

High-performance modeling acoustic and elastic waves using the Parallel Dichotomy Algorithm.

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Abstract

A high-performance parallel algorithm is proposed for modeling the propagation of acoustic and elastic waves in inhomogeneous media. An initial boundary-value problem is replaced by a series of boundary-value problems for a constant elliptic operator and different right-hand sides via the integral Laguerre transform. It is proposed to solve difference equations by the conjugate gradient method for acoustic equations and by the GMRES(k) method for modeling elastic waves. A preconditioning operator was the Laplace operator that is inverted using the variable separation method. The novelty of the proposed algorithm is using the Dichotomy Algorithm (Terekhov, 2010), which was designed for solving a series of tridiagonal systems of linear equations, in the context of the preconditioning operator inversion. Via considering analytical solutions, it is shown that modeling wave processes for long instants of time requires high-resolution meshes. The proposed parallel fine-mesh algorithm enabled to solve real application seismic problems in acceptable time and with high accuracy. By solving model problems, it is demonstrated that the considered parallel algorithm possesses high performance and efficiency over a wide range of the number of processors (from 2 to 8192).

Keywords: Acoustic waves, Elastic waves, Tridiagonal matrix algorithm (TDMA), Parallel Thomas Algorithm, Parallel Dichotomy Algorithm, Laguerre transform

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1. Introduction

Steadily growing number of processors opens up new opportunities for solving complex applied problems, for example, elastodynamic problems [1, 2, 3]. In this case, quite efficient algorithms are numerical-analytical algorithms [4, 5], where the solution is represented, via the integral time transformation, as the Fourier series in terms of some orthonormal system of functions. The expansion coefficients are determined numerically as a solution of boundary-value problems for the elliptic type of equation [6, 7, 8].

Many publications [9, 10, 11, 12, 13, 14], are concerned with development and investigation of parallel numerical elliptic differential operator inversion algorithms. Nevertheless, this problem remains quite urgent. The explanation is that the steady growth of the number of processors integrated within one computer system imposes new demands to scalability of parallel algorithms. For instance, methods effective for a small number of processors ($p < 32$), e.g., the cyclic reduction algorithm [15, 16], become ineffective because the communication costs prevail over the computational ones. This necessitates further development of parallel numerical algorithms that allow using modern computational resources with the greatest efficient factor.

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Publications [17, 18, 19, 20, 21, 22] propose different approaches to solving elliptic equations of second order with inseparable variables, where the iterative process is reduced to multiple Laplacian inversion. However, realization of efficient procedure [17, 23, 24, 25] for the Laplacian inversion requires solving tridiagonal systems of linear equations, which, on a multiprocessor system, is a nontrivial problem. This difficulty can be overcome by using the Dichotomy Algorithm [26], which was developed for inversion of one and the same tridiagonal matrix for many right-hand sides. The Dichotomy Algorithm was chosen because for this class of problems it ensures almost linear dependence of the speedup coefficient in a wide range of the number of processors. In terms of accuracy, the number of arithmetic operations, and the number of communications, the Dichotomy Algorithm is practically equivalent to the cyclic reduction method [15, 27]. However, with comparable levels of transferred data, the real time of interprocessor communications for the Dichotomy Algorithms is much less. The explanation is that the main communication operation of the Dichotomy Algorithm, that is, all-reduce-to-one(+), possesses the associative property, which allows reducing the time of interprocessor communications due to their optimization [28, 29]. In the present paper, taking into account the high efficiency of the Dichotomy Algorithm, we will consider the possibility of using it within the scope of numerical-analytical approach for modeling the propagation of acoustic and elastic waves.

The peculiarity of the Dichotomy Algorithm is that it was designed for solving problems with the same tridiagonal matrix and different right-hand sides. Choosing the integral transformation, we considered the fact that prior to solving tridiagonal systems, it is necessary to perform preparatory calculations with a volume $O(N)$, where N is the dimension of the system of equations. Really, after applying the time Fourier transform to the acoustic equation we obtain the boundary-value problem for the Helmholtz equation

$$\Delta u_n + k_n^2 u_n = f_n, \quad n = 1, 2, \dots \quad (1)$$

In this case, the dependence of the differential operator on the number of calculated harmonic prevents effective usage of the Dichotomy Algorithm because only one right-hand side will correspond to the same matrix. The exception is the case of Toeplitz tridiagonal matrices [30] for which the volume of preparatory computations is $O(N/p + \log_2 p)$ rather than $O(N)$, where p is the number of processors. Thus, for solution of problem (1) in the Cartesian coordinate system, the Dichotomy Algorithm can be applied, e.g., in the context of the variable separation method that requires inversion of Toeplitz (quasi-Toeplitz) matrices.

In the present work, we consider media of 2.5D geometry. In this case, in the cylindrical coordinate system, for the Laplace operator inversion, it is necessary to solve tridiagonal SLAEs of the general form. For this case, we considered the Laguerre transform [4], after applying it to the acoustic equation, it is required to invert one and the same differential operator for all right-hand sides

$$\Delta u_n - \lambda^2 u_n = f_n + \sum_{i=1}^{n-1} \alpha_{n,i} u_i, \quad n = 1, 2, \dots \quad \alpha_{n,i}, \lambda \in R. \quad (2)$$

The fact that the preparatory computations in the context of the Dichotomy Algorithm are performed once for all right-hand sides allows one to neglect preparatory expenses. Thus, it becomes possible to use the Dichotomy Algorithm for solving problem (2) by methods demanding inversion of general tridiagonal matrices.

In the present paper, using the Laguerre transform and the Dichotomy Algorithm we considered the high-performance parallel algorithm for modeling acoustic and elastic waves in 2.5D media. At present, applied geophysics problems have to be solved for steadily increasing times and recording systems. On the other hand, improvement of practical observing systems necessitates increasing the calculation accuracy. In the paper, by considering analytical solutions we have shown that modeling wave processes for longer instants of time requires higher resolution meshes. We illustrated the possibility of effectively using thousands of processors within one calculation. This enabled practical real-time and high-accuracy computing on current computers.

2. Problem Statement and Solution Algorithm

2.1. Acoustic Equation

In the cylindrical coordinate system (r, z) , in the half-space $z \geq 0$ we will consider the problem of modeling the propagation of acoustic waves from a point source

$$\rho(\mathbf{x}) \frac{\partial^2 u}{\partial t^2}(\mathbf{x}, t) = \nabla [\kappa(\mathbf{x}) \nabla u(\mathbf{x}, t)] + \frac{1}{2\pi} \frac{\delta(\mathbf{x} - \mathbf{x}_0)}{r} f(t), \quad t > 0, \quad \mathbf{x} = (r, z). \quad (3)$$

Suppose that problem (3) is solved with homogeneous initial conditions

$$u|_{t=0} = \frac{\partial u}{\partial t} \Big|_{t=0} = 0. \quad (4)$$

Assume that at $z = 0$ the surface is free, and the auxiliary boundaries are entered along the coordinates r and z

$$\frac{\partial u}{\partial z} \Big|_{z=0, l_2} = u|_{r=l_1} = 0. \quad (5)$$

The boundaries $r = l_1$ and $z = l_2$ are chosen such that waves reflected from them do not arise for the calculated instant of time. In addition we demand that

$$\frac{\partial u}{\partial r} \Big|_{r=0} = 0. \quad (6)$$

Let us represent for the solution of problem (3)-(6) as the Fourier-Laguerre series[4]

$$R_m(\mathbf{x}) = \int_0^\infty u(\mathbf{x}, t) (ht)^{-\frac{\alpha}{2}} l_m^\alpha(ht) dt \quad (7)$$

with the inversion formulas

$$u(\mathbf{x}, t) = (ht)^{\frac{\alpha}{2}} \sum_{m=0}^\infty R_m(\mathbf{x}) l_m^\alpha(ht), \quad (8)$$

where $l_m^\alpha(ht)$ are the orthonormal Laguerre functions [31], which are represented via classical Laguerre polynomials as follows

$$l_m^\alpha(ht) = \sqrt{\frac{hm!}{(m+\alpha)!}} (ht)^{\frac{\alpha}{2}} e^{-\frac{ht}{2}} L_m^\alpha(ht).$$

Here, m is Laguerre polynomial degree and h is the transformation parameter. The necessary and sufficient parameter for satisfying the initial data is $\alpha \geq 2$ (α is the order of Laguerre functions).

