

Application of the Parallel Dichotomy Algorithm for solving Toeplitz tridiagonal systems of linear equations with one right-hand side.

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Abstract

Based on a modification of the "Dichotomy Algorithm" (Terekhov, 2010), we propose a parallel procedure for solving tridiagonal systems of equations with Toeplitz matrices. Taking the structure of the Toeplitz matrices, we may substantially reduce the number of the "preliminary calculations" of the Dichotomy Algorithm, which makes it possible to effectively solve a series as well as a single system of equations. On the example of solving of elliptic equations by the Separation Variable Method, we show that the computation accuracy is comparable with the sequential version of the Thomas method, and the dependence of the speedup on the number of processors is almost linear. The proposed modification is aimed at parallel realization of a broad class of numerical methods including the inversion of Toeplitz and quasi-Toeplitz tridiagonal matrices.

Keywords: Parallel Dichotomy algorithm, Tridiagonal matrix algorithm (TDMA), Thomas algorithm, Poisson equation, Toeplitz matrixes, Fourier Method

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1. Introduction

The realization of many numerical algorithms, such as the Multigrid Line Relaxation [1–3], ADI and Separation Variable Method [2, 4–6], Cyclic Reduction Method [4, 5] for solving elliptic equations and also the problems of construction of splines [7, 8] etc. requires solving tridiagonal systems of equations with Toeplitz matrices [9, 10]

$$T = \begin{pmatrix} t_0 & t_1 & & & 0 \\ t_{-1} & t_0 & t_1 & & \\ & \ddots & \ddots & \ddots & \\ & & t_{-1} & t_0 & t_1 \\ 0 & & & t_{-1} & t_0 \end{pmatrix} \equiv \text{tridiag}\{\dots, t_{-1}, t_0, t_1, \dots\}. \quad (1)$$

Since, in solving modern problems of mathematical modeling, the size and the number of such problems can reach several tens of thousands, such computations must be performed on a supercomputer.

A lot of versions of parallel Thomas algorithms for general tridiagonal matrices [11–18], as well as for Toeplitz matrices [19–21], have been worked out as of today. Algorithms have been proposed that take into account the presence of diagonal dominance[22]. In [23], on the example of the realization of the ADI method, the approach was considered in which combination of computations and interprocessor exchanges

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makes it possible to increase the paralleling efficiency. In [24], a method called the Dichotomy Algorithm was proposed for solving a series of problems with a constant matrix and different right-hand sides

$$A\mathbf{X}_m = \mathbf{F}_m, \quad m = 1, \dots, M, \tag{2}$$

$$A = \text{tridiag}\{\dots, c_i, b_i, a_i, \dots\}, \quad i = 1, \dots, N, \quad c_1 = a_N = 0,$$

where M is the number of problems in the series. The advantage of the Dichotomy Algorithm consists in that it makes it possible to attain a thousandfold speedup for problem (2) not only in theory but also in practice. Aiming at a further development of this approach, we, based on a modification of the Dichotomy Algorithm, will propose a parallel algorithm for solving not only a series but a single system of linear algebraic equations (SLAE) with Toeplitz matrices.

A sufficient condition for the applicability of the Dichotomy Algorithm is the diagonal dominance of the matrix of the SLAE. As regards accuracy, the number of arithmetic operations, and the number of communication interactions, the Dichotomy Algorithm is almost equivalent to the Cyclic Reduction method [25, 26] However, for comparable data volumes, the real time of interprocessor interactions in the Dichotomy Algorithm is much smaller. This is explained by the fact that all interprocessor exchanges may be carried out via a sequence of calls to the collective operation "All-to-One-Reduce(+)" [27]. The account of such properties as the associativity and commutativity of the operation "+" taken over the distributed data makes it possible to reduce the time of communication interactions by optimizing them [28–32]. While the organization of exchanges via a multiple call to the nonblocking¹ function "All-to-One-Reduce(+)" makes it possible to reduce the time of synchronization of processor elements (PE). Indeed, if, in one group of processors², there exist two free PEs with prepared data then the execution of the collective operation "(+)" over this group of processors can start to even if the previous call on all processors is not finished. Thus, the structure of the Dichotomy Algorithm yields ample opportunities for the minimization of the data transfer time as well as the PE synchronization time. In the cyclic reduction method, the fixed order of elimination of the unknowns, on the one hand, restricts optimization of communication interactions, and on the other, requires synchronization of the computations on each reduction order.

The presence of a preliminary step with $O(N)$ arithmetic operations spent, where N is the dimension of the SLAE, does not make it possible to use the Dichotomy Algorithm effectively for solving one problem. However, for Toeplitz matrices, an economical preliminary procedure can be constructed with the number of the arithmetic operations of order $O(N/p + \log_2 p)$, where p where is the number of the processors. Thus, a modification of the preliminary step in the Dichotomy Algorithm enables us to effectively solve not only a series but a single SLAE with a Toeplitz matrix.

The structure of the article is as follows. In Section 2, we expose the Dichotomy Algorithm for the general case. In Section 3, we propose an economical preliminary procedure for the inversion of tridiagonal matrices in the Toeplitz class. We consider the problems of the stability of the dichotomy process and the accuracy of the so-obtained solution for systems with or without diagonal dominance. In Section 4, we give the results of numerical experiments. Section 5 is devoted to the summary of the work we have done.

2. The Dichotomy Algorithm

Before starting the exposition of the Dichotomy Algorithm, consider the question of mapping the data of the problem onto many processors.

2.1. Data decomposition

Let p be the number of the PEs. Partition the vector of the right-hand side and the solution vector \mathbf{F} and \mathbf{X} into subvectors $\mathbf{Q}_i, \mathbf{U}_i$ as follows:

¹This requirement is necessary for the realization of the Dichotomy Algorithm (see Subsection 2.5)

²A communicator in the terminology of the MPI.

$$\mathbf{F} = (\mathbf{Q}_1, \mathbf{Q}_2, \dots, \mathbf{Q}_p)^\top = (f_1, f_2, \dots, f_{size\{\mathbf{F}\}-1}, f_{size\{\mathbf{F}\}})^\top, \quad (3)$$

$$\mathbf{X} = (\mathbf{U}_1, \mathbf{U}_2, \dots, \mathbf{U}_p)^\top = (x_1, x_2, \dots, x_{size\{\mathbf{X}\}-1}, x_{size\{\mathbf{X}\}})^\top. \quad (4)$$

Denoting by $size\{\mathbf{V}\}$ the number of the components of a vector \mathbf{V} , require the fulfillment of the following conditions:

$$size\{\mathbf{Q}_i\} = size\{\mathbf{U}_i\} \geq 2, \quad i = 1, \dots, p,$$

$$\sum_{i=1}^p size\{\mathbf{Q}_i\} = \sum_{i=1}^p size\{\mathbf{U}_i\} = size\{\mathbf{X}\}.$$

Assume that the pair of subvectors $(\mathbf{Q}_i, \mathbf{U}_i)$ belongs to the PE with the number i and the row of the matrix A having number j belongs to the PE containing the pair of the elements (x_j, f_j) of (3),(4).

