Parallel numerical simulation of wave propagation in 3D elastic medium with application of the Laguerre transform

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Abstract. *In this paper, we apply an approach for numerical simulation of elastic waves in heterogeneous medium, based on the implementation of integral Laguerre transform with subsequent domain decomposition. Following the Laguerre transform, we obtain a system with strictly negative definite elliptic operator, which doesn't depend on separation parameter. Therefore, parallel calculations can be organized by means of the additive Schwarz method and systems of linear algebraic equations in each subdomain can be solved by means of LU factorization. In the paper we study this approach in 3D case.*

Keywords

Laguerre transform, additive Schwarz method, wavefield, parallel calculations.

1 Introduction

The large-scale numerical simulation of elastic wave propagation in realistic 3D heterogeneous media is impossible without parallel computations based on domain decomposition. So far, the most popular approach here is to use explicit finite-difference schemes based on staggered grids, despite drawbacks such as the necessity to perform data send/receive at each time step, full re-simulation of the wavefield for each new source, and hard disk data storage for implementation of a reverse-time migration. In this regard, considerable attention has recently been given to the development of alternative techniques for simulation of seismic waves, especially, the ones working in the temporal frequency domain [1]. However, the use of such methods for general heterogeneous media also faces a range of significant issues. The main issue is a consequence of the indefiniteness of the impedance matrix. This property brings about a very slow rate of convergence for the iterative procedures solving the linear algebraic equations resulting from the finite dimensional approximation of the elastic wave equations in the temporal frequency domain.

2 Statement of the problem. Solution algorithm

Let us consider a system of second order elastic equations for a volumetric source with zero initial conditions.

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial}{\partial x_j}\left(C_{ijkl} \frac{\partial u_k}{\partial x_l} \right) + \delta(\bar{x} - \bar{x}_0)\, f(t), \quad (1)$$

Here ρ is density, C_{ijkl} is stiffness tensor, $\bar{x}_0$ reflect spacial coordinate of the source, $f(t)$ is the source function. In order to restrict the target area, we use a certain modification of the elastic Perfectly Matched Layer (PML) presented in [2]. Such a modification was proposed and implemented by G.V. Reshetova and V.A. Tcheverda [3]. Let us use Laguerre transform in order to exclude time variable t from (1) and solve system in spatial space. The integral Laguerre transform for the function $u(x,z,t) \in L_2(0,\infty)$ is given by the following relation:

$$u_n(x,z) = \int_0^\infty u(x,z,t)\cdot(ht)^{-\frac{\alpha}{2}} l_n^\alpha(ht)dt \quad (2)$$

with the inversion formula

$$u(x,z,t) = \sum_{n=0}^\infty u_n(x,z)(ht)^{\frac{\alpha}{2}} l_n^\alpha(ht) \quad (3)$$

Here $l_n^\alpha(ht)$ are orthonormal Laguerre functions

$$l_n^\alpha(ht) = \sqrt{\frac{n!}{(n+\alpha)!}(ht)^{\frac{\alpha}{2}} e^{-\frac{ht}{2}} L_n^\alpha(ht)}$$

with, $h \in R_+, \alpha \in Z_+$ and $L_n^\alpha(ht)$ being classical Laguerre polynomials [4].
Application of the integral Laguerre transform to the system of elastic equations (1) transforms it to the system of elliptic second order partial differential equations with a negative definite operator:

$$Lu_n = g_n$$

Here u_n are unknown coefficients from (3) and g_n are right hand sizes depending on source and on $u_1 ... u_{n-1}$. The finite different approximation gives a system of linear algebraic equations with a sparse nine-diagonal negative definite matrix. It is worth mentioning that the matrix of this system does not depend on the separation parameter *n*.