As a result, the initial boundary-value problem (3)-(6) is reduced to the boundary-value problems in the spectral domain

$$\left\{ \begin{array}{l} \nabla [\kappa(\mathbf{x}) \nabla R_m(\mathbf{x})] - \rho(\mathbf{x}) \frac{h^2}{4} R_m(\mathbf{x}) = -\frac{1}{2\pi} \frac{\delta(\mathbf{x} - \mathbf{x}_0)}{r} f_m + \rho(\mathbf{x}) h^2 \sqrt{\frac{m!}{(m+\alpha)!}} \sum_{k=0}^{m-1} (m-k) \sqrt{\frac{(k+\alpha)!}{k!}} R_k(\mathbf{x}), \\ \frac{\partial R_m}{\partial r} \Big|_{r=0} = \frac{\partial R_m}{\partial z} \Big|_{z=0, l_2} = R_m|_{r=l_1} = 0, \end{array} \right. \quad (9)$$

where $f_m = \int_0^\infty f(t) (ht)^{-\frac{\alpha}{2}} l_m^\alpha(ht) dt$.

This method can be considered as an analog of the spectral-difference method, based on the Fourier transform [8], but in this case, but the role of "frequency" belongs to the parameter m that determines the degree of the polynomials. Contrary to the Fourier method, the harmonic separation parameter is present only in the right-hand side.

2.2. Elastic Medium

To describe the propagation of elastic waves in a inhomogeneous half-space, we will consider the equations of motion in the cylindrical coordinate system [3]

$$\rho \frac{\partial \mathbf{W}^2}{\partial t^2} = (\lambda + \mu) \nabla (\nabla \cdot \mathbf{W}) + \mu \nabla^2 \mathbf{W} + \nabla \lambda (\nabla \cdot \mathbf{W}) + \nabla \mu \times (\nabla \times \mathbf{W}) + 2 (\nabla \mu \cdot \nabla) \mathbf{W} + \rho \mathbf{F}. \quad (10)$$

Here, \mathbf{W} is the displacement vector, $\lambda > 0$ and $\mu > 0$ are Lamé coefficients, \mathbf{F} is the force vector describing the action of space-localized axially symmetric source.

Let us consider the case of the cylindrical coordinate system (2.5D), where $\mathbf{W} = (u_r, u_z)^T$, $\mathbf{F} = (F_r, F_z)^T$, $\lambda = \lambda(r, z)$, $\mu = \mu(r, z)$ and $\rho = \rho(r, z)$. Assume that at $z = 0$, the surface is free, with auxiliary boundaries along the coordinates r and z , as in the case of the acoustic equation. Problem (10) is solved with homogeneous initial conditions.

Represent the solution of problem (10) as the Fourier-Laguerre series

$$u_r(\mathbf{x}, t) = (ht)^{\frac{\alpha}{2}} \sum_{m=0}^{\infty} Q_m(\mathbf{x}) l_m^\alpha(ht), \quad u_z(\mathbf{x}, t) = (ht)^{\frac{\alpha}{2}} \sum_{m=0}^{\infty} U_m(\mathbf{x}) l_m^\alpha(ht). \quad (11)$$

As a result, defining the expansion coefficients Q_m and U_m necessitates solving a number of problems of the form

$$\left\{ \begin{aligned} & \frac{\partial}{\partial r} \left[(2\mu + \lambda) \frac{\partial Q_m}{\partial r} + \lambda \left(\frac{\partial U_m}{\partial z} + \frac{Q_m}{r} \right) \right] + \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial Q_m}{\partial z} + \frac{\partial U_m}{\partial r} \right) \right] + \frac{2\mu}{r} \left(\frac{\partial Q_m}{\partial r} - \frac{Q_m}{r} \right) - \rho \frac{h^2}{4} Q_m = \\ & = -\rho F_r f_m + \rho h^2 \sqrt{\frac{m!}{(m+\alpha)!}} \sum_{k=0}^{m-1} (m-k) \sqrt{\frac{(k+\alpha)!}{k!}} Q_k, \\ & \frac{1}{r} \frac{\partial}{\partial r} \left[r \mu \left(\frac{\partial Q_m}{\partial z} + \frac{\partial U_m}{\partial r} \right) \right] + \frac{\partial}{\partial z} \left[(\lambda + 2\mu) \frac{\partial U_m}{\partial z} + \lambda \left(\frac{\partial U_m}{\partial r} + \frac{Q_m}{r} \right) \right] - \rho \frac{h^2}{4} U_m = \\ & = -\rho F_z f_m + \rho h^2 \sqrt{\frac{m!}{(m+\alpha)!}} \sum_{k=0}^{m-1} (m-k) \sqrt{\frac{(k+\alpha)!}{k!}} U_k, \end{aligned} \right. \quad (12)$$

where the boundary conditions on the free surface take the form [1, 2, 3]

$$\tilde{\tau}_{rz} = \left\{ \frac{\partial U_m}{\partial z} + \frac{\partial Q_m}{\partial r} \right\} \Big|_{z=0} = 0, \quad (13)$$

$$\tilde{\sigma}_{zz} = \left\{ \lambda \left(\frac{\partial U_m}{\partial r} + \frac{U_m}{r} \right) + (\lambda + 2\mu) \frac{\partial Q_m}{\partial z} \right\} \Big|_{z=0} = 0. \quad (14)$$

