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**DIRECT METHODS   
FOR SOLVING SYSTEM OF LINEAR EQUATIONS**

*Practice 4. Solving of sparse systems by direct methods in heat conduction problem in a plate. MKL PARDISO usage.*

Nizhni Novgorod

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# Objectives

The objective of the given laboratory work is to investigate some methods for solving system of linear equations with a sparse matrix by example of stationary problem of heat distribution in a rectangular plate with specified temperature boundary conditions.

# Abstract

A stationary problem of heat distribution in a rectangular plate with specified temperature boundary conditions is considered in the work. Heat distribution is described by a partial differential equation of the second order, solving of which is reduced to solving of a linear algebraic equation system with a block five-diagonal matrix. It is proposed to study the Cholesky method during this work and apply its implementation from the MKL PARDISO library for solving the stationary problem of temperature distribution in a plate. Along with this, it is supposed to develop implementation using MKL LAPACK, compare the efficiency of solving the problem by means of MKL PARDISO and MKL LAPACK, and perform scalability analysis for the application that uses the parallel solver MKL PARDISO.

# GUIDELINES

A stationary problem of heat distribution in a rectangular plate with specified temperature boundary conditions is considered in the work. A mathematical model for this process is a partial differential equation of the second order. To solve such equations numerically, the finite differences method may be used: a discrete grid is introduced in the parameters space and the differential equation is approximated by a linear algebraic equation with a five-diagonal matrix. This matrix is symmetric positive definite.

The Cholesky method was considered earlier for solving a sparse SLAE with a symmetric positive definite matrix. This method allows to represent a matrix *A* as a product *UTU*, where *U* is an upper triangular matrix (this is equivalent to the representation *LLT*, where *L* is a lower triangular matrix). Solving of the original system is reduced to solving of two triangular systems.

When the matrix *A* is sparse, decomposition can generate new nonzero elements in the factor *U*. Fill-in depends on the structure of the original matrix. In some problems, the fill-in is large enough, i.e. the upper triangle of the matrix *U* becomes dense. To maintain decomposition sparsity, *reordering* is used – the original matrix *A* is multiplied by a permutation matrix *P*, i.e. *PAPT*. Reordering changes a pattern of the original matrix using the symmetric permutations of rows and columns, but retains its sign-definiteness, thus allowing applying the Cholesky factorization to the new matrix. Solving of the system *Ax*=*b* with a sparse symmetric positive definite matrix is reduced to solving of the equivalent system (*PAPT*)*Px*=*Pb* to within a permutation of the vector *x.*

MKL PARDISO uses the Cholesky decomposition for solving SLAE. The solver performs the following sequence of operations:

1. Matrix reordering.
2. Decomposition of the reordered matrix. The symbolic and numerical phases are performed at this step. The first phase constructs a pattern of the matrix *U* and allocates memory necessary for storing this matrix; the second phase calculates the values of the nonzero elements.
3. Solving of two triangular systems (the backward phase of the method).

Note that the PARDISO developers support solving of SLAE with other types of matrices, basing on their decomposition. In particular, when solving a SLAE with a symmetric nonpositive definite matrix, a work scheme for the solver is the same, while the reordered matrix is decomposed into the form of , where is a block diagonal matrix and is an upper triangular matrix.

Along with using MKL PARDISO, the MKL LAPACK library can be applied for solving this problem. The functions of MKL LAPACK are focused on work with band matrices, i.e. they do not include searching for a permutation that minimizes fill-in of the factor. As a result, the band is filled and the matrix is not sparse anymore.

The experiments results show that for the problems of small size, the MKL LAPACK library demonstrates a greater performance, whereas for the problems of large size it is much more profitable to use MKL PARDISO. Also, according to the experiments results, there is no speedup when using the parallel algorithm with the number of threads more than 4. This is explained by the fact that the considered scheme for solving SLAE does not have large internal parallelism because of certain data dependencies in the factorization algorithm for the matrices of such type.

# recommendations for students

The numerical methods for partial differential equations are stated in [1], [2]. Using of these methods reduces solving of a differential equation to solving of a large sparse SLAE. How to work with sparse systems (algorithms, storage structures) is discussed in [3] in detail. The documentation for the Intel® Math Kernel Library used in the laboratory work is available on the Internet [4].

# References

1. David R. Kincaid and E. Ward Cheney. Numerical analysis : mathematics of scientific computing. Brooks/Cole Publishing Company, 1991.
2. Richard L. Burden, J. Douglas Faires. Numerical Analysis. Brooks Cole, 2000.
3. Sergio Pissanetzky. Sparse matrix technology. Academic Press, 1984.
4. Official Website Intel® MathKernelLibrary [http://software.intel.com/en-us/articles/intel-math-kernel-library-documentation/].

# exercises

1. Estimate the complexity of the Cholesky method for the case of five-diagonal matrix considered in the work.
2. Estimate the complexity of the phases of SLAE solving (reordering, symbolic and numerical factorization, etc.)
3. Compute analytically the fill-in of the factor for the heat conduction matrix without reordering and compare it with the fill-in value calculated by PARDISO when factoring the matrix with a direct permutation.
4. Implement the Gaussian method for solving SLAE with a five-diagonal matrix considered in the work (both sequential and parallel versions). Perform the scalability analysis for the application using the parallel implementation of the Gaussian method.

# test questions

1. What is the complexity of the Cholesky method?
   1. *n*3+O(*n*2)
   2. + 1/3*n*3+O(*n*2)
   3. 2/3*n*3+O(*n*2)
2. How many nonzero diagonals is there in the SLAE matrix appearing when solving numerically the Dirichlet problem for the Poisson equation in a two-dimensional region?
   1. +5
   2. 7
   3. 3
3. Specify the main purpose for reordering SLAE:
   1. Minimization of the number of performed operations
   2. Minimization of the solution error
   3. + Minimization of the fill-in of the factor
4. What phase of solving SLAE is the most time-consuming?
   1. The symbolic decomposition
   2. + The numerical decomposition
   3. The backward phase
5. What factorization is performed when solving SLAE with a symmetric nonpositive definite matrix by means of MKL PARDISO?
   1. +, where is a block diagonal matrix, is an upper triangular matrix.
   2. , where is a block matrix, is an upper triangular matrix.
   3. , where is a block diagonal matrix, is a lower triangular matrix.
6. What storage format id used in MKL PARDISO for storing sparse matrices?
   1. The coordinate format.
   2. + Compressed Row Storage format.
   3. Compressed Column Storage format.
7. Why the reordering phase is used in MKL PARDISO when applying the Cholesky factorization?
   1. In order to retain the original matrix pattern in the decomposition.
   2. In order to change the original matrix pattern.
   3. + In order to maintain decomposition sparsity.
8. When solving SLAE with the help of the Cholesky decomposition, three phases are performed in MKL PARDISO – reordering, factorization and solving of the systems with triangular matrices. What functions should be called in order to implement the specified sequence of actions?
   1. The functions PARDISO\_PERM, PARDISO\_FACT, PARDISO\_SUBS.
   2. + The function PARDISO with the different sets of parameters according to the corresponding phase.
   3. The functions dss\_reorder, dss\_factor, dss\_solve.
9. The developers of MKLPARDISO provide an additional way to call through the DirectSparseSolver (DSS) interface. What functions initializes the solver work?
   1. +dss\_create
   2. dss\_init
   3. dss\_initialize