Parallelization of the algorithm is implemented on the base of the domain decomposition and the additive Schwarz method [5], [6]. The basic idea of this method is to search for the solution not in the original computational domain, if it is too large, but to decompose it to elementary subdomains (Figure 1.a) of an appropriate size and to resolve the problem in each of these subdomains. In particular, to resolve the boundary value problem in the domain D with the boundary S, it is decomposed to two overlapping subdomains D1 and D2 (Figure 1.b), so two new boundaries S1 and S2 are introduced. The Schwarz alternations start with computation of solutions within subdomains D1 and D2 with arbitrary boundary conditions on S1 and S2, respectively. For each subsequent iteration (m+1), the solution in D1 is constructed using as boundary conditions on S1 the trace of a solution in D2 computed by the previous iteration (m). The same procedure is used to update the solution in D2. The convergence of iterations for this version of the additive Schwarz method is ensured by the negative definiteness of the operator and overlapping of the neighboring subdomains.

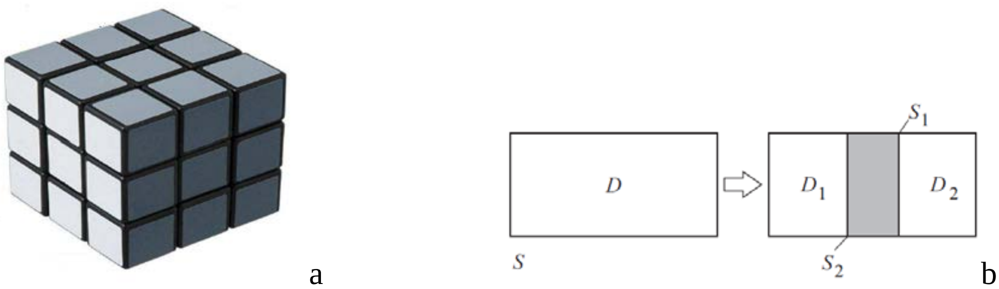

Fig. 1. a. 3D domain decomposition; b. The overlapping domain decomposition and Schwarz iterations

3 Organization of parallel calculations

Since system of linear algebraic equations (SLAE), obtained after approximation (2), does not depend on the separation parameter, it is reasonable to use direct solver on the base of LU decomposition: in each subdomain it can be done only once, saved in the RAM and subsequently be used for all right-hand sides.

In order to perform the LU factorization and to solve a SLAE for a large number of right-hand sides we use Intel Math Kernel Library (Intel MKL) PARDISO direct solver that is optimized under Intel processor architecture and is parallelized via OpenMP. In order to improve the factorization performance, algorithms of Intel MKL PARDISO are based on a Level-3 BLAS update. Moreover, there are additional features in PARDISO, which can improve the performance, in particular, leftlooking [7] and two-level [8] factorization algorithms. The first algorithm improves the scalability on a small number of threads while the second – on many threads (more than eight). The computational cost of solving SLAE with many right-hand sides (RHS) is the same or higher than those needed for factorization. A solving step in Intel MKL PARDISO is optimized both for one RHS and for many RHS.

In spite of using the effective matrix format CSR (compress sparse row), which are designed to store sparse matrices, tests showed that memory "bottle neck" is storing LU factors, which are results of decomposition of initial matrix A. For example to solve 2D problem in domain 1600x1600 need to have about 8 GB RAM. It not so bad, because many modern high performance systems have such resources. However, if we try to solve 3D problem with not so big sizes, very huge size of RAM is required. So, the problem 80x80x80 fit in the 8GB RAM.

Improving the algorithms of matrix decomposition is one of main lines of development in computational mathematic. Nevertheless, the fill-in of LU factors cannot be significantly decreased even via modern packages like METIS or SCOTCH. These packages are based on row-column reordering of an initial matrix by using Nested Dissection (ND) algorithm [9]. However for 3D problems need to find another approaches to decrease fill-in. One of them is low-rank approximation method, H-technique and H-matrices. The fact is that diagonal blocks of LU-factors can be effectively represented in H-format; non-diagonal blocks and Schur complement can be approximated by low-rank matrices [10]. Therefore, computational resources can be significantly decreased [11]. The FLOPS and memory estimation for different algorithms of factorization stage are provided in the Table 1.