2.3. Approximation of equations

On a rectangular mesh $\bar{\omega} = \bar{\omega}_r \times \bar{\omega}_z = \omega \cup \gamma$, where

$$\bar{\omega}_r = \{r_i = (i - 0.5)h_r, i = 1, \dots, N_r, h_r = l_1/(N_r - 0.5)\},$$

$$\bar{\omega}_z = \{z_k = (k - 0.5)h_z, k = 1, \dots, N_z, h_z = l_2/(N_z - 0.5)\},$$

$$\omega = \bar{\omega} \cap G, \quad \gamma = \bar{\omega} \cap \Gamma,$$

conform problem (9) with the difference problem

$$Ay_m = f, \quad m = 1, 2, \dots, \quad A : H \longrightarrow H, \quad (15)$$

where the difference operator $A = A^* > 0$ is given by a scheme of the second order of accuracy [6, 32]

$$(\Lambda_r + \Lambda_z) y_m - w(x) y_m = -\phi(x), \quad x \in \bar{\omega}, \quad (16)$$

$$\Lambda_r y = \begin{cases} \frac{1}{h_r} a_1 y_r, & i = 1 \\ (a_1 y_{\bar{r}})_r, & 1 \leq i \leq N_1 - 1 \end{cases}, \quad \Lambda_z y = \begin{cases} \frac{1}{h_z} a_2 y_z, & k = 1 \\ (a_2 y_{\bar{z}})_z, & 1 \leq k \leq N_2 - 1, \\ \frac{1}{h_z} a_2 y_{\bar{z}}, & k = N_2 \end{cases} \quad (17)$$

$$a_1(i, k) = \bar{r}_i \kappa(\bar{r}_i, z_k), \quad a_2(i, k) = r_i \kappa(r_i, \bar{z}_k), \quad w(i, k) = \rho(r_i, z_k) \frac{h^2}{4} r_i,$$

$$\phi(i, j) = -\frac{1}{2\pi} \frac{\delta(i - i_0, j - j_0)}{r_i} f_m + \rho(\mathbf{x}) h^2 \sqrt{\frac{m!}{(m + \alpha)!}} \sum_{k=0}^{m-1} (m - k) \sqrt{\frac{(k + \alpha)!}{k!}} y_k(\mathbf{x}), \quad \mathbf{x}_0 = (i_0 h_r, j_0 h_z). \quad (18)$$

where $\bar{r}_i = r_i + 0.5h_r$, $\bar{z}_k = z_k + 0.5h_z$; $y_{\bar{r}}$, $y_{\bar{z}}$ and y_r , y_z are the "backward" and "forward" difference relationships with respect to z and r [17, 6]. The boundary condition on the side $r = l_1$ is approximated exactly $y_{N_1, k} = 0$, $k = 1, \dots, N_2$. For solving problem (16), we use the conjugate gradient method [33].

Conform the problem (10) on a mesh $\bar{\omega}$ with the difference problem

$$Cy_m = f, \quad m = 1, 2, \dots, \quad C : H \rightarrow H. \quad (19)$$

A number of works [34, 35] describe the problem of constructing the discrete analog of problem (12). For this reason, in the present paper we performed approximation by the finite-volume method with second order of accuracy. For solving problem (19), by virtue of the non self-adjoint difference operator C , we will use the GMRES(k) method, where k is the restart parameter [33]. Note, when using the Laguerre transformation, the difference operator is always positive-definite. This guarantees convergence of the GMRES(k) method for any $k \geq 1$ [33].

2.4. Preconditioning

By choosing a preconditioning procedure, one can affect substantially the convergence of iterative algorithms of solving a system of linear equations and, as a result, the elapsed time. Besides standard requirements [17, 33] upon a preconditioning operator, such as

- energy equivalence of operator B to operator A in the sense of inequalities¹

$$\gamma_1 (Bu, u) \leq (Au, u) \leq \gamma_2 (Bu, u); \quad 0 < \gamma_1 \leq \gamma_2, \quad A = A^* > 0, \quad B = B^* > 0, \quad (20)$$

$$\gamma_1 = \min_{x \neq 0} \frac{(Ax, x)}{(Bx, x)}, \quad \gamma_2 = \max_{x \neq 0} \frac{(Ax, x)}{(Bx, x)};$$

- operation of inversion of operator B must be less time-consuming than for operator A ,

¹For the non self-adjoint case, see, e.g., [17, 33, 36].

we require efficiency of a procedure preconditioning of operator inversion on a multiprocessor computer system. Since not all preconditioning procedures can be efficiently implemented with the use of hundreds of processors (e.g., ILU expansion [33]), the latter requirement drastically limits the class of possible preconditioners.

In [26], based on the Dichotomy Algorithm, the author proposed a high-performance parallel implementation of the variable separation method [17, 24, 37] for the Laplace operator inversion. The use of the Dichotomy Algorithm for solving tridiagonal systems of linear equations ensures linear dependence of the speedup coefficient on the number of processors. Thus, for problem (15), following works [17, 18, 19, 20, 21, 22], as the preconditioner operator we will consider²

$$B \equiv \Lambda_r + \Lambda_z - d \quad (21)$$

with the coefficients

$$a_1(i, k) = \bar{r}_i \tilde{\kappa}, \quad a_2(i, k) = r_i \tilde{\kappa}, \quad d(i, k) = r_i \frac{h^2}{4} \tilde{\rho}.$$

For problem (19), the preconditioner is given as

$$K \equiv \begin{bmatrix} B_1 & 0 \\ 0 & B_2 \end{bmatrix}, \quad (22)$$

where $B_1 \equiv \Lambda_r + \Lambda_z - d$ with the coefficients

$$a_1(i, k) = \bar{r}_i \widetilde{(\lambda + 2\mu)}, \quad a_2(i, k) = r_i \tilde{\mu}, \quad d(i, k) = r_i \frac{h^2}{4} \tilde{\rho} + \frac{(\lambda + 2\mu)}{r_i}$$

and $B_2 \equiv \Lambda_r + \Lambda_z - d$ with the coefficients

$$a_1(i, k) = \bar{r}_i \tilde{\mu}, \quad a_2(i, k) = r_i \widetilde{(\lambda + 2\mu)}, \quad d(i, k) = r_i \frac{h^2}{4} \tilde{\rho}$$

By virtue of the assumption that the contrast of the medium is moderate and the use of a supercomputer implies a great number of mesh nodes, this class of preconditioners enables a good convergence rate. Moreover, the sought solution will be achieved in the number of iterations, which does not practically depend on the number of mesh nodes [17].

Since in the proposed scheme of solution of to problem the main computational and communication costs fall on the preconditioner inversion, the algorithm efficiency, as a whole, is determined by performance of the parallel procedure of solution of the problems $B_\alpha y = \phi$.

3. Numerical Experiments

3.1. Parallel Performance

For estimating the performance of the proposed algorithm, using Fortran-90 and the MPI paradigm, we implemented numerical procedures for solving problems (3) and (10). The Fast Fourier transform, which is necessary for the preconditioner inversion, was done using FFTW library [38]; the tridiagonal systems of linear equations were solved using the Dichotomy Algorithm [26, 30]. Calculations were performed on MBC-100k supercomputer (from the Interdepartment Supercomputer Center of the Russian Academy of Sciences) and on NKS-30t supercomputer (from the Siberian Supercomputer Center of the Siberian Branch of the Russian Academy of Sciences). The computer are based on Intel Xeon four-core processors operating at 3 GHz and connected via the Infiniband communication medium.

²Introduce the notation $\tilde{f} = \frac{1}{2} (\min_{x \in G} f(\mathbf{x}) + \max_{x \in G} f(\mathbf{x}))$.