Introduce in addition the following notations:

- Denote the first and the last elements of a vector \mathbf{V} by $first\{\mathbf{V}\}$ and $last\{\mathbf{V}\}$.
- Denote by $\{A\}_l^t$ the matrix obtained from a matrix A by throwing off all rows and columns with the numbers less than l or greater than t .
- Denote by $\{\mathbf{V}\}_l^t$ the subvector obtained from a vector \mathbf{V} by throwing off the components with the numbers less than l or greater than t .
- Define \mathbf{e}_k as a coordinate vector in \mathfrak{R}^n .

2.2. The Dichotomy of a SLAE

The Dichotomy Algorithm is a representative of the class of algorithms known as "Divide & Conquer" [17, 33, 34]. On each dichotomy level, the tridiagonal system of equations obtained at the previous step is partitioned into three independent subsystems of lesser dimensions (Fig. 2) by computing the solutions in the $first\{\mathbf{U}_m\}$, $last\{\mathbf{U}_m\}$ components (Fig. 1).

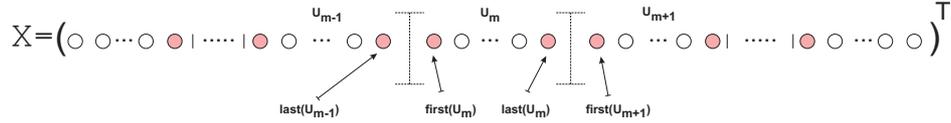


Figure 1: The first and last elements of the solution vector.

Thus, on the first dichotomy level, we construct two components of the solution vector

$$(\mathbf{X})_{m_L} \equiv first\{\mathbf{U}_m\}, \quad (\mathbf{X})_{m_R} \equiv last\{\mathbf{U}_m\}, \quad (5)$$

situated on the m th processor. The calculation of these components makes it possible to replace the initial system by three independent problems

$$\{\mathbf{A}\mathbf{X}\}_1^{m_L-1} = \{\mathbf{F}\}_1^{m_L-1} - a_{m_L-1} (\mathbf{X})_{m_L} \mathbf{e}^L, \quad (6)$$

$$\{\mathbf{A}\}_L^{m_R-1} \begin{pmatrix} x_{m_L+1} \\ x_{m_L+2} \\ \dots \\ x_{m_R-1} \end{pmatrix} = \begin{pmatrix} f_{m_L+1} - c_{m_L+1} (\mathbf{X})_{m_L} \\ f_{m_L+2} \\ \dots \\ f_{m_R-1} - a_{m_R-1} (\mathbf{X})_{m_R} \end{pmatrix}, \quad (7)$$

$$\{\mathbf{A}\mathbf{X}\}_{m_R+1}^n = \{\mathbf{F}\}_{m_R+1}^n - c_{m_R+1} (\mathbf{X})_{m_R} \mathbf{e}^R. \quad (8)$$

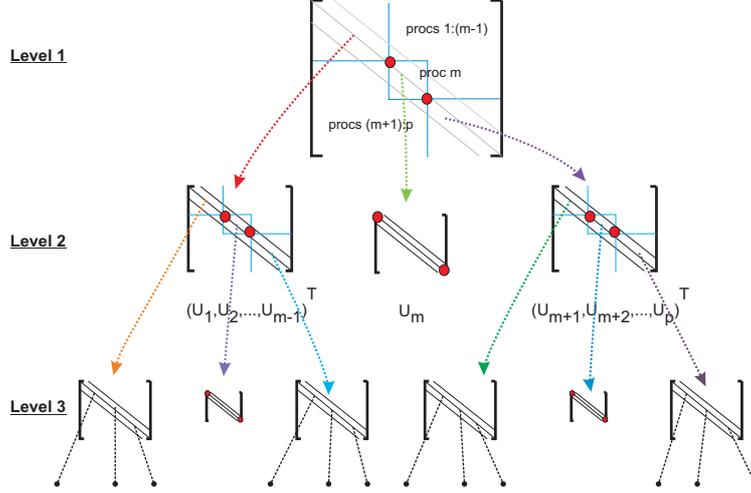


Figure 2: Partition of a tridiagonal SLAE into independent subsystems.

$$\mathbf{e}^R = (1, 0, 0, \dots, 0)^T, \quad \mathbf{e}^L = (0, \dots, 0, 0, 1)^T.$$

On the second dichotomy level, we similarly separate systems (6) and (8). As a result, in $\lceil \log_2 p \rceil$ steps, the initial system of equations (2) will split into p independent subsystems of the form (7). The solution to (7) on each processor may be found independently with the use of any sequential version of the Thomas algorithm [5, 35] for $O(\text{size}\{\mathbf{X}\}/p)$ arithmetic operations.

2.3. The Main Formulas

The process of the calculation of the *first* $\{\mathbf{U}_m\}$, *last* $\{\mathbf{U}_m\}$ components consists in two steps: a preliminary step carried out once for all right-hand sides of (2) and the dichotomy process at which the solution is computed for each right-hand side.

At the preliminary step, on the m th processor locally without communication interactions, we compute two rows of the matrix A^{-1}

$$A^T \mathbf{G}_m^L = \mathbf{e}_{m_L}, \quad A^T \mathbf{G}_m^R = \mathbf{e}_{m_R}, \quad (9)$$

where m_L, m_R are defined in (5) and \mathbf{e}_k is an ort.

The vectors $\mathbf{G}_m^{\mathbf{R},\mathbf{L}}$ have the sense of the difference Green's function [36] for the corresponding three-point boundary value problem.

Remark 1. In [24], the system of linear algebraic equation with symmetric and asymmetric tridiagonal matrices were separately considered (Lemma 1 and Section 3.6). However, with allowance for the property $(A^T)^{-1} = (A^{-1})^T$, the preliminary procedure can be essentially simplified reducing to the calculation of the vectors $\mathbf{G}^{\mathbf{R},\mathbf{L}}$ following (9). This makes possible, on the one hand, not to consider the case with an asymmetric matrix and, on the other hand, to exclude the situation like overflow, which may take place in explicit calculation of the inverse matrix entries.

In addition, at the preliminary step, we compute two vectors

$$\begin{aligned} \mathbf{Z}_m^L &= (z_1^L, z_2^L, \dots, z_{m_L-1}^L, 1)^T, \\ \mathbf{Z}_m^R &= (1, z_{m_R+1}^R, \dots, z_{N-1}^R, z_N^R)^T, \end{aligned} \quad (10)$$

where the components of the vectors are found as solutions to the systems

$$\{A\}_1^{m_L-1} \{\mathbf{Z}^L\}_1^{m_L-1} = -a_{m_L-1} \mathbf{e}^L, \quad (11)$$

$$\{A\}_{m_R+1}^N \{\mathbf{Z}^R\}_{m_R+1}^N = -c_{m_R+1} \mathbf{e}^R. \quad (12)$$

Thus, the costs of the preliminary computations for the Dichotomy Algorithm will constitute $size\{\mathbf{Z}_m^{R,L}\} = O(N)$. Therefore, it is appropriate to apply the Dichotomy Algorithm for solving several SLAE with constant matrix and different right-hand sides. In this case, the preliminary computations may be neglected.

