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# Simulation of seismic wave propagation in 3D heterogeneous media: a parallel computing approach

Santa Agreste and Angela Ricciardello Department of Mathematics Messina University, Italy {sagreste,aricciardello}@unime.it

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# Abstract

The use of parallel computing makes it feasible to simulate realistic seismological events, whose reconstruction requires wide domains, high frequencies and the introduction of the dissipation terms. The propagation problem of seismic waves is a key feature of the earthquake dynamics that we are interested in numerically modeling and simulating. In particular, in this work we present several preliminary results about the load balancing for the parallel resolution of a simulation of the propagation of seismic waves in a 3D heterogeneous medium. The Finite Element Method is employed for the spatial discretization by using non-structured tetrahedral meshes. The Newmark method is used for the time discretization. With the aim to study a priori the load balancing, we introduce two performance indices: closing nodes and node balancing. In particular, the first one estimates the amount of processor data, the latter provides information on work-load distribution. The variation of these indices as functions of the number of processors and of the number of nodes of the grid is then investigated.

Keywords: Seismic Wave Propagation, Finite Element Method, Mesh Generation, Domain Decomposition, Parallel Computing

AMS Subject Classification: 65Y05, 68W10, 65M60, 86A15

# 1. Introduction

In the context of numerical simulations of seismic events, the seismic wave propagation problem is accomplished by numerically solving the partial differential equations of elastic wave propagation. A numerical approximation of these equations over the spatial domain can be realized by means of Finite Difference (FDM) [1], Finite Element (FEM) [2–4], Finite Volume (FVM) [5,6] and Spectral Element (SEM) [7,8] methods.

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In this work, we adopt FEM because the integro-differential formulation let to consider the elastic parameters with discontinuities and the free boundary conditions are automatically satisfied. Moreover, it exploits for non-structured meshes, that are suitable to numerically reconstruct the near surface geology, because they better reconstruct the topography of the site [9].

However, FEM usually requires huge computational resources, *i.e.*, a large amount of memory and a long computational time. For this reason, the large scale of the problem associated with modeling strong motion in 3D is usually managed by using techniques of high performance computing. Nevertheless, parallel platforms supporting FEM are difficult to built up. Indeed, a simulation based on FEM and on non-structured meshes involves indirect addressing to work with very large matrices. Further, an amiss load partitioning among processors may engender a high computational cost [2].

This paper deals with the investigation of the load balancing that can be obtained by solving a 3D seismic problem in a parallel computing environment. The seismic wave propagation is described by the heterogeneous elastic equations supplemented by suitable initial and boundary conditions (IBVP). Details on our model are provided in Section 2. With the aim to realize a parallel code for solving this problem, a suitable analysis of mesh partitioning and data parceling is here presented. The main idea behind our parallel approach is to split the global problem (that may be very large) in local ones that have the same structure as the original one but with a smaller size.

To this purpose, a significant support is given by two efficient tools available in the literature: *LaGrit*, to implement the mesh, and METIS, for the domain decomposition. In order to analyze *a priori* the load balancing, we introduce two performance indices: the index of *closing nodes* (CN) and the index of *node balancing* (NB). They depend on the number of grid nodes, processors and nodes shared by processors (called *overlapping nodes*). The CN index is used to estimate the size of local mass matrices, while the NB index gives information on the goodness of the node distribution among processors. In the last section of the paper, several experimental tests are discussed. They show that, analyzing the trend of the indices introduced above, it is possible to estimate *a priori* the optimal number of required processors according to the dimension of the problem.

## 2. The seismic wave propagation model

We introduce the mathematical formulation of the seismic wave propagation in heterogeneous media. Let  $\mathbb{R}^3$  be the three–dimensional real space and  $\mathbf{x} = (x, y, z) \in \mathbb{R}^3$  a generic vector; let f(x, y) be a regular function in  $\mathbb{R}^2$ , we define the 3D domain  $\Omega$  as

$$\Omega = \left\{ (x, y, z) \in \mathbb{R}^3 : z > f(x, y), (x, y) \in \mathbb{R}^2 \right\}$$

whose boundary

$$\partial \Omega = \left\{ (x, y, z) \in \mathbb{R}^3 : z = f(x, y), (x, y) \in \mathbb{R}^2 \right\}$$

describes the so-called *free-surface* of  $\Omega$ .