Table 1 and Fig. 1.a represent measurement results of performance for the conjugate gradient method; Table 2 and Fig. 1.b show those for the GMRES(10) method. Implementing these algorithms, we achieved a nearly linear dependence of the speedup on the number of processors for meshes of different resolution. Within one calculation, we managed to involve a considerable number of processors (from 1024 to 8192) with an efficiency of 90% to 50%, respectively. The achieved performance and scalability are provided due to using the Dichotomy Algorithm in the context of the parallel preconditioner inversion. Thus, the algorithm will substantially increase the efficiency of usage of supercomputer computational resources in solving elliptic equations. Thus, in solving applied geophysics problems.

size	2048x2048		4096x4096		8192x8192		16384x16384		32768x32768	
NP	T	S	T	S	T	S	T	S	T	S
64	1.4e-02	-	8.0e-02	-	3.5e-01	-	1.7	-	-	-
128	7.3e-03	122	6.3e-02	138	1.8e-01	124	7.2e-01	151	3.9	-
256	6.3e-03	<u>142</u>	1.8e-02	284	9.0e-02	254	4.3e-01	253	2.15	172
512	-	-	1.1e-02	465	5.0e-02	448	2.0e-01	544	1.01	463
1024	-	-	1.0e-02	<u>512</u>	2.7e-02	829	1.0e-01	1088	5.4e-01	924
2048	-	-	-	-	2.3e-02	973	7.0e-02	1554	3.2e-01	1560
4096	-	-	-	-	2.0e-02	<u>1120</u>	5.8e-02	<u>1875</u>	2.1e-01	<u>2377</u>

Table 1: Calculation time (T) and speedup (S) versus the number of processors for one iteration of the CG method.

size	2048x2048		4096x4096		8192x8192		16384x16384		32768x32768	
NP	T	S	T	S	T	S	T	S	T	S
64	0.53	-	3.51	-	14.6	-	-	-	-	-
128	0.27	125	1.58	142	7.3	128	31.3	-	-	-
256	0.17	<u>200</u>	0.72	312	3.8	245	15.5	258	-	-
512	0.32	106	0.38	591	1.93	484	8.4	476	35	-
1024	-	-	0.35	<u>641</u>	1	934	4.5	890	17.1	1047
2048	-	-	0.5	450	0.8	1168	2.63	1523	9.62	1862
4096	-	-	-	-	0.76	<u>1229</u>	2.3	<u>1741</u>	5.7	3132
8192	-	-	-	-	-	-	-	-	4.15	<u>4318</u>

Table 2: Calculation time (T) and speedup (S) versus the number of processors for one cycle of the GMRES(10) method.

Dupros et al. [39] considered a parallel algorithm for solving the dynamic problem of the elasticity theory. They demonstrated the possibility of using 1024 processors. Up to 256 processors, the authors have obtained a high speedup; however, the algorithm efficiency was lower in the range from 256 to 1024 processors. Our algorithm ensures a high efficiency in the range from 64 to 8192 processors, the software implementation been much simpler.

As a result of numerical experiments it has been found that the execution time of the first iteration for the CG and GMRES(k) methods is several times greater than that of subsequent ones. This is explained by application of dynamic optimization of interprocessor communications on the level of MPI-Reduce(" + ") after repeated execution of the main communication operation " + " in the context of the Dichotomy Algorithm. In this case, due to the associative addition, the order of processor exchanges is set such that to minimize as much as possible the communication time. Thus, the possibility of applying the algorithms of dynamic optimization of the communication interactions ensures the high performance of the Dichotomy Algorithm. We should note that for the cyclic reduction method, a fixed order of elimination of unknowns prevents optimization of the communication interactions to a full extent. For this reason, in practice, the Dichotomy Algorithm possesses a much higher performance than the cyclic reduction method.

It is known that the efficiency of variational methods for solving SLAEs on a supercomputer decreases because of intensive communication interactions while computing $\| \cdot \|$ on distributed data. This problem can be solved by means of modifications of the known algorithms [36]. Let us compare estimates of the communication time for computing $\| \cdot \|$ for the CG and GMRES(k) methods and the communication time

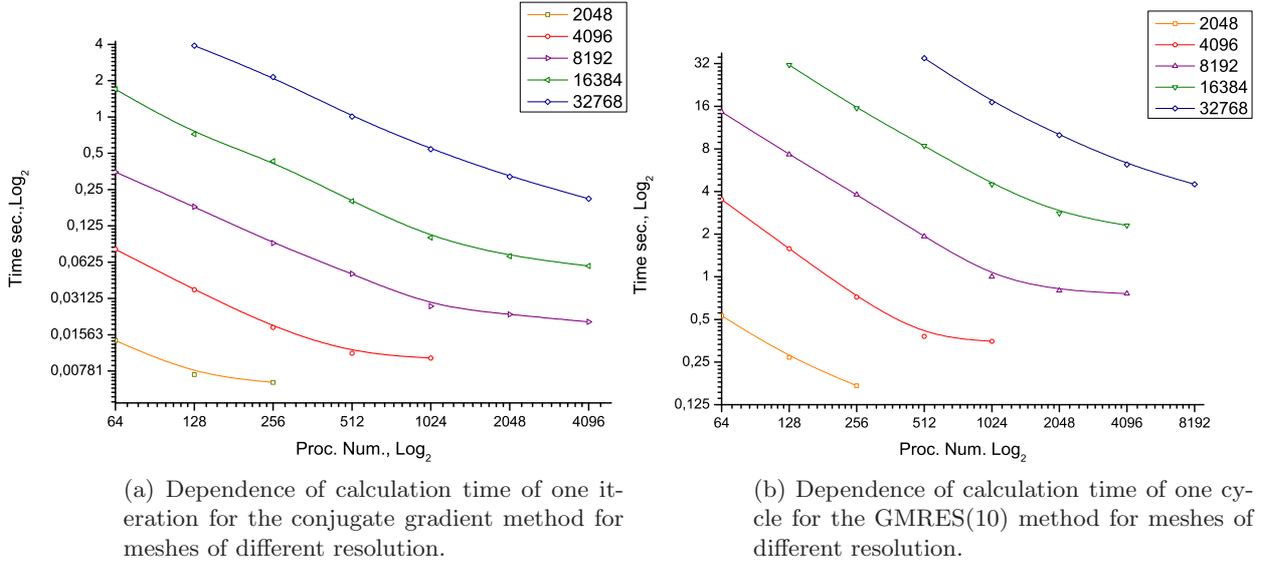


Figure 1:

of the Dichotomy Algorithm:

$$T_p^{\|\cdot\|, all-reduce} = 2 \log_2(p) \alpha + \frac{p-1}{p} (\gamma + 2\beta),$$

$$T_p^{Dichotomy} = \alpha [\log_2(p) + 1] \log_2(p) + l \left(\log_2(p) - \frac{p-1}{p} \right) (\gamma + 2\beta).$$

From this it follows that for computer systems with a low latency (α) and for $l \gg 1$, the communication time for calculating $\|\cdot\|$ is insignificant, compared to the communication costs of the Dichotomy Algorithm. Thus, the chosen precondition procedure does not need modifications of the CG and GMRES(k) methods.

3.2. Acoustic Waves

The use of mesh methods in spatial derivative approximation cause a numerical effect called a "phase error" [8]. In modeling wave propagation processes for long instants of time, this effect determines considerably the accuracy of the solution. For this reason, from the view of practice, an urgent problem is choosing the number of mesh nodes per characteristic wavelength. The high performance of the proposed algorithm allows one to estimate the accuracy of solution for meshes with a high resolution ($h_\alpha = 1/100\lambda \div 1/150\lambda$).

Tables 1 and 2 show that calculation of acoustic waves requires much less count time than that of elastic waves. Hence, we first consider the problem of modeling acoustic wave propagation in a homogeneous medium $\rho, \kappa \equiv const$. This made it possible to investigate the accuracy of solution for meshes with much more nodes and with less computational costs.

