Two-dimensional frequency-domain visco-elastic full waveform inversion: Parallel algorithms, optimization and performance

R. Brossier

Geôazur, Université de Nice-Sophia Antipolis - CNRS, 250 rue Albert Einstein, 06560 Valbonne, France

1. Introduction

Quantitative imaging of the subsurface is essential for geotechnical and civil engineering applications, for seismic hazard and natural resources exploration, and for our geodynamics knowledge. The physical properties of the subsurface are often estimated through seismic-wave analysis, with wave travel-times generally used to perform tomography of the Earth interior. In the 1980s, the full waveform inversion (FWI) method was introduced by Tarantola (1984) to exploit the complete information contained in the waveforms of seismograms, and to infer high-resolution models of the subsurface. FWI was originally developed in the time-domain (Tarantola, 1984, 1987), and it has become tractable and popular in the frequency-domain since the pioneering work of Pratt and Worthington (1990) and Pratt (1990). FWI is currently a field of active research, and particularly for active seismic surveys at various scales. Computationally efficient frequency-domain FWI was designed by limiting the inversion to a few discrete frequencies, taking advantage of the redundant wavenumber cover provided by wide-aperture surveys (Sigure and Pratt, 2004; Brenders and Pratt, 2007a). Frequency-domain FWI potentially provides high-resolution quantitative images of physical parameters, although it suffers from two main difficulties.

The first of these difficulties relates to the computational cost of the forward problem; namely, the numerical resolution of the wave equation in heterogeneous media for multiple sources. In two dimensions, the forward problem can be solved efficiently in the frequency-domain (Marfurt, 1984), leading to the resolution of a linear system per frequency, the right-hand side of which is the source. This system is solved efficiently for multiple sources with a direct solver, which performs one LU factorization of the matrix, followed by a forward and a backward substitution per source. For the acoustic wave equation, optimal finite-difference (FD) schemes have been designed for optimal use of the CPU core-memory when used with direct solvers (Jo et al., 1996; Hustedt et al., 2004). However, these optimal schemes are difficult to design for the elastic wave equation, because the numerical scheme directly depends on the Poisson ratio of the medium, which leads to stability issues when considering free-surface boundary conditions and liquid/solid interfaces (Stekl and Pratt, 1998). Moreover, FD suffers from the usual limitation linked to Cartesian regular grids: the grid interval is defined by the smallest propagated wavelength to avoid numerical dispersion, or by complex interface geometries, which require fine discretization to avoid parasite diffractions from the corners of the Cartesian grid. These two constraints generally
lead to local oversampling of the medium, and therefore a waste of computational resources (Saenger and Bohlen, 2004; Bohlen and Saenger, 2006). To deal with non-regular grids, finite element (FE) methods can be considered with either low interpolation orders (Marfurt, 1984; Bielak et al., 2003), or high interpolation orders, using the so-called spectral element method (Komatitsch and Vilotte, 1998; Chaljub et al., 2003). These methods require, however, explicit boundary conditions for modelling the water/solid contact, and are generally developed for quadrangle grids, which leads to meshing issues. Another alternative is the finite element discontinuous Galerkin (DG) method (Käser and Dumbser, 2006; Dumbser and Käser, 2006; Brossier et al., 2008). This DG method allows for the use of triangular/tetrahedral meshes, and it is suitable for the handling of strong physical contrasts in the medium, including liquid/solid contact. The DG method is chosen in the present study to perform the FWI forward problem in the frequency-domain.

The second difficulty of FWI is related to the ill-posedness and nonlinearity of the inverse problem, which is generally formulated as a least-squares local optimization (Tarantola, 1987; Pratt and Worthington, 1990), so as to manage the numerical cost of the forward problem. The ill-posedness of FWI mainly arises from the lack of low frequencies in the source bandwidth and the incomplete illumination of the subsurface provided by conventional seismic surveys. Consequently, the problem is highly non-linear and the results strongly depend on the accuracy of the starting model in the framework of local optimization and on the presence of noise. Several hierarchical multi-scale strategies that proceed from low frequencies to higher frequencies have been proposed to mitigate the nonlinearity of the inverse problem (Pratt and Worthington, 1990; Bunks et al., 1995; Sigurge and Pratt, 2004; Brossier et al., 2009a). Subsets of data and parameter classes can also be hierarchically inverted to mitigate the nonlinearity and nonuniqueness issues in the framework of elastic inversion (Sears et al., 2008; Brossier et al., 2009b).

To tackle targets of realistic size and complexity with FWI, efficient algorithms must be implemented for modern computational platforms for both the forward and the inverse problems. An example of such algorithms is presented in Sourbier et al. (2009a), who implemented a parallel FWI algorithm for large-scale distributed-memory platforms in the framework of the two-dimensional (2D) acoustic monoparameter approximation, with a FD forward problem and steepest-descent-based optimization scheme.