Then, the wave propagation is described by the following IBVP, for heterogeneous media, that is a simplification of the model presented in [10], without dissipation term,

(1) 
$$\begin{cases} \rho(\mathbf{x}) \frac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla \cdot \sigma + \mathbf{F}(\mathbf{x}, t), & \forall (\mathbf{x}, t) \in \Omega \times (0, +\infty) \\ \sigma = (\lambda(\mathbf{x}) + \mu(\mathbf{x})) \nabla \mathbf{u}, \\ \mathbf{u}(\mathbf{x}, 0) = 0, & \forall \mathbf{x} \in \Omega, \\ \frac{\partial}{\partial t} \mathbf{u}(\mathbf{x}, 0) = 0, & \forall \mathbf{x} \in \Omega, \\ \frac{\partial}{\partial \mathbf{n}} \sigma(\mathbf{x}, t) = 0, & \forall (\mathbf{x}, t) \in \partial\Omega \times (0, +\infty), \end{cases}$$

where **u** is the displacement, the functions  $\rho(\mathbf{x})$  (mass density),  $\lambda(\mathbf{x})$  and  $\mu(\mathbf{x})$  (the Lamé constants) characterize the elasticity of the medium, and  $\mathbf{F}(\mathbf{x},t)$  is the external forces; moreover, t is the time,  $\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$ , and **n** is the outward normal unit to  $\partial\Omega$ .

## 3. Numerical dicretization

We adopted the FEM to numerically integrate the IBVP defined in (1) on non-structured meshes with a step dh depending on the maximum frequency  $f_{max}$  and on the minimum wave velocity  $v_{min}$  in  $\Omega$  as follows:

$$dh = \frac{v_{min}}{n f_{max}}$$

where *n* represents the number of evaluations per wavelength needed to cover the minimum frequency for a non dispersive propagation, [25]. The various experimentation provided in [26] shows that n = 6 is a value that guarantees the accuracy of the numerical solution. In order to avoid the reflections at the boundary, we introduce the so-called *absorbing boundary* conditions [11–16], a numerical scheme that makes the perimeter of the

computational grid transparent to outward moving waves. In this case, we assumed the Caserta–Firmani–Ruggiero transparent conditions [3]. In the weak formulation we adopted the Galerkin method [17], yielding

(2) 
$$M^2 \frac{d^2 \mathbf{U}}{dt^2} + M^1 \frac{d \mathbf{U}}{dt} + M^0 \mathbf{U} = \mathbf{f}.$$

 $M^2$ ,  $M^1$  and  $M^0$  are sparse square matrices of order equal to 3 times the node number. Their entries are the integral on  $\Omega$  of a combination of the basis functions  $N(\mathbf{x})$  or their derivatives (see [18] for details).

The time discretization has been implemented through the Newmark method, [27,28] with time step  $\delta t \leq dh/v_{max}$ , and parameters  $\gamma_1 = 1/4$  and  $\gamma_2 = 1/2$ . The optimal choice of these parameters, has been largely investigated and discussed in [26]. So, we get

(3) 
$$\begin{cases} A\ddot{\mathbf{U}}^{n+1} = \mathbf{b}^{n+1}, \\ \dot{\mathbf{U}}^{n+1} = \dot{\mathbf{U}}^n + \delta t \left( (1 - \gamma_2) \ddot{\mathbf{U}}^n + \gamma_2 \ddot{\mathbf{U}}^{n+1} \right), \\ \mathbf{U}^{n+1} = \mathbf{U}^n + \delta t \dot{\mathbf{U}}^n + \frac{\delta t^2}{2} \left( (1 - \gamma_1) \ddot{\mathbf{U}}^n + \gamma_1 \ddot{\mathbf{U}}^{n+1} \right), \end{cases}$$

with

$$A = M^{2} + \gamma_{2} \delta t M^{1} + \gamma_{1} \frac{\delta t^{2}}{2} M^{0},$$
  
$$\mathbf{b}^{n+1} = \mathbf{f}^{n+1} - \left[ (1 - \gamma_{2}) M^{1} + \frac{\delta t^{2}}{2} (1 - \gamma_{1}) M^{0} \right] \ddot{\mathbf{U}}^{n} - (M^{1} + \delta t M^{0}) \dot{\mathbf{U}}^{n} - M^{0} \mathbf{U}^{n}.$$

#### 3.1. Mass matrix properties

In the following we refer to the matrix A defined above as mass matrix. Note that the matrix A is sparse and its entries corresponding to inner nodes are symmetric, while those corresponding to boundary ones are not symmetric. For this reason, we re-order the nodes: first of all, we tidy up the inner nodes and then, in queue, the boundary ones. Such a simple strategy allows us to minimize the matrix allocation, storing it by means of an innovative version of CSR format [19]. So, we actually store less than half of the entries of the mass matrix.

In Fig. 1, we show the sparsity of the matrix A with 1.728 nodes, after their re-ordering. It is characterized by an arrow structure, whose non symmetric part is delimited by red lines. The entries of A are  $(3 \cdot 1.728) \times (3 \cdot 1.728) = 26.873.856$ , and non-zero elements are 203.454. By adopting the strategy presented above, we only store 135.630 elements.