For problem (3), a point source was situated at the origin of coordinates; the time dependence was given as

$$f(t) = \exp \left[-\frac{(2\pi f_0(t-t_0))^2}{\gamma^2} \right] \sin(2\pi f_0(t-t_0)), \quad (23)$$

where $f_0 = 30\text{Hz}$, $t_0 = 0.2s$, $\gamma = 4$.

Approximation of Eq. (9) was done on the uniform mesh $\bar{\omega}$ with $N_1 = N_2 = 2^k$ nodes, $k = \{12, 13, 14, 15\}$. The number of addends in series (8) was $n = 3000$; the expansion parameters were $\alpha = 9$, $h = 400$. The distances were measured in wavelength λ .

The time dependencies of the wavefield amplitudes for four receivers situated on the free surface at different lengths from the source are represented in Fig. 2. It is seen that the accuracy of the obtained solution for different instants of time depends substantially on the number of mesh nodes per characteristic wavelength. For instance, for first instants of time, for achieving a reasonable calculation accuracy, the mesh with a space step $h_r = h_z = 1/40\lambda$ is sufficient (Fig. 2.a); for longer time intervals it is required to decrease the mesh step in order to keep a reasonable level of the calculation accuracy.

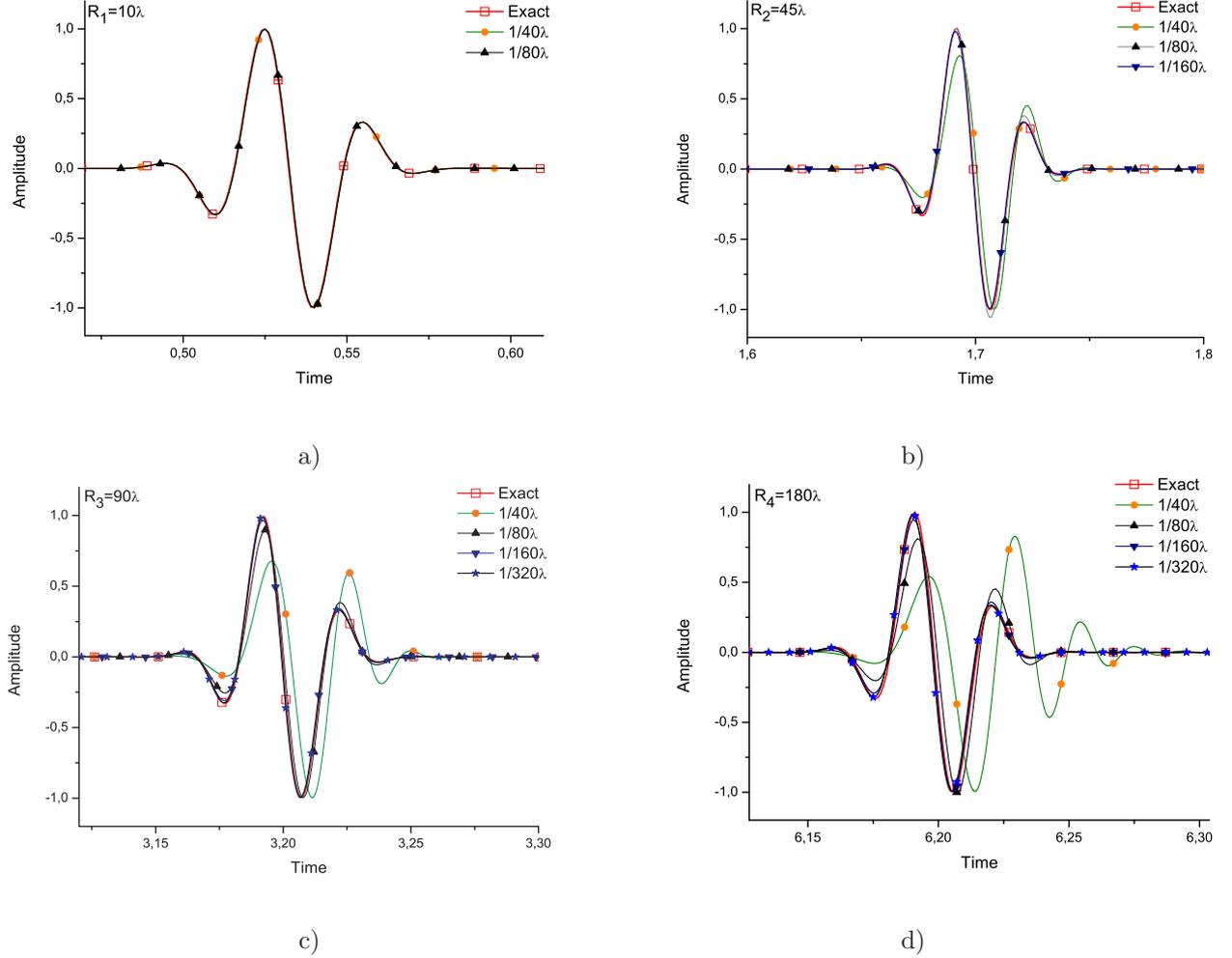


Figure 2: The time dependence of solution $u(\mathbf{x}_i, t)$ for the acoustic equation, where $\mathbf{x}_i = (R_i, 0)$, $i = 1, 2, 3, 4$.

Figure 3 represents dependence of the accuracy of the obtained solution on the receiver position for meshes with different resolution:

$$\epsilon(\mathbf{x}_i) = \sqrt{\frac{\int_0^{t_1} [u_{exact}(\mathbf{x}_i, t) - u_h(\mathbf{x}_i, t)]^2 dt}{\int_0^{t_1} [u_{exact}(\mathbf{x}_i, t)]^2 dt}}, \quad \mathbf{x}_i = (ih_r, 0), \quad i = 1, \dots, N_1,$$

where $u_{exact}(r, 0, t) = \frac{1}{2\pi} \frac{f(t - r/\sqrt{k/\rho})}{r}$ is the exact solution and u_h is the numerical solution obtained on the mesh with the space step $h_r = h_z = h$.

It can be easily found that when the time interval of modeling is increased m times, the space step must be decreased $\approx \sqrt{m}$ times; this agrees with theoretical estimates for approximation methods of the second

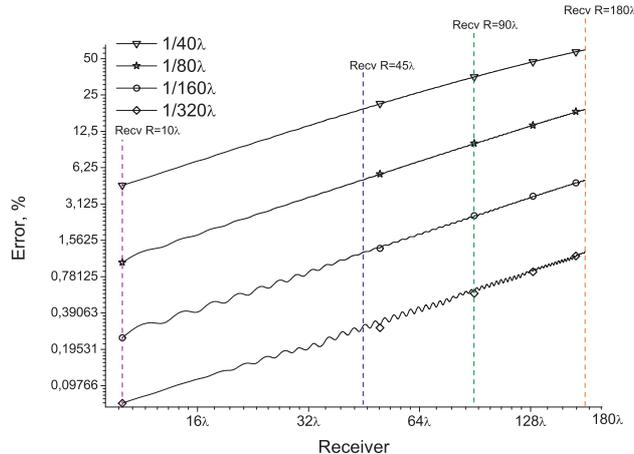


Figure 3: Dependence of the solution accuracy on the position of receiver (3.2) for the meshes of different resolution.

order of accuracy [8]. Thus, for acoustic wave simulation for long time intervals, it is necessary to use meshes with a sufficient number of nodes in order that numerical effects caused by the model resolution do not predominate.