Like in the Partition Algorithm [17, 33], the Dichotomy Algorithm is based on the superposition principle [37]. That is, the components of the solution vector are expressed via the sum of the general solution to the homogeneous equation and a partial solution to the nonhomogeneous equation. However, in the Dichotomy Algorithm, this principle is realized in a somewhat different manner.

Suppose that $\forall i \neq m, \|\mathbf{Q}_i\| = 0$. Then the components of (5) satisfy the identity [24]

$$(\mathbf{X})_{m_L} = \sum_{j=m_L}^{m_R} (\mathbf{F})_j (\mathbf{G}_m^L)_j, \quad (\mathbf{X})_{m_R} = \sum_{j=m_L}^{m_R} (\mathbf{F})_j (\mathbf{G}_m^R)_j. \quad (13)$$

The remaining components of the solution vector may be determined from the auxiliary vectors $\mathbf{Z}_m^{R,L}$ as follows:

$$(\mathbf{X})_i = \begin{cases} (\mathbf{Z}_m^L)_i (\mathbf{X})_{m_L}, & i \leq m_L \\ (\mathbf{Z}_m^R)_i (\mathbf{X})_{m_R}, & i \geq m_R. \end{cases} \quad (14)$$

If we consider all possible cases $m = 1, \dots, p$ when $\|\mathbf{Q}_m\| \neq 0$ while $\forall i \neq m \|\mathbf{Q}_i\| = 0$ and then sum up the so-obtained solutions (14), we come to the formula for computing the *first, last*-elements

$$(\mathbf{X})_k = \begin{cases} \sum_{j=1}^{m-1} \beta_j^R (\mathbf{Z}_j^R)_k + \sum_{j=m}^p \beta_j^L (\mathbf{Z}_j^L)_k, & (\mathbf{X})_k = first\{\mathbf{U}_m\}, \\ \sum_{j=1}^m \beta_j^R (\mathbf{Z}_j^R)_k + \sum_{j=m+1}^p \beta_j^L (\mathbf{Z}_j^L)_k, & (\mathbf{X})_k = last\{\mathbf{U}_m\}, \end{cases} \quad (15)$$

where

$$\beta_m^L = \sum_{j=m_L}^{m_R} (\mathbf{F})_j (\mathbf{G}_m^L)_j, \quad \beta_m^R = \sum_{j=m_L}^{m_R} (\mathbf{F})_j (\mathbf{G}_m^R)_j. \quad (16)$$

Here the indices m_R, m_L are found locally on each processor by (5).

The vectors u_m, v_m are the solution to the interior difference boundary value problem with respect to the subvector \mathbf{U}_m , whereas the vectors $\mathbf{Z}_m^{R,L}$ are the solution to the exterior boundary value problem. This difference is of principle. So, in the realization of the Dichotomy Algorithm, the computation of the *first, last*-components is reduced to the calculation of the sums (15), whereas, in the Partition Algorithm, it is necessary to solve a "reduced" [17, 33] SLAE of dimension $2p-2$ by means of some parallel variant of the Gauss Elimination Method. Since the computation of the sums on a multiprocessor computing system can be realized with a greater efficiency than the Gauss elimination method, the Dichotomy Algorithm makes it possible to reach a greater productivity for the problems of the form (2) than the Partition Algorithm.

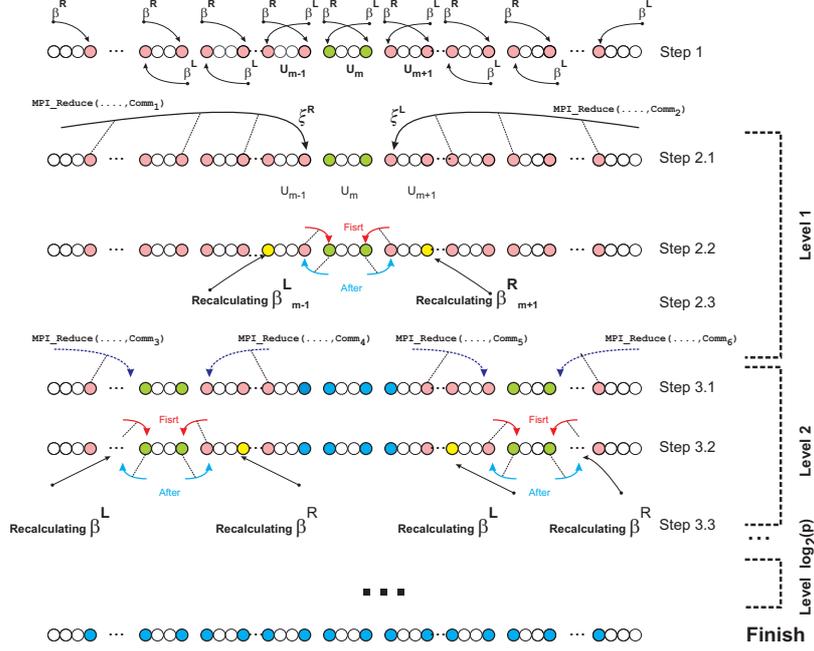


Figure 3: The MPI-realization of the Dichotomy Process.

2.4. MPI realization of the Dichotomy Algorithm

Fig. 3 contains the MPI-realization of (15) for partitioning the system $A\mathbf{X} = \mathbf{F}$, $size\{\mathbf{F}\} = N$.

Assume that the vectors $\mathbf{G}_m^{R,L}, \mathbf{Z}_m^{R,L}$ are already defined at the preliminary step. Then, at step 1 of the Dichotomy Process, by (16) each processor computes two local quantities $\beta_m^{R,L}$, where m is the processor number. The arithmetic costs at this step are $O(size\{\mathbf{U}_i\})$ for each PE. In the sequel, in the separation of the systems, the quantities $\beta_m^{R,L}$ will be recomputed for a number of operations of order $O(1)$.

At the first dichotomy level, consisting of steps 2.1–2.2–2.3, we compute two components of (5) with the use of (15) as follows.

At step 2.1, by calling the collective function *mpi_Reduce* over the communicators $Comm_1, Comm_2$, we compute the quantities

$$\xi^R = \sum_{j=1}^{m-1} \beta_j^R (\mathbf{Z}_j^R)_{m_L}, \quad \xi^L = \sum_{j=m+1}^p \beta_j^L (\mathbf{Z}_j^L)_{m_R}. \quad (17)$$

At step 2.2, processor $m-1$ sends³ to processor m the quantity ξ^R and processor $m+1$, the quantity ξ^L .

Now, the sought components situated on the m th processor may be computed as [24]

$$\begin{aligned} (\mathbf{X})_{m_L} &= first\{\mathbf{U}_m\} = \xi^R + \xi^L \frac{(\mathbf{G}_m^L)_{m_R}}{(\mathbf{G}_m^R)_{m_R}} + \beta_m^L, \\ (\mathbf{X})_{m_R} &= last\{\mathbf{U}_m\} = \xi^R \frac{(\mathbf{G}_m^R)_{m_L}}{(\mathbf{G}_m^L)_{m_L}} + \xi^L + \beta_m^R. \end{aligned} \quad (18)$$

³This exchange is designated as "First" in Fig. 2.

