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Fast Solvers for Systems of Linear Equations with Block-Band Matrices

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Abstract. This article deals with parallel iterative algorithms for linear systems with block-band matrices. The algorithms can be used in mathematical modeling of the problems involving finite difference and finite element methods. The solvers are adjusted to the problem and to the computing systems, which use special precompilers. Applications of the algorithms to the ACELAN-COMPOS software package focused on the new material modeling, is described. To achieve a high performance, both parallel programming techniques and the optimization of the processor memory hierarchy are used. The results of numerical experiments confirm the efficiency of the methods and algorithms.

AMS subject classifications: 65F08, 65F50

Key words: High performance computing, parallel computing, iterative algorithm, sparse matrix, system of linear algebraic equations.

1. Introduction

In many problems of mathematical modeling, there is a need to solve systems of linear algebraic equations with large sparse matrices. Iterative algorithms are used to solve such problems [9,23].

This work continues the series of publications of the authors [26,28,30]. The solvers presented in this article are embedded in the ACELAN COMPOS application software package for modeling the properties of new materials [18,20]. In recent years, the main distinguishing feature of processors is that the execution time of arithmetic operations is more than an order of magnitude bigger than the time of reading the arguments of such operations from RAM [16]. In this work, we use structures for efficient data storage and fast algorithms. Numerical experiments demonstrate the high efficiency of the methods

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presented. While in [26, 28] the solver was applied to the matrices obtained by a finite difference method, we extend the capabilities of the solver to matrices arising in finite element methods.

Since the solver in the application software package is focused on a certain set of similar problems, the solver is assumed to be parameterized. The parameters of the solver are both the characteristics of the input data of the problem (for example, the number of unknown functions and the number of differential equations in the model, the numerical solution of which leads to the system of linear algebraic equations) and the characteristics of the computing system (the amount of cache memory, parallelization capabilities).

Block-band matrices arise when regular grids are used on the domains having the form of rectangular parallelepipeds. If the region has a different shape, then curved orthogonal grids can sometimes be used to obtain a system of linear algebraic equations with a block-band matrix [15, 17]. The solution of linear systems with such matrices can be accelerated by employing specific data structures and parallel methods that can operate with blocks [1, 2, 11]. Such solvers are usually iterative due to the need to keep low memory profile, which is usually not possible for direct solvers. An important part of the development of such iterative solver is convergence analysis [10] and multi-stage performance analysis [3, 5]. Asynchronous parallel nonlinear multi-splitting programs and their convergence analysis were presented in [1]. Designing proper preconditioner is another vital part of solver development for specific matrix structures [4, 6–8].

An important feature of the ACELAN COMPOS package solver presented in this work is that not only the initial data of the mathematical model but also the solver is formed in the package. In addition, the precompiler — i.e. the preliminary compiler in [26, 28], is modified. The presented precompiler merges loops that have different for-loop headers [27]. Information dependency analysis is used for the correctness and effectiveness of the merge. The use of the precompiler is justified by the fact that the modern optimizing compilers such as GCC, LLVM, ICC do not optimize programs efficiently enough [14]. A precompiler is a preliminary compiler that converts a C program into a faster program of the same language. The precompiler presented in the paper, is developed on the basis of OPS (Optimizing Parallelizing System) [13, 21] and shows acceleration by 1.25 times. Ways to get further performance are outlined.

2. Features of Block-Band Matrices

The block-band matrices are a kind of sparse matrices. Sparse matrices are stored in memory [22] only by values of non-zero elements and their row and column numbers (3 numbers). Block-band matrices can be stored only by non-zero diagonals [26, 28], which are stored as arrays. In this case, column and row numbers should not be stored. The amount of memory used is 2 times less than for sparse matrices of the general form.

Band matrices arise in finite-difference and finite-element methods — cf. Figs. 1 and 2, when covering a rectangular parallelepiped with a Cartesian grid [2–8, 10, 11]. If we consider a system of differential equations, the matrix of the system of linear algebraic equations is a block-band matrix — cf. Fig. 3. The elements of this matrix are blocks (matrices)