We will note that for solving the problem, higher-order schemes [40, 34] are suitable. In the context of the parallel algorithm, increasing approximation order does not cause loss of efficiency because the preconditioning for higher-order schemes can be done with the second order. Naturally, in this case the number of iterations for the CG and GMRES(k) methods for achieving the desired accuracy will be a bit more, but the behavior of the dependence of the speedup on the number of processors will not change.

3.3. Solid layer over Solid Half Space

Although early results on elastic wavefield modeling have been obtained long ago [41], [42], however, they were rather qualitative because of a large step of the space mesh $h = 1/5\lambda \div 1/2\lambda$. Considerably increased computer performance and also development of multiprocessor computer systems have made it possible to increase the calculation accuracy [43, 44, 45]. However, in spite of available theoretical estimates of the dependence of solution accuracy on mesh step [8], the problem of practical choosing a space step of meshes is still urgent. By solving the acoustic equation, it was illustrated that calculations for long instants of time require meshes with many nodes. Taking into account that the proposed parallel algorithm possesses high performance, we will analyze issues of accuracy for problem (10) for meshes $h = h_r = h_z = \{1/10\lambda_s, 1/20\lambda_s, 1/45\lambda_s, 1/90\lambda_s\}$, where $\lambda_s = \min V_s/f_0$. Here, V_s is the S -wave propagation velocity and f_0 is the source frequency.

Let us consider a problem on elastic wave propagation in a thin layer whose seam thickness is comparable with the wavelength (Fig. 4.a). The wavefield source is a source of the type of "center of pressure" [2]:

$$F_r = \frac{1}{2\pi} \frac{d}{dr} \left[\frac{\delta(r)}{r} \right] \delta(z-d), \quad F_z = \frac{1}{2\pi} \frac{\delta(r)}{r} \frac{d}{dz} \delta(z-d). \quad (24)$$

The time dependence of the pulse $f(t)$ was determined in (23), where $f_0 = 30\text{Hz}$, $t_0 = 0.2\text{s}$ and $\gamma = 4$. The source is placed at the depth $d = 10\text{m}$. In the calculations, the instants of time were $t \in (0, 5)\text{s}$. The number of terms of series (11) was $n = 2000$ with the parameters $\alpha = 8$ and $h = 600$.

In problems of simulation of wavefields, in particular, seismic ones, the governing factor is choosing model problems to estimate accuracy of numerical algorithms. A common method applied for layered media is the method proposed in [46, 47] and extended in [48, 49], etc. The drawback of the method is that it introduces interference (artifacts). The use of minor matrices [50] made it possible to extend applicability of the matrix method, but did not eliminated artifacts. In the present paper, we evaluate the accuracy of the proposed

parallel algorithm with the use of the approach described in [51, 52]. The essence of the method is that the sought-for boundary-value problem of second order in the spectral domain is reduced to two Cauchy problems of first order, to which there exists a stable analytical solution. As a consequence, this made it possible to remove all constraints on the powers of layers, frequencies, and recording systems. Comparison of the modeling results and results obtained by means of the analytical method made it possible to estimate the dependence of the numerical solution accuracy on the space mesh step.

The medium model and a snapshot of the wavefield for the component $u_z(r, z)$ at $t = 3s$. are represented in Fig. 4.a. Figures 4.b,c and Figs. 5.a,b show the component u_z as a function of time for a receiver situated on the free surface at $r = 1500$.

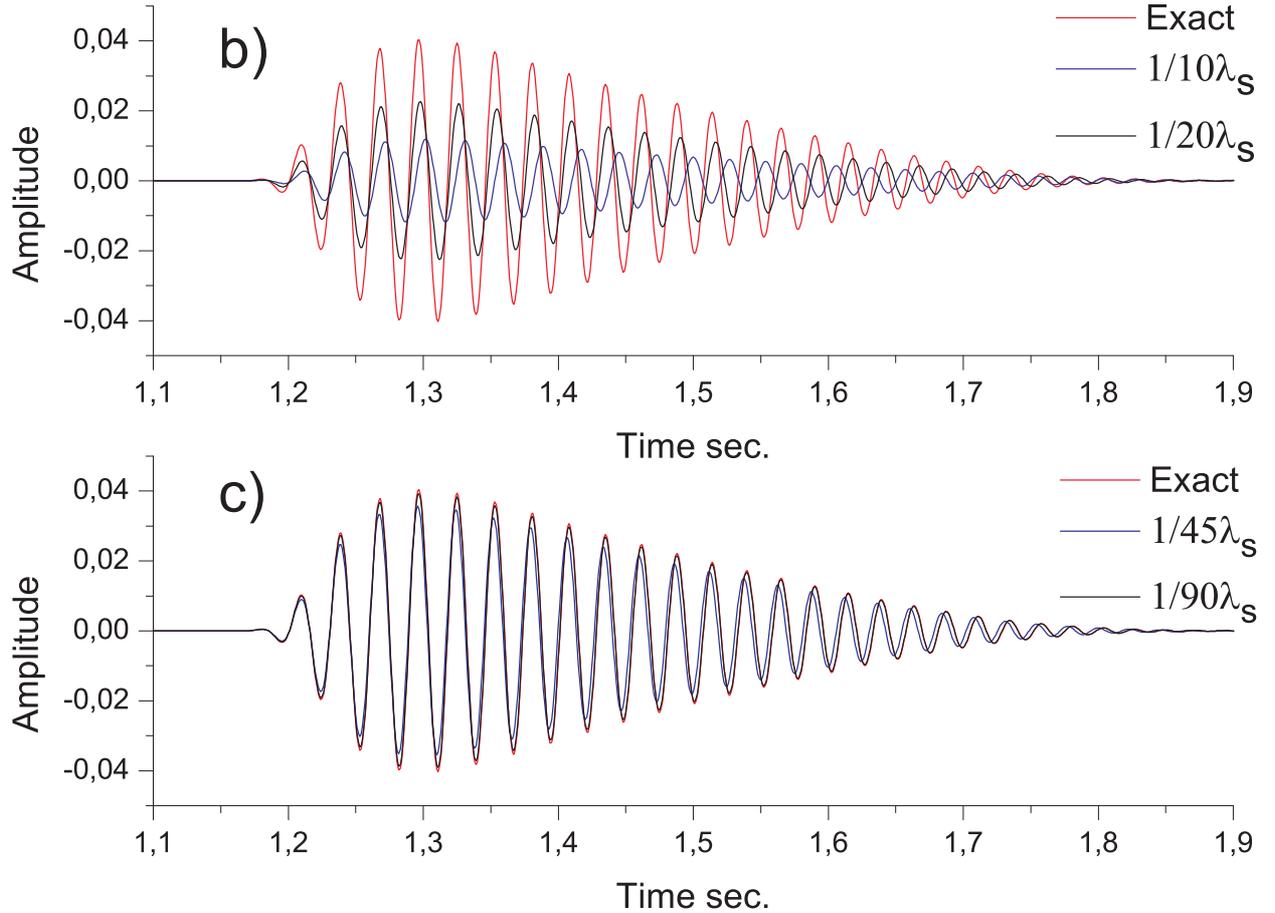


Figure 4: (a) A snapshot for the displacement vector component $u_z(z, r)$ at $t = 3s$ in the presence of a thin layer. The time dependence of amplitude $t \in [1.1, 1.9]s$ for detector receiver $u_z(1500m, 0)$ for calculations on the meshes: (b) $N_r \times N_z = \{4096 \times 4096, 8192 \times 8192\}$; (c) $N_r \times N_z = \{16384 \times 16384, 32768 \times 32768\}$.