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Figure 1. Sparsity of the matrix A relative to a grid with 1728 nodes. The red lines represent the bound between inner and border nodes.

# 4. The parallel scheme

The complexity of simulating the wave propagation in wide and heterogeneous media, by adopting high frequencies, forces this problem to be dealt with high performance computing techniques. In fact, FEM usually requires huge resources, *i.e.*, a large amount of memory and a high computational cost, that may exceed the software and hardware capabilities of a monoprocessor. The time integration of the linear system (3) takes a long computational time in such a way that days are needed to simulate one minute of soil shaking even if the fastest optimized sequential algorithm is adopted. For this reason, in this section we present a novel parallel approach to decompose the original problem into sub-problems with smaller size. We adopt some tools available in the literature, such as LaGrit [20] and METIS [21], to achieve our goal. The discretization of the physical domain is obtained by using LaGrit, a library developed by Los Alamos National Security, LLC at Los Alamos National Laboratory (LANL) with the U.S. Department of Energy (DOE). The mesh generation uses a Delaunay tetrahedralization algorithm that respects material interfaces [22,23]. The obtained mesh is partitioned by adopting METIS. We have chosen this library because it is a good tool able to quickly produce high-quality partitions also for a wide grid. Moreover, by minimizing the edgecut, the applied partitioning algorithm also minimizes the connections between processors.

#### 4.1. Mesh partitioning

Once LaGrit generates the mesh, the set of its constituting elements are partitioned into *initial subdomains*, by using METIS. It is important to remark that the obtained sets of tetrahedra and nodes are disjoint. Then, to attain the *complete subdomains*, we add to the initial node partition the vertices of tetraedra which are not included yet. They are shared by more than one subdomain and are called *overlapping nodes*. Fig. 2 illustrates the result of the Delaunay tetrahedralization algorithm applied to a homogeneous cube with side L = 700 meters,  $v_{min} = 1,800$  Km/s and  $f_{max} = 15$ Hz. The overlapping nodes are pointed out.



Figure 2. 16464 elements are given by the Delaunay tetrahedralization of a homogeneous cube with side L = 700 meters,  $v_{min} = 1,800$  Km/s and  $f_{max} = 15$  Hz. As shown, they are distributed among 10 processors. Overlapping nodes are emphasized too.

## 4.2. Parceling

Once *initial subdomains* are achieved, our aim is to distribute them among processors. If the physical domain is homogeneous, each subdomain is mapped one-to-one into a processor. Note that it is important to generate a global-to-local map, which allows the identification of a node on a processor by its global label, and vice versa [2,24].

When *initial subdomains* are distributed among processors, each of them identifies the *overlapping nodes*, by means of an efficient procedure, and generates its *complete subdomain*. Then, the local mass matrix, which is a non-zero one with a symmetric pattern, is assembled. Nodes are re-ordered in such a way that the nodes lying on the physical domain, called *boundary nodes*, are enqueued. Thus, after a suitable re-ordering of local nodes, as described in the previous section, we can store only about half of the entries of the matrix, by means of the optimized CSR format.

All the local mass matrices have the same features of the global one. Indeed, the structure of the matrix and its properties are preserved. Thus, they are arrow matrices, with a symmetric pattern and diagonally dominant almost everywhere. For the sake of simplicity, we consider the mass matrix depicted in Fig. 1 and we split the original problem among 4 processors, so obtaining the local matrices shown in Fig. 3. In this case, the global matrix has  $1728 \times 1.728 = 2.985.984$  blocks  $3 \times 3$ , and only 22.606 entries are non-zero. The matrix in Fig. 3(a) has  $541 \times 541 = 292.681$  blocks  $3 \times 3$ , and only 6.317 entries are non-zero. The matrix in Fig. 3(b) has  $545 \times 545 = 297.025$  blocks  $3 \times 3$ , and only 6.427 entries are non-zero. The matrix in Fig. 3(c) has  $534 \times 534 = 285.156$  blocks  $3 \times 3$ , and only 6.266 entries are non-zero. The matrix in Fig. 3(d) has  $548 \times 548 = 300.304$  blocks  $3 \times 3$ , and only 6.426 entries are non-zero.

## 5. Numerical results

Once local mass matrices are stored, each processor solves the linear system (3) reduced to its own subdomain. The local solutions are assembled with the aim of reconstructing the global one. In particular, on the overlapping nodes we applied a weighted mean, where the weights are proportional to the node multiplicity in each subdomain. For this reason, it is important to know *a priori* the role played by the *overlapping nodes* in the decomposition of the problem among processors. In this section, we present some results on the load balancing associated with the mesh partitioning. With this aim, we study CN and NB indices.