Tab.1. Computation resources of LU-decomposition for 3D problem (NxNxN mesh points)

	LU decomposition	***ND algorithm***	***Low-rank approximation***
FLOPS	$O(N^8)$	$O(N^6)$	$O(N^4)$
Memory consumption	$O(N^5)$	$O(N^4)$	$O(N^3)$

4 Numerical experiments

Numerical experiments were carried out on the high performance computer of the Moscow State University with a hybrid parallel architecture: 519 nodes, each of them consists of two quad-core processors and has 8 GB RAM.
The first experiments were performed to understand the dependence of the number of iterations on the number of subdomains is analyzed. These results are presented in Table 2. We have considered a simplest situation: a homogeneous elastic medium, separated by various number of subdomains, as showed in Figure 2. The system (1) is solved for each type of decomposition, the number of Schwarz iterations is measured.

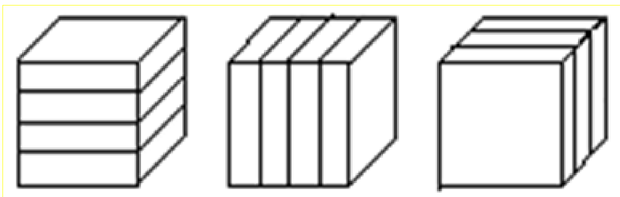

Fig. 2. 1D decomposition of computational domain

Tab.2. Dependence of number of Schwarz iterations on number of subdomains

Number of subdomains	2	3	4	5	6	7	8
Number of iterations	3	4	5	6	7	8	9

In the second experiment, computational domain consists of inhomogenous medium with two layers as presented in Figure 3a. Each layer has own wave propagation velocities (in the top level $V_p = 3600$ m/s, in the low one $V_p = 5000$ m/s, $V_s = \frac{V_p}{\sqrt{3}}$) and common density $\rho = 1500 kg/m^3$. As the source function, we chose Ricker impulse with dominant frequency 30 Hz. It is located in the center of computational domain, which separated by 27 subdomains as showed in Figure 1a. Each subdomain is handled by own cluster node with 8GB RAM. The neighborhood subdomains exchanges between each other by solution after each Schwarz iteration. The size of the computational domain was 800x800x800m. The result of this experiment is presented in Figure 3b (snapshots in two projections).

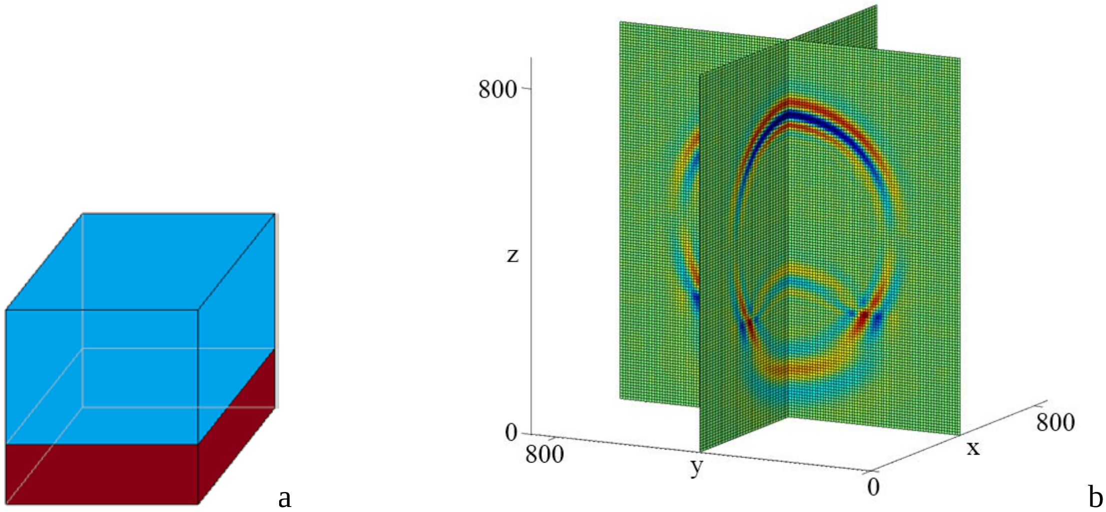

Fig. 3. a. Inhomogeneous layered medium; b. The result of this experiment – snapshots in two projections

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