Figure 4.b and Fig. 5.a evidence that the meshes with steps $1/10\lambda_s$ and $1/20\lambda_s$ ensure no accuracy. Thus, the mesh with $1/45\lambda_s$ or $1/90\lambda_s$ can ensure an acceptable level of accuracy for initial instants of times (Fig. 4.b and Fig. 5.a). For final instants of time (Fig. 4.c and Fig. 5.b) the calculations have to be done on the mesh with $1/90\lambda_s$. The results of evaluating the accuracy of solution for the problem of the elasticity theory are in good agreement with the results obtained for the acoustic equation. Therefore, we can state that the main factor determining the accuracy of solution in wave process simulation is the number of mesh nodes per wavelength. Also, modeling of real space-time scales requires modeling meshes with a higher resolution.

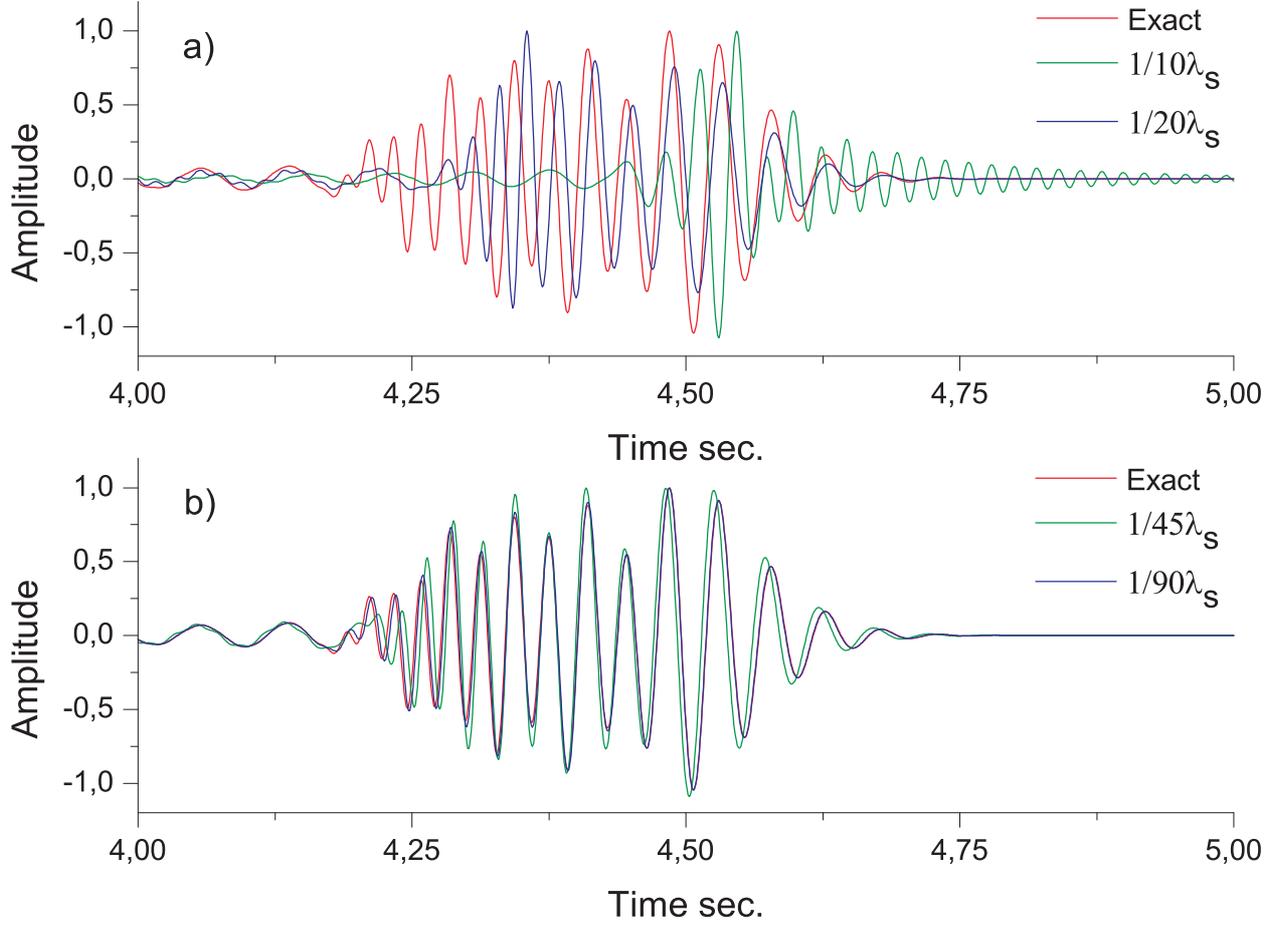


Figure 5: The time dependence of amplitude $t \in [4, 5]s$ for detector receiver $u_z(1500m, 0)$ for calculations on the meshes: (a) $N_r \times N_z = \{4096 \times 4096, 8192 \times 8192\}$; (b) $N_r \times N_z = \{16384 \times 16384, 32768 \times 32768\}$.

3.4. Marmousi

For illustrating the ability of the proposed algorithm to perform (for an acceptable time) elastic wavefield simulation for real application problems, we will consider problem (10) for the Marmousi medium (Fig. 6.a) [53].

The calculations were done for $t \in (0, 6]s$ on the meshes with $N_r \times N_z = \{8192 \times 2048, 16384 \times 4096, 32768 \times 8192\}$ nodes, which corresponded to a space step $h_r = h_z = \{1.5m, 0.75m, 0.375m\}$. The wavefield was modeled from a source of the type of center of pressure (23),(24) with the parameters $f_0 = 10Hz$, $t_0 = 1s$ and $\gamma = 4$. The number of terms of series (11) was $n = 1200$ with the parameters $\alpha = 8$ and $h = 300$. Figure 6.b shows a snapshot of a wavefield for the displacement vector component $u_r(r, z)$ at $t = 6s$; Figs. 7.a,b represent dependencies of the component $u_r(r, z)$ along straight lines "Slice-R" and "Slice-Z". Comparing results obtained for different meshes, we conclude that an acceptable accuracy for the final instant of time is achieved in calculations with the mesh space step $h_r = h_z = 0.75m$, which corresponds to $\{N_r \times N_z\} = \{16384 \times 4096\}$ nodes. For this mesh, according to Table 3, computing will take 4.7 hours with 1024 processors. The efficiency is about 90%. We should note that sometimes it is reasonable to perform computing using more processors, but with a lower efficiency, because in this case the amount of storage is increased. This makes it possible to choose greater values of k for the GMRES(k) method and, thereby ensure a higher convergence rate[33].

NP	256	512	1024	2048	4096
Mesh	Time Hours				
8192 × 2048	3.1	1.6	1.4	2.4	4.2
16384 × 4096	17	8.6	4.7	3.8	4
32768 × 8192	68	34	19.6	12	11

Table 3: Calculation time versus the number of processors for meshes of different resolution for the Marmousi medium.