Remark 2. The quantities $(\mathbf{G}_m^R)_{m_L}/(\mathbf{G}_m^L)_{m_L}$ and $(\mathbf{G}_m^L)_{m_R}/(\mathbf{G}_m^R)_{m_R}$ make it possible to "transfer" the boundary condition from the component *first* to the component *last* and vice versa, i.e., inside the vector \mathbf{U}_m .

Furthermore, to exclude the thus-found components from the system of equations, processor m sends⁴ to processor $m - 1$ the quantity $\delta^L = \left(\xi^L \frac{(\mathbf{G}_m^L)_{m_R}}{(\mathbf{G}_m^R)_{m_R}} + \beta_m^L \right) (\mathbf{Z}_m^L)_{m_L-1}$ and to processor $m + 1$, the quantity

$$\delta^R = \left(\xi^R \frac{(\mathbf{G}_m^R)_{m_L}}{(\mathbf{G}_m^L)_{m_L}} + \beta_m^R \right) (\mathbf{Z}_m^R)_{m_R+1} \text{ respectively.}$$

At step 2.3, the vector of the right-hand side of SLAE (6),(7),(8) is modified, and the processors with numbers $m - 1, m + 1$ recompute the quantities

$$\begin{aligned} \hat{\beta}_{m-1}^R &= \beta_{m-1}^R + \delta^L, & \hat{\beta}_{m+1}^L &= \beta_{m+1}^L + \delta^R, \\ \hat{\beta}_{m-1}^L &= \beta_{m-1}^L + \delta^L \frac{(\mathbf{G}_{m-1}^L)_{t_R}}{(\mathbf{G}_{m-1}^R)_{t_R}}, & \hat{\beta}_{m+1}^R &= \beta_{m+1}^R + \delta^R \frac{(\mathbf{G}_{m+1}^R)_{q_L}}{(\mathbf{G}_{m+1}^L)_{q_L}}, \end{aligned} \quad (19)$$

where $(\mathbf{X})_{t_R} \equiv \text{last}\{\mathbf{U}_{m-1}\}$, $(\mathbf{X})_{q_L} \equiv \text{first}\{\mathbf{U}_{m+1}\}$,

On the next dichotomy level, an analogous separation process is applied to subsystems (6),(8), where the quantities (19) are used instead of $\beta_{m-1,m+1}^{R,L}$. Moreover, the steps having numbers $s.1, s.2, s.3$, (where $s = 1, 2, \dots, \lceil \log_2 p \rceil$) are equivalent to steps 2.1, 2.2, 2.3. However, on the s th level, 2^{s-1} already independent systems obtained at the previous step are separated independently.

2.5. Optimization of the Communication Costs

Since the number of arithmetic operations at the step of solving the "reduced" SLAE is relatively small, the communication cost of the algorithm of solving this subproblem defines the efficiency of the Partition Algorithm. The "reduced" system may be solved by the Cyclic Reduction Method [13, 38]. In [24] it was shown that the estimates of the computation time for the Dichotomy Algorithm and the Cyclic Reduction coincide in order if, first, the delay time α before the data transfer is insignificant and, second, not one but several series of problems are solved simultaneously

$$\begin{aligned} T_p^{Dichotomy} &= \alpha \lceil \log_2(p) \rceil \log_2(p) + l \left(\log_2(p) - \frac{p-1}{p} \right) (\gamma + 2\beta) \approx \\ &\approx 2 \log_2(p) (l\beta + l\gamma/2), \\ T_p^{Cyclic\ Reduction} &= 2 \log_2(p) (\alpha + l\beta + l\gamma) \approx 2 \log_2(p) (l\beta + l\gamma). \end{aligned}$$

Here β is the time of transfer of a real number from one PE to another, γ is the time spent on the operation of addition of two numbers, l is the number of the series of the simultaneously solved SLAEs.

In comparison with the Partition Algorithm + the Cyclic Reduction, the Dichotomy Algorithm gives a higher speedup coefficient due to lesser time costs for the synchronization of the computations as well as on the data exchange between the PEs.

The reduction of the communication time is possible due to the fact that the main communication operation ("+") of the Dichotomy Algorithm is associative. The architecture of modern supercomputers is such that the time of pairwise interactions may differ substantially for different processors [39–41]. The associativity of the computations makes it possible to define the order of the interactions of the PEs on the level of a communication library or a programming language so as to minimize the time of data exchanges by taking into account the architecture of the supercomputer.

⁴This exchange is designated as "After" in Fig. 2.

The reduction of the interprocessor exchange time is not a sufficient condition for the efficiency of the parallel algorithm since it is necessary to take into account the presence of synchronization of the computations. It often happens that most of the PEs expect the computation results from several PEs, which leads to the decrease of the total efficiency due to down-time periods of the computational resources. In the context of the Dichotomy Algorithm, the problem of minimization of the synchronization time is solved as follows. First, the number of groups of interacting processors increases with the number of the dichotomy level but the number of processes in each of them decreases; hence, so does the time of interprocessor exchanges. Second, the Dichotomy Algorithm almost does not require to synchronize the computations in passing from one dichotomy level to another (especially, on the first levels, where the number of communications is maximal). Thus, for beginning the process of partitioning the system of equations on dichotomy level $s + 1$, it is first necessary to modify the quantities (19) at step $s.3$. However, the processors that do not compute the $\hat{\beta}_m^{\text{R,L}}$ at step $s.3$ may start the summation of the series (17) at step $(s + 1).1$ without waiting for the result of the previous steps. Thus, on a majority of the processors, steps $s.2, s.3$, and $(s + 1).1$ may be carried out with a high degree of parallelism.

3. The Parallel Dichotomy Algorithm for Toeplitz Matrices

The realization of the Dichotomy Algorithm on a parallel computational system may be regarded as the solution of two separate subproblems:

1. Minimization of the number of arithmetic operations in the computation of the auxiliary vectors $\mathbf{Z}_m^{\text{R,L}}, \mathbf{G}_m^{\text{R,L}}$.
2. Minimization of the time of the communications and synchronization in the realization of (15).

Since, at the second step of the Dichotomy Algorithm, the form of the SLAE does not matter, we, in order to guarantee the possibility of solving not only a series but a single equation with matrix of the form (1), pose the problem of reducing the number of arithmetic operations at the preliminary step. Note that, in view of (15),(16) we do not need to determine all components of the auxiliary vectors but only those used. Thus, we need to find only $O(N/p)$ components of $\mathbf{G}_m^{\text{R,L}}$ and $\lceil \log_2 p \rceil$ components of $\mathbf{Z}_m^{\text{R,L}}$.

3.1. Optimization of the Preliminary Computations

For a general matrix (2), finding the necessary components $z_i^{\text{R,L}}, g_i^{\text{R,L}}$ from (9),(10) requires $O(N)$ arithmetic operations. For Toeplitz matrices, the components of the auxiliary vectors may be found in a lesser number of operations in accordance with the following theorem.