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(a) Processor 0: local mass matrix



(c) Processor 2: local mass matrix



(b) Processor 1: local mass matrix



(d) Processor 3: local mass matrix

Figure 3. Sparsity of the matrices obtained by splitting the original problem among 4 processors. The red lines evidence the limit between inner and boundary nodes.

## 5.1. CN index

The CN index represents the mean of the overlapping nodes as a function of the number of nodes,

$$\beta = \frac{N_O}{N}$$

where

- $N_O$  is the total number of overlapping nodes assigned to each processor;
- N is the number of total nodes.

It gives information on how much the overlapping nodes weight upon the dimension of the local mass matrix. In fact, if the work–load is equally distributed among  $n_p$  processors, then the initial number of nodes on processor is  $N/n_p$ . For the sake of simplicity, we suppose that the number c of

overlapping nodes is the same on each processor. Thus, as  $c = \beta N/n_p$ , the size of local matrix A is

size(A) = 
$$\frac{N}{n_p} + c = \frac{N}{n_p} (1 + \beta)$$
.

We obtain an analogous result also when c is not constant.



Figure 4. CN index:  $\beta$  is the ratio of the total number of overlapping nodes and the total number of nodes. It is useful to estimate the dimension of local mass matrices. We present the trend of the parameter  $\beta$  versus the number of processors from 4 to 128. Several examples are shown fixing the number of the elements.

We remark that:

- if β = n<sub>p</sub> 1, we have the worst case, because each processor has N nodes. In fact each processor sends its local nodes to all the others. In other words, the set of overlapping nodes coincides with the set of total nodes with multiplicity n<sub>p</sub>.
- if  $\beta << 1$ , then the local matrix size is not much increased by the overlapping nodes in such a way that they do not weight on local matrix dimension and we get

size(A) 
$$\approx \frac{N}{n_p}$$
.

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Fig. 4 shows the trend of closing nodes versus the number of processors. Each line represents this parameter corresponding to a fixed number of nodes. The curves are increasing independently the node number. Anyway, the various experimental tests, we have carried out, show that a good arrangement between local mass matrix size and the number of employed processors occurs when  $\beta < 0.25$ .

## 5.2. NB index

The NB index represents the balance of node distribution among processors. It is given by

$$\alpha = \frac{N_t}{N \cdot n_p}$$

where

•  $N_t$  is the number of nodes counted with their multiplicity (an inner node has multiplicity 1, while an overlapping node has multiplicity equal to the number of processors sharing it);

• N is the number of total nodes;

•  $n_p$  is the number of processors.

The following points are worth of being underlined:

- if  $\alpha = 1$ , then the number of nodes distributed in each subdomain corresponds exactly to the number of total nodes. This is the *unbalanced case*. In fact, the local domain coincides with the global one, and then each processor solves the complete problem.
- if  $\alpha = 1/n_p$ , the nodes are uniformly distributed among each subdomain, so that they are exactly  $N/n_p$  in each processor. This means that the work-load is equally distributed among processors. Nevertheless, it is an ideal case because the set of overlapping nodes can not be empty.

Fig. 5 shows the trend of CN index versus the number of processors. Each curve represents this parameter corresponding to a fixed number of nodes. Note that the red star points identify the case  $\alpha = 1/n_p$ , that is the ideal one. As expected,  $\alpha$  approaches the ideal curve as the number of nodes increases. Anyway, the several tests performed show that when  $\alpha < 0.025$ , it is not necessary to increase the number of employed processors, according to the  $\beta$  results.

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Figure 5. NB index:  $\alpha$  is the ratio of the sum of nodes of each processor and the total nodes number times the number of processors. This parameter provides another evaluation of the matrix size growth caused by the overlapping nodes. We present the trend of the parameter  $\alpha$  versus the number of processors from 4 to 128. Several examples are shown fixing the number of nodes.

## 6. Conclusions

The aim of this work was to describe some preliminary results of our portable, computationally efficient and readable parallel code developed for simulating 3D wave propagation in heterogeneous media with arbitrary topography. For this reason, first of all we presented an accurate and *a priori* analysis of the performance and the work–load balance among processors. To do so, we introduced the *node balancing* and *closing node* indices. The numerical results presented in this work provide useful information to approach the ideal case of load balance and so determine the optimal number of required processors according to the dimension of the problem.

Our next step will be the implementation of a suitable parallel algorithm for solving the achieved local linear systems. Even though many tools for solving PDEs by using FEM currently exist, current work is in progress to optimize the solver associated with our type of problems. Preliminary numerical simulations have been performed showing that we can correctly and efficiently simulate the dynamics of interaction between the seismic radiation caused by earthquakes and the near surface geology. This will be the subject of a forthcoming paper.

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