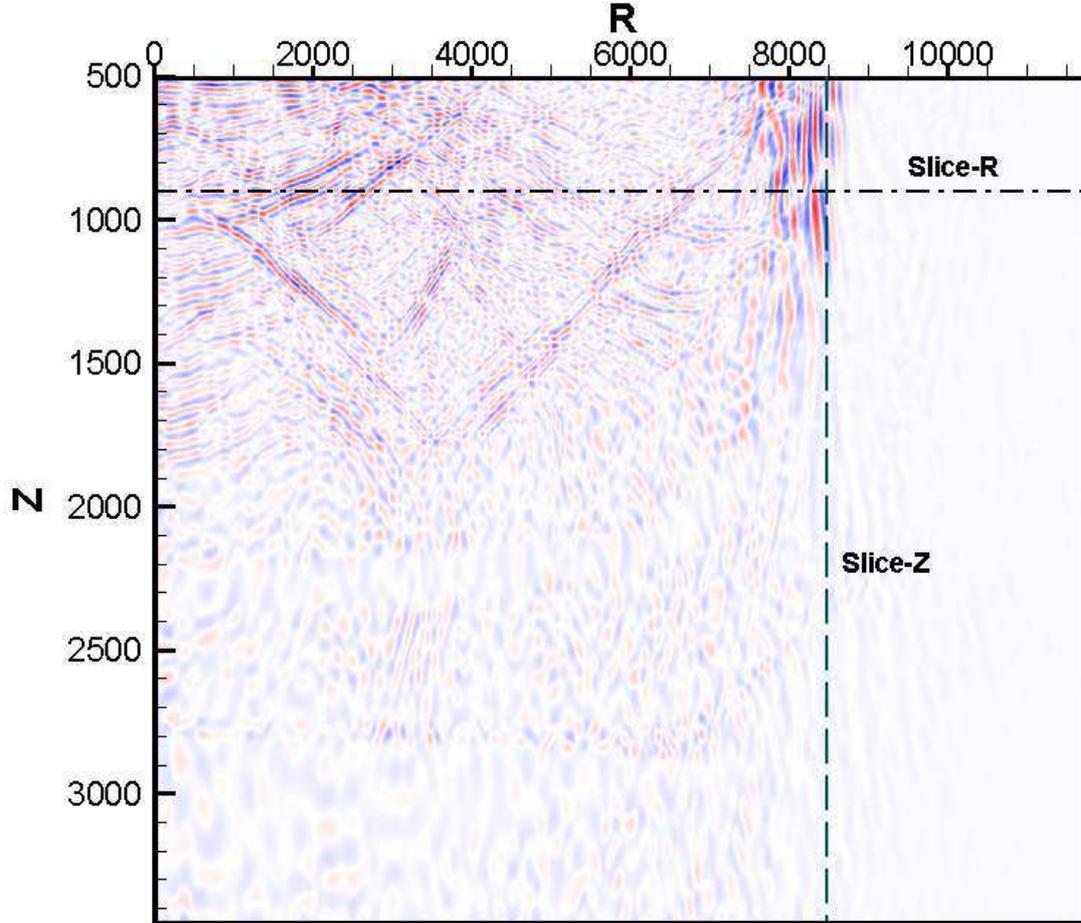


Figure 6: (a) Marmousi model ($z \geq 500m$): P,S – wave velocities; (b) a snapshot for the displacement vector component $u_r(r, z)$ at $t = 6$ s.

The numerical experiments have shown that the proposed algorithm enables not only to perform modeling, but also to solve real application geophysics problems. For doing so, both a supercomputer with a moderate number of processors ($64 \div 256$) and multiprocessor systems integrating thousands of computing elements are used effectively.

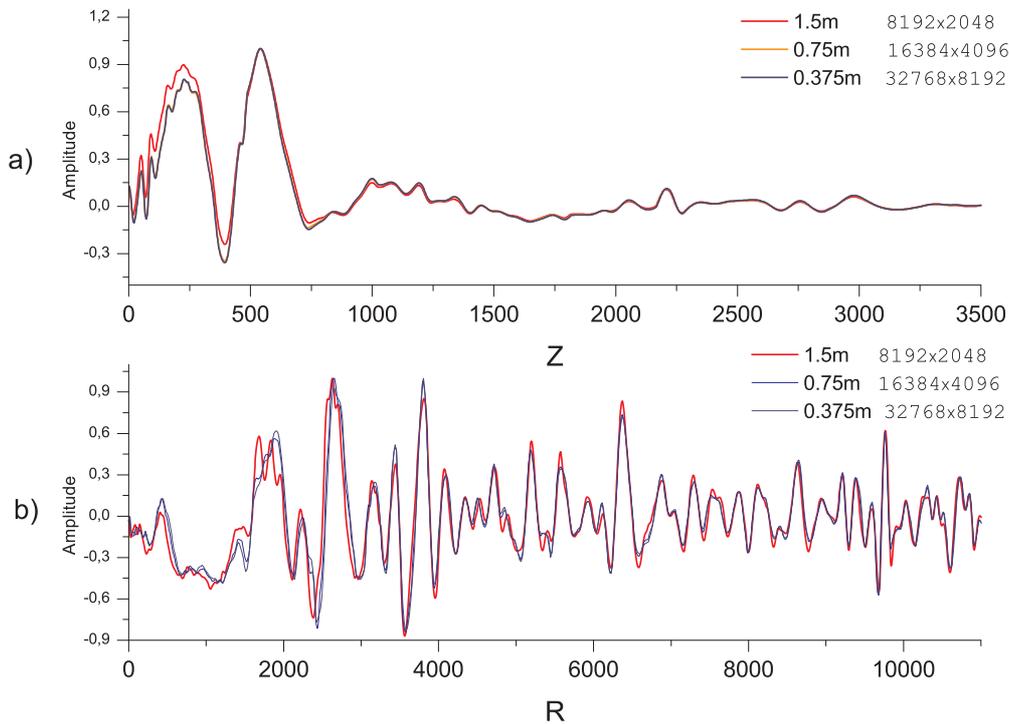


Figure 7: Dependence of the field amplitude for the component u_r at $t = 6$ along straight lines (a) Slice-Z and (b) Slice-R.

4. Conclusions

We have proposed the parallel algorithm for solving an acoustic equation and dynamic problem of the elasticity theory in a cylindrical coordinate system (2.5 D). The Laguerre time transform was used to perform changing from the initially boundary-value problem to the problem of inversion of the same elliptic second-order operator for different right-hand sides. The difference equations resulting from elliptic operator approximation were solved by the CG method or the GMRES method. Choosing the Laplace operator as the preconditioning one allowed for a high convergence rate of the iterative process for media with a moderate contrast.

The nearly linear dependence of the speedup and the high scalability of the parallel algorithm on the number of processors were ensured due to the Dichotomy Algorithm in the context of the variable separation method for inverting the preconditional operator. The proposed algorithm has validated its efficiency in calculations with 64 to 8192 processors. Thus, the high performance of the Dichotomy Algorithm and its simple implementation enable efficient parallelization of economic numerical procedures that require multiple solution of tridiagonal systems of equations.

The main conclusion is that the wave process modeling for longer time intervals requires increasing number of space mesh nodes. This causes the necessity of applying high-performance computer systems for solving application problems. It has been shown that the proposed parallel algorithm, which based on the known economic numerical methods and the Dichotomy Algorithm, makes it possible to efficiently involve thousands of processors within one calculation. This enables to perform practical calculations for real models of media, times, and distances with the desired accuracy.

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