Theorem 1. [5, 10, 37] *Assume that we need to solve a SLAE*

$$T\mathbf{Y} = \mathbf{F}$$

with matrix (1) of order N . Then the n th component of the solution may be calculated as

$$y_n = \sum_{k=1}^{n-1} \frac{(q_1 q_2)^{n-k} (q_2^{N+1-n} - q_1^{N+1-n}) (q_2^k - q_1^k)}{(q_2 - q_1) (q_2^{N+1} - q_1^{N+1})} \cdot \frac{f_k}{t_1} + \sum_{k=n}^N \frac{(q_2^{N+1-k} - q_1^{N+1-k}) (q_2^n - q_1^n)}{(q_2 - q_1) (q_2^{N+1} - q_1^{N+1})} \cdot \frac{f_k}{t_1}, \quad (20)$$

$$q_1 = \frac{-t_0 + \sqrt{t_0^2 - 4t_{-1}t_1}}{2t_1}, \quad q_2 = \frac{-t_0 - \sqrt{t_0^2 - 4t_{-1}t_1}}{2t_1}.$$

Moreover, the solution does not exist if $q_1^{N+1} = q_2^{N+1}$ but $q_1 \neq q_2$.

Involving the fact that the right-hand sides in (9),(11),(12) may contain a unique nonzero component, it is easy to prove that, for computing one component of the vectors $\mathbf{Z}_m^{\text{R,L}}, \mathbf{G}_m^{\text{R,L}}$, by (20) we will need $O(1)$ arithmetic operations. Therefore, at the preliminary step as well as at the step of the partition of the SLAE,

it will be necessary to carry out $O(N/p + \log_2 p)$ arithmetic operations. Thus, the Dichotomy Algorithm for Toeplitz matrices may be applied not only to a series but to a single problem.

A similar economic preliminary procedure may be constructed for matrices of a somewhat more general kind than (1). For example, in [10, 42], explicit expressions are given for computing the elements of the inverse matrix to a matrix of the form

$$A = \begin{pmatrix} t_0 + \psi & t_1 & & & 0 \\ & t_{-1} & t_0 & t_1 & \\ & & \ddots & \ddots & \ddots \\ & & & t_{-1} & t_0 & t_1 \\ 0 & & & & t_{-1} & t_0 + \chi \end{pmatrix}. \quad (21)$$

Thus, if, for some tridiagonal matrix, it is possible to compute a separate component of the vectors $\mathbf{Z}_m^{\text{R,L}}, \mathbf{G}_m^{\text{R,L}}$ for $O(1)$ arithmetic operations then, in this case, it is possible to effectively solve a series as well as a single problem.

3.2. Inversion of the Operator ∇^2

In solving the first boundary value problem for the Poisson equation by such methods as the Multigrid Line Relaxation, the Variable-Separation Method etc., it is necessary to solve a series of equations of the form

$$\begin{cases} \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + \lambda_k y_i = -f_i, \quad \lambda_k \in R \quad 1 \leq i \leq N-1, \quad k = 1, \dots, M, \\ y_0 = \mu_1, \quad y_N = \mu_2. \end{cases} \quad (22)$$

Consider an economic algorithm for computing of the components of the vectors $\mathbf{Z}_m^{\text{R,L}}, \mathbf{G}_m^{\text{R,L}}$ for problems (22). It is known [5, 10, 43] that the solution to (22) is given by (20) and may be written down in the form

$$y_n = \frac{U_{N-n-1}(x)}{U_{N-1}(x)} \left[\mu_1 + \sum_{k=1}^{n-1} U_{k-1}(x) f(k) \right] + \frac{U_{n-1}(x)}{U_{N-1}(x)} \left[\mu_2 + \sum_{k=n}^{N-1} U_{N-k-1}(x) f(k) \right], \quad (23)$$

where $x = 1 - h^2 \lambda / 2 \neq \cos \frac{k\pi}{N}$, $k = 1, 2, \dots, N-1$ and $U_n(x)$ is the Chebyshev polynomial of the second kind of n degree [44, 45].

With (5) taken into account, the solution to (10) on the m th processor has the form

$$\begin{aligned} z_i^{\text{R}} &= \frac{U_{N-i-1}(x)}{U_{N-m_R-1}(x)}, \quad m_R \leq i \leq N, \\ z_i^{\text{L}} &= \frac{U_{i-1}(x)}{U_{m_L-1}(x)}, \quad 1 \leq i \leq m_L. \end{aligned} \quad (24)$$

The solution to (9) has the form

$$\begin{aligned} g_i^{\text{L}} &= \frac{U_{N-i-1}(x)}{U_{N-1}(x)} U_{m_L-1}(x), \quad m_L \leq i \leq m_R, \\ g_i^{\text{R}} &= \frac{U_{i-1}(x)}{U_{N-1}(x)} U_{N-m_R-1}(x), \quad m_L \leq i \leq m_R. \end{aligned} \quad (25)$$

Since the necessary components of $\mathbf{G}_m^{\text{R,L}}$ are situated successively (16), having computed $g_{m_R, m_L}^{\text{R,L}}$ by (25), it is more economic to compute the remaining components by solving the systems

$$\{\mathbf{A}\mathbf{G}^{\text{R}}\}_{m_L+1}^{m_R-1} = -t_{-1} g_{m_L}^{\text{R}} \mathbf{e}^{\text{R}} - t_1 g_{m_R}^{\text{R}} \mathbf{e}^{\text{L}}, \quad (26)$$

$$\{\mathbf{A}\mathbf{G}^{\text{L}}\}_{m_L+1}^{m_R-1} = -t_{-1} g_{m_L}^{\text{L}} \mathbf{e}^{\text{R}} - t_1 g_{m_R}^{\text{L}} \mathbf{e}^{\text{L}}. \quad (27)$$

3.3. Accuracy analysis

Since the values of $U_k(x)$ outside the interval $[-1, 1]$ begin to increase rapidly with k , we cannot exclude an overflow-type situation in a program realization of (24),(25) for $|x| > 1$ [46, 47]. To overcome this difficulty, we do the following. Let N_0 be the degree of the polynomial greater than which the quantity $U_k(x)$, $k > N_0$, $|x| > 1$ cannot be computed because the result exceeds the boundary of the admissible values of the real variable. A Chebyshev polynomial of the second kind admits the representation [44]

$$U_n(x) = \frac{1}{2\sqrt{x^2-1}} \left[\left(x + \sqrt{x^2-1}\right)^{n+1} - \left(x + \sqrt{x^2-1}\right)^{-(n+1)} \right], \quad |x| \geq 1. \quad (28)$$

Then the relation

$$\left(x + \sqrt{x^2-1}\right)^{-(n+1)} \ll \left(x + \sqrt{x^2-1}\right)^{(n+1)}, \quad (29)$$

holds $\forall n > N_0$, from which $\forall n > N_0$ we may assume with a good accuracy that

$$U_n(x) \simeq \frac{1}{2\sqrt{x^2-1}} \left(x + \sqrt{x^2-1}\right)^{n+1}. \quad (30)$$

Now, substituting (30) into (25) and collecting similar summands, we infer

$$\begin{aligned} g_i^L &\simeq \frac{1}{2\sqrt{x^2-1}} \left[\eta^{(m_L-i)} + \eta^{(-2N-i+m_L)} - \eta^{(-2N+m_L+i)} - \eta^{(-m_L-i)} \right], \quad m_L \leq i, \\ g_i^R &\simeq \frac{1}{2\sqrt{x^2-1}} \left[\eta^{(i-m_R)} + \eta^{(-2N+i-m_R)} - \eta^{(-2N+m_R+i)} - \eta^{(-i-m_R)} \right], \quad m_R \geq i, \end{aligned} \quad (31)$$

where $\eta = x + \sqrt{x^2-1}$.

