysis: a) boundary value problem describing the flow around wing profiles of Zhukovsky, discretized by the boundary element method; b) anomalous diffusion in a bounded domain modeled with fractional Laplacian, where the finite element method is applied for discretization. In both cases, the continuous problems are reduced to systems of linear algebraic equations with dense matrices. It has been shown that the structure of these matrices is suitable for the application of a hierarchical method using HSS compression. An important part is the comparative analysis of the

computational efficiency of software packages implementing block LU factorization, as a variant of Gaussian elimination. The general conclusion is that the MKL software package has better performance than the analyzed alternative parallel implementations of block LU factorization. The main focus of the dissertation is the analysis of the possibility to improve the computational efficiency of solving systems of linear algebraic equations with dense matrices using a block hierarchical method using HSS compression. This method is implemented in the STRUMPACK software package. The performance of the hierarchical algorithm for systems of linear algebraic equations, obtained by applying the boundary element method and the finite element element for the considered elliptic boundary value problems, is analyzed. The analysis shows that these dense matrices have a suitable structure for applying the hierarchical method. This means that low-rank off-diagonal blocks are obtained in the HSS compression process. The sequential experiments confirm the estimates of the computational complexity of the analyzed block methods. For both problems, the hierarchical solver has better performance than the Gaussian solver from the MKL package - the most efficient of the software tools analyzed in this paper using LU factorization. When applying the hierarchical method, an approximate solution of the system is found, and its accuracy depends on the accuracy of the HSS compression. For the problem of flow around Zhukovsky's wing profiles, the relative errors for the respective ε_{rel} thresholds are larger, which, however, is compensated by the higher performance. The structure of the obtained dense matrix is not suitable for HSS compression. To improve it, five reordering methods have been proposed. The presented analysis shows the advantages of the methods of nested desections and recursive bisection. The computational efficiency and accuracy of the hierarchical solver based on HSS compression for a parabolic problem with fractional diffusion in space have been studied. An implicit Euler differece scheme with a constant time step is used for discretization in time. In this formulation of the problem, finding the numerical solution is reduced to solving a sequence of systems of linear algebraic equations with the same matrix. Thus, at each time step, a system with the transition matrix is solved, which is factorized once. Solving such systems with the help of HSS compression has a lower computational complexity - O (nr), compared to the case when LU factorization in the Gaussian method - O (n^2). For the considered parabolic problem, the times of the hierarchical solver are better in both sequential and parallel experiments. At the same time, thanks to the unconditional stability of Euler's implicit method, the relative error of the solution remains close to the set relative threshold ε_{rel}.

8. Main scientific and applied scientific contributions. The performance of the following software packages for solving linear systems with dense matrices using block LU factorization has been studied: - for general purpose processors (CPUs) - the Intel Math Kernel Library (MKL) package and the Parallel Linear Algebra Software for Multicore Architectures (PLASMA) open access library; - for accelerators with Intel's Many Integrated Core (MIC) architecture - MKL and the Matrix Algebra on GPU and Multicore Architectures (MAGMA) open access package. The results of numerical experiments for systems obtained by approximation with the boundary element method of the boundary value problem for laminar flow around Zhukovsky wing profiles are in accordance with the asymptotic estimates of the computational complexity. The comparative analysis shows better performance and very good parallel scalability of the MKL package. The computational complexity, parallel efficiency and relative error of a hierarchical semi-separable compression (HSS) method are studied. Numerical experiments are performed with the STRUctured Matrices PACKage (STRUMPACK), in which a parallel solver based on HSS compression and ULV-like factorization is implemented. Comparative analysis includes two types of dense matrices that are obtained after discretization. It is shown that for the problem of flow around Zhukovsky profiles discretized by the boundary element method, the sequential numbering of the nodes along the boundary of the profiles leads to a matrix with a structure suitable for HSS compression. This is not the case for the fractional diffusion boundary value problem, discretized by the finite element method. In order to improve the efficiency of the

hierarchical semi-separable compression, five methods for reordering of the unknowns have been proposed and studied. For three of them have been developed new algorithms and software implementations. The comparative analysis shows a significant improvement of the results when applying the methods of nested disections and recursive bisection. A method, algorithm, and program realization have been developed for numerical solution of a parabolic equation with a fractional diffusion operator in space. An implicit Euler method with constant time step and with lumped mass matrix is applied for time discretization. It has been proven that for this time dependent problem, the computational complexity of the individual parts of the algorithm creates conditions for the advantage of the hierarchical method based on the HSS compression. This is confirmed by the performrd numerical experiments. Thus, for all dimensions of the discrete problems in space, as well as for all settings of the relative error threshold, the variant of the program using the solver from the STRUMPACK package has better performance than the one using the MKL.

Conclusion. My assessment of the scientific and scientific-applied contributions of Dimitar Georgiev Slavchev in his dissertation on "Composite numerical methods and scalable block algorithms" in connection with the procedure for obtaining the educational and scientific degree "Doctor" at the Institute of Information and Communication Technologies - BAS (IICT-BAS) is definitely positive. These contributions comply with the requirements of the Law on the Development of the Academic Staff of the Republic of Bulgaria. The minimum national requirements and those of IICT-BAS have been met. I recommend Dimitar Georgiev Slavchev to be awarded the educational and scientific degree "Doctor" in the professional field 4.5 Mathematics, doctoral program "Computational Mathematics".

29.04.2022 Prepared the oppinion:

Sofia /Prof. DSc

На основание ЗЗЛД