Since the exponents in (31) are at most zero and $|x| > 1$, the situation of an overflow of variables is excluded.

Remark 3. In solving tridiagonal systems of dimension less than N_0 , the computations of the components of the auxiliary vectors should be performed by (24),(25), (28) so as to avoid loss of accuracy because of a possible violation of (29).

Remark 4. If $|x| < 1$ then $U_k(x) \leq k + 1$. Hence no overflow of variables arises for $x \neq \cos \frac{k\pi}{N}$, $k = 1, 2, \dots, N-1$ and reasonable N .

3.4. Stability analysis

It is proved in [24] that a sufficient condition of stability for the Dichotomy Algorithm is given by the diagonal dominance of the matrix of the SLAE

$$|b_i| \geq |a_i| + |c_i|, \quad i = 2, \dots, N-1, \quad (32)$$

$$|b_1| \geq |a_1|, \quad |b_N| \geq |c_N|, \quad (33)$$

and at least one of the inequalities is strict.

For problem (22) in the case of $\lambda \leq 0$, the matrix of the SLAE has diagonal dominance, which guarantees the stability of the Dichotomy Algorithm. However, for $\lambda > 0$, there is no diagonal dominance and accumulation of roundoff error can happen. This follows from the fact that, by the failure of the maximum principle [36, 48], the components of the vectors $\mathbf{Z}_m^{\text{R,L}}$ may have their modulus greater than one (Fig. 4). In this case, the error of the computation of the *first*, *last*-components committed on the s th dichotomy level passes to $s+1$ level by means of (19) and is then "strengthened" by multiplying by $|\mathbf{Z}_m^{\text{R,L}}| \leq \gamma$ in (15). Thus, if the number of the dichotomy levels is great and γ is much greater than 1 then an accuracy loss is possible.

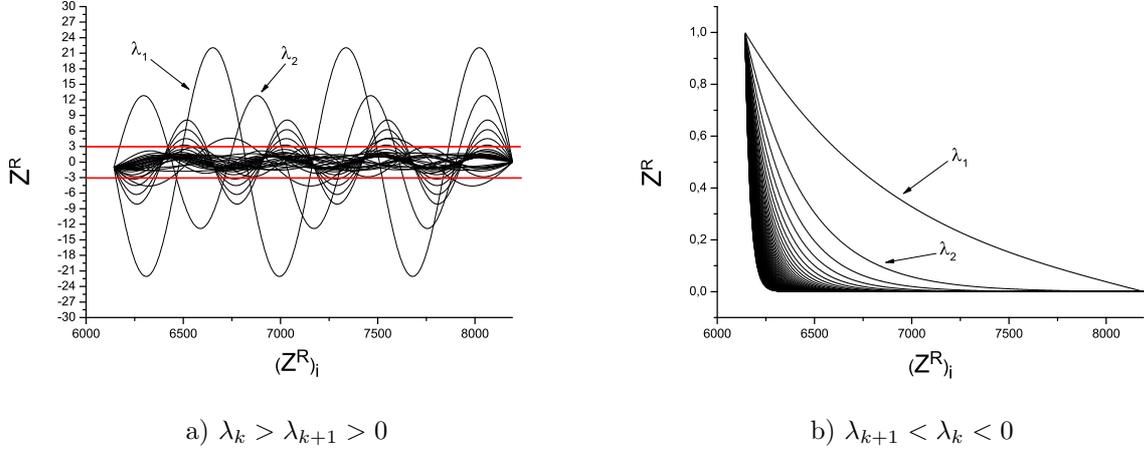


Figure 4: The values of the components of \mathbf{Z}_2^R for the case $N = 8192$, $p = 4$ in solving (22) for different values λ .

If we take the estimate

$$\varepsilon_i = \prod_{j=1}^l \left| \left(\mathbf{z}_{n_j}^{\text{R,L}} \right)_i \right| \varepsilon \leq \gamma^l \varepsilon, \quad (34)$$

as the maximal error of the computation of the component $(\mathbf{X})_i$, where l is the number of the dichotomy step at which the sought component will be computed, ε is the initial error. Then, for example, for $p = 4096$, $l = 12$ and $\gamma < 3$, the computation error at worst goes six digits to the right, which is acceptable for many problems. Thus, for $\gamma > 1$, we need to perform an a priori (34) as well as an a posteriori check of the accuracy of the so-obtained solution.

3.5. Inversion of the Operator ∇^2 for 3D Case.

For solving the 3D problems, it is necessary to provide the possibility of using a large number of processors for algorithms efficient with respect to the number of arithmetic actions. From the viewpoint of data decomposition between the processors, the best choice is the variable directions method (ADI) [5], where at each step of the iteration process the tridiagonal SLAEs should be solved for all the three directions, which allows one to use a large number of processors within the limits of one calculation. Unfortunately, compared to the 2D case, the 3D-ADI algorithm is not efficient because of its low convergence rate [36]. Thus, via the Fourier transform it is reasonable to solve not a 3D problem but a series of independent 2D problems:

$$\frac{y(l)_{i+1,j} - 2y(l)_{i,j} + y(l)_{i-1,j}}{h_1^2} + \frac{y(l)_{i,j+1} - 2y(l)_{i,j} + y(l)_{i,j-1}}{h_2^2} - \frac{4}{h_3^2} \sin^2 \left(\frac{\pi(l-1)}{2(N_3-1)} \right) y(l)_{i,j} = -f(l)_{i,j},$$

$$i = 2, \dots, N_1 - 1, \quad j = 2, \dots, N_2 - 1, \quad l = 2, \dots, N_3 - 1. \quad (35)$$

For solving the problem (35), we can use the parallel version of the variable separation method [24]. However, this algorithm drastically limits the number of used processors because the tridiagonal SLAEs are solved only in one direction and, consequently, only the one-dimensional data decomposition will be efficient because for other directions it is necessary to use the fast Fourier transform algorithm. In order to overcome the problems of data decomposition and ensure efficiency of the method in terms of the number of operations, for solving the problems (35), one should use the 2D-ADI method [24]. The calculation efficiency is achieved due to the fact that as the value of l increases from 2 to $N_3 - 1$ the condition number for an equation of the form (35) decreases as well as the necessary number of iterations of the ADI algorithm, Fig. 6.a. Thus, the hybrid parallel algorithm under consideration is comparable in efficiency with the variable separation method, however, contrary to the latter, it allows 2D efficient data decomposition between the processors.

4. Numerical Experiments

For estimating the efficiency of the above-proposed modification of the dichotomy algorithm for Toeplitz matrices, consider the following boundary value problem

$$\Delta u = f(x), \quad x \in G \subset \mathfrak{R}^\alpha, \quad \alpha = 2, 3, \quad u|_\Gamma = 0. \quad (36)$$

For solving the difference problem in *Fortran* – 90 with the use of the communication MPI–library, we have realized the variable separation method following the scheme of [24]. For the 2D problem the approximation of (36) was carried out with the second order of accuracy on a uniform mesh with the number of the points $N_1 = N_2 = 2^k$, $k = 13..16$ and with the number of the points $N_1 = N_2 = N_3 = 2^k$, $k = 9..13$ for the 3D problem. For estimating the cost of the preliminary computations, the calculation of the vectors $\mathbf{G}_m^{\text{R,L}}$, $\mathbf{Z}_m^{\text{R,L}}$ for problem (36) was realized in two variants: by (9),(10) for an arbitrary symmetric matrix and by (31),(10) for Toeplitz matrices. Since the matrix of the SLAE is not used at the second stage of the dichotomy algorithm, one MPI-realization of (15),(16) is enough for these cases. The calculation was performed on the "Lomonosov" supercomputer of Moscow State University. The supercomputer comprises Intel Xeon X5570 four-core processors operating at 2.93 GHz in the Infiniband QDR communication environment. Each computational node contains two processors and 12 GB of RAM.

For the 2d problem the dependencies of the time of the preliminary computations, the time of the dichotomy process ($\mathbf{T}_{\text{Stage}_1}^{\text{General}}$, $\mathbf{T}_{\text{Stage}_1}^{\text{Toeplitz}}$, $\mathbf{T}_{\text{Stage}_2}$), and the speedup on the number of the processors are given in Tables 1 and in Fig. 5. We can see from Tables 1 that the time ($\mathbf{T}_{\text{Stage}_1}^{\text{General}}$) necessary for the computation of the vectors $\mathbf{G}_m^{\text{R,L}}$, $\mathbf{Z}_m^{\text{R,L}}$ for general matrices is independent of the number of processors and is proportional to the number of unknowns. This is due to the fact that the total dimension of the auxiliary vectors has order $O(N)$. Thus, if we neglect the fact that the matrices are Toeplitz for (36) then the time costs for the preliminary computations will be $O(N_1 N_2)$. For Toeplitz matrices, the use of (24),(31), in comparison with the general case (9),(10) makes possible to decrease the computation time of the auxiliary vectors ($\mathbf{T}_{\text{Stage}_1}^{\text{General}}$ vs. $\mathbf{T}_{\text{Stage}_1}^{\text{Toeplitz}}$) by several orders. As a result, it becomes possible to efficiently solve SLAEs with both one and several right-hand sides because the time needed for the preliminary stage of the dichotomy algorithm for the Toeplitz matrices becomes comparable to that needed for carrying out the dichotomy process (Fig. ??) for one right-hand side. For solving a SLAE with one right-hand side, we should take into account the preliminary dichotomy algorithm costs. In this case, the speedup value will be 1.5 – 2.5 times less than that in solving a SLAE for several right-hand sides, i.e. when the preliminary computations independent of the number of the right-hand-sides can be neglected.

$N_1 \times N_2$	8192x8192		16384x16384		32768x32768		65536x65536	
$\mathbf{T}_{\text{Stage}_1}^{\text{General}}$	$\approx 3.3\text{sec.}$		$\approx 13 \text{ sec.}$		$\approx 53 \text{ sec.}$		$\approx 246 \text{ sec.}$	
num. proc.	$\mathbf{T}_{\text{Stage}_1}^{\text{Toeplitz}}$	$\mathbf{T}_{\text{Stage}_2}$	$\mathbf{T}_{\text{Stage}_1}^{\text{Toeplitz}}$	$\mathbf{T}_{\text{Stage}_2}$	$\mathbf{T}_{\text{Stage}_1}^{\text{Toeplitz}}$	$\mathbf{T}_{\text{Stage}_2}$	$\mathbf{T}_{\text{Stage}_1}^{\text{Toeplitz}}$	$\mathbf{T}_{\text{Stage}_2}$
32	0.2	3.9e-01	0.75	1.6	-	-	-	-
64	0.1	1.9e-01	0.33	0.84	-	-	-	-
128	5.6e-02	1.0e-01	0.17	0.4	0.81	1.77	-	-
256	3.7e-02	4.9e-02	0.12	0.2	0.41	0.89	1.62	3.83
512	3.0e-02	2.6e-02	8.0e-02	0.12	0.24	0.58	0.84	1.92
1024	2.6e-02	1.6e-02	6.5e-02	6.5e-02	0.17	0.28	0.51	1.0
2048	2.6e-02	1.4e-02	5.8e-02	4.2e-02	0.13	0.15	0.36	0.59
4096	2.5e-02	1.6e-02	5.5e-02	6.0e-02	0.12	0.10	0.30	0.35

Table 1: The dependence of the computation time \mathbf{T} on the number of processors for the 2D Poisson equation. Here $\mathbf{T}_{\text{Stage}_1}^{\text{Toeplitz}}$, $\mathbf{T}_{\text{Stage}_1}^{\text{General}}$ are the times of the preliminary stage of the dichotomy algorithm for the Toeplitz matrices and general matrices respectively; $\mathbf{T}_{\text{Stage}_2}$ is the time of the implementation of the dichotomy process for any tridiagonal matrix.

We see that the dichotomy algorithm ensures a speedup close to that linear. For a large number of processors, no substantial decrease of efficiency occurs because of the predominance of inter-processor exchanges. This is ensured by dynamic optimization of the communication interactions. Indeed, calling the

function `MPI_Reduce` for the first time, we can collect information about the time of the interaction between the processors, the volume of the data transferred etc. for each communicator. This will make possible to optimize the processes of data exchange for subsequent calls of `MPI_Reduce` [28? –31]. The dependence of the computation time on the number of processors in the case of the use of dynamic optimization and without it is given in Fig. 5.b. For a small number of processors $p < 512$, dynamic optimization does not influence the computation time much since, in this case, the computational costs exceed those communicational. However, as the number of the processors increases, the effect caused by optimization becomes more than substantial. Thus, the high efficiency of the dichotomy algorithm is provided, on the one hand, by the low costs of the synchronization of the computations, and on the other, by the possibility of reduction for the data transfer time by static and dynamic optimization of the communication interactions.

For the case of solving the 3D Poisson equation, the dependence of the calculating time and the speedup on the number of processors is given in Table 2 and in Fig. 6.b. As for the 2D problem, the speedup nearly linearly depends on the number of processors. Owing to the high scalability of the dichotomy algorithm, the calculation time, with increasing number of processors, reaches a stationary value and then does not grow. The use of the efficient modification of the preliminary procedure of the dichotomy algorithm for the Toeplitz tridiagonal matrices has made it possible to reduce the time of preliminary calculations from several hours to several fractions of second.

$N_1 \times N_2 \times N_3$	512 ³		1024 ³		2048 ³		4096 ³		8192 ³	
num. proc.	$\mathbf{T}_{\text{Stage}_1}^{\text{Toeplitz}}$	$\mathbf{T}_{\text{Stage}_2}$								
64	2.1e-2	0.76	6.5e-2	4.8	-	-	-	-	-	-
128	1.9e-2	0.42	5.5e-2	2.5	1.6e-1	31.1	-	-	-	-
256	1.8e-2	0.23	4.6e-2	1.3	1.3e-1	7.7	-	-	-	-
512	1.7e-2	0.14	4.2e-2	0.75	1.1e-1	16.6	-	-	-	-
1024	1.5e-2	0.08	3.8e-2	0.44	9.5e-2	3.8	2.3e-1	24	-	-
2048	1.5e-2	0.06	3.7e-2	0.28	8.7e-2	2.0	2.2e-1	13.3	-	-
4096	1.6e-2	4.6e-2	4.1e-2	0.17	8.6e-2	1.1	2.1e-1	7.1	-	-
8192	1.6e-2	3.9e-2	3.3e-2	0.12	8.5e-2	0.72	2.1e-1	3.71	-	-
16384	1.6e-2	3.3e-2	3.7e-2	9.8e-2	8.3e-2	0.46	1.8e-1	1.76	0.37	23.9

Table 2: The dependence of the computation time \mathbf{T} on the number of processors for solving of the 3D Poisson equation. Here $\mathbf{T}_{\text{Stage}_1}^{\text{Toeplitz}}$ is the time of the preliminary stage of the dichotomy for the Toeplitz matrices; $\mathbf{T}_{\text{Stage}_2}$ is the time of the implementation of the dichotomy process for any tridiagonal matrix.

5. Conclusions

In this article, we have proposed a parallel algorithm for solving tridiagonal systems of equations with Toeplitz matrices demonstrating high efficiency including for thousands of processors. The method is based on the Dichotomy Algorithm devised for solving a series of tridiagonal systems of linear equations with constant matrix and different right-hand sides. The fact that, for Toeplitz matrices, each component of the solution vector may be calculated without solving the SLAE makes it possible to substantially reduce the computation time at the preliminary step of the Dichotomy Algorithm. As a result, it became possible to effectively solve not only a series but a single system of equations. The reduction of the time for the preliminary computations is also very important in solving a series of problems with a large number of unknowns, since, if we disregard the special structure of the matrix, the delay before the direct start of solving the equation may be substantial.

In some algorithms considered above, the presence of diagonal dominance for the matrix of the SLAE is taken into account, which enables us to reduce the number of interprocessor exchanges. Sometimes this imposes the constraint that the size of systems of the form of (7) must be at least some threshold value; otherwise, we have an accuracy loss [22]. Thus, the maximal number of the processors that may be used for solving the problem depends on the presence of diagonal dominance. If we use the Dichotomy Algorithm, such dependencies do not arise, and the solution satisfies (with the computer accuracy in mind)

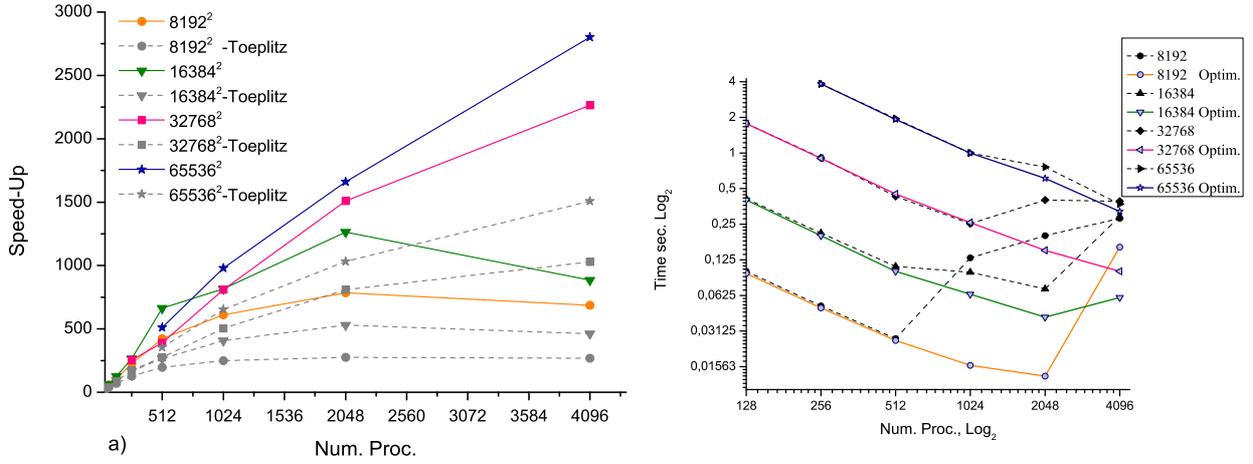


Figure 5: a) Dependence of the speedup on the number of the processors for the 2D Variable-Separation Method for general (without the preliminary stage time) and Toeplitz (including the preliminary stage time) matrices. b) The influence of the dynamic optimization of inter-processor interactions on the computation time.

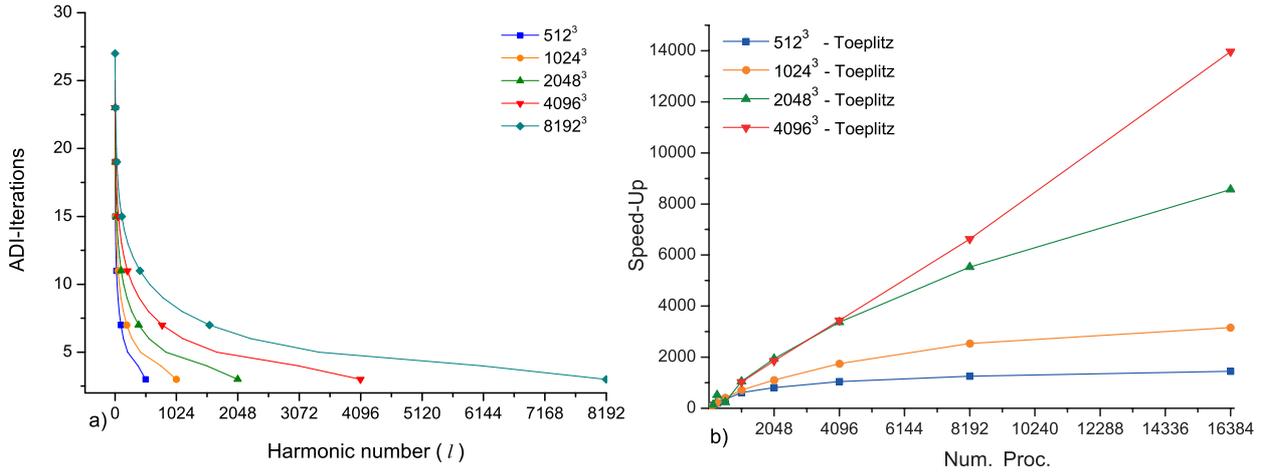


Figure 6: a) The number of ADI method iterations versus the harmonic number in solving problems of the form (35). b) Speedup versus the number of processors in solving the 3D Poisson equation.

the initial system of equations for any number of the processors. As a result, the process of paralleling of the already existing numerical methods including the inversion procedure of a tridiagonal SLAE is substantially simplified.

Computational experiments confirm that dynamic optimization on the level of the MPI-library makes it possible to substantially reduce the time of interprocessor exchanges. The effect caused by optimization is especially noticeable in computations with the use of a large number of processors. Thus, the above-proposed algorithm for solving tridiagonal systems of equations with Toeplitz matrices makes it possible to attain a high computation speed in a wide range of processors and guarantee high transferability of the software.

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