The present study presents the implementation of a massively parallel frequency-domain FWI algorithm for imaging 2D viscoelastic media. The second section will focus on the forward problem solution, as performed with a low-order DG method. In the third section, the inversion algorithm is presented, with special emphasis on the reconstruction of multi-parameter classes from vectorial wavefields using a quasi-Newton method. The last section will review the parallel implementation of the algorithm, with an analysis of its performance on a distributed-memory platform.

### 2. Forward problem

#### 2.1. Theory and discretization

Two-dimensional, elastic, frequency-domain FWI requires the frequency-domain solutions of the 2D P-SV wave equations for heterogeneous media and multiple sources. We consider the first-order hyperbolic system where both particle velocities \((V_x, V_z)\) and stresses \((\sigma_{xx}, \sigma_{zz}, \sigma_{xz})\) are unknown quantities, as described by the system:

\[
-\frac{i}{\omega}V_x = \frac{1}{\rho(x)} \left\{ \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xz}}{\partial z} \right\} + f_x
\]

\[
-\frac{i}{\omega}V_z = \frac{1}{\rho(x)} \left\{ \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{zz}}{\partial z} \right\} + f_z
\]

where \(\lambda\) and \(\mu\) are the Lame coefficients, \(\rho\) is the density, and \(\omega\) is the angular frequency. Source terms are either point forces \((f_x, f_z)\) or applied stresses \((\sigma_{xx0}, \sigma_{zz0}, \sigma_{xz0})\). The symbol \(i\) denotes the purely imaginary term defined by \(i = \sqrt{-1}\). Only isotropic media are considered in this analysis. The intrinsic attenuation of the medium is easily taken into account in the frequency-domain using complex-valued wave velocities. In the present study, the Kolsky–Futterman model (Kolsky, 1956; Futterman, 1962) without the dispersion term is considered in this analysis. The intrinsic attenuation of the medium is easily taken into account in the frequency-domain using complex-valued wave velocities. In the present study, the Kolsky–Futterman model is used (Toksöz and Johnston, 1981). Please note, however, that the dispersion term could be included without extra cost in the formulation.

A change in variable is applied to the system of Eqs. (1) to develop a pseudo-conservative formulation that is useful for the derivation of the DG formulation. We now consider the following vector with three components \((T_1, T_2, T_3) = (\sigma_{xx} + \sigma_{zz})/2, (\sigma_{xx} - \sigma_{zz})/2, \sigma_{xz}/2\).

Note that, when considering this variable change, \(T_1\) represents the hydrostatic pressure measured in liquids. In the case of liquid/solid propagation, such as in marine seismic experiments, the \(T_1\) variable provides direct access to the pressure measured by hydrophones, while \(T_2\) and \(T_3\) are zero in liquid, relative to the deviatoric part of the stress tensor.

Moreover, we must consider a finite domain, and therefore, we apply perfectly matched layer (PML) absorbing conditions (Berenger, 1994) through the functions \(s_x, s_z\), defined in the direction \(r\) as \(s_r = 1/(1 + j\gamma_r/\omega)\), where \(\gamma_r\) is zero inside the computational domain and nonzero inside the absorbing layers. The new differential system that includes the PML functions, which is equivalent to the system of Eqs. (1), can be written as

\[
-\frac{i}{\omega}pV_x = s_x \left( \frac{T_1 + T_2}{\rho} \right) + s_z \left( \frac{T_1}{\rho} \right) + \rho f_x
\]

\[
-\frac{i}{\omega}pV_z = s_z \left( \frac{T_3}{\rho} \right) + s_z \left( \frac{T_2}{\rho} \right) + \rho f_z
\]

\[
-\frac{i}{\omega}T_1 = s_x \left( \frac{\partial V_x}{\partial x} + \frac{\partial V_z}{\partial z} \right) - \frac{i\omega}{\lambda + \mu} T_1
\]

\[
-\frac{i}{\omega}T_2 = s_z \left( \frac{\partial V_x}{\partial x} - \frac{\partial V_z}{\partial z} \right) - \frac{i\omega}{\mu} T_2
\]

\[
-\frac{i}{\omega}T_3 = s_z \left( \frac{\partial V_x}{\partial x} + \frac{\partial V_z}{\partial z} \right) - \frac{i\omega}{\mu} T_3
\]

To derive the DG formulation, the model is first discretized with polygonal cells. For each cell, the system of Eqs. (2) is multiplied by a low-order DG method based on Lagrange polynomials that can be easily defined and integrated on triangle shapes. The system of Eqs. (2) is then integrated over each cell, which leads to the so-called weak formulation of the system. We assume that the physical properties of the medium are constant inside each cell, and we use centred numerical fluxes to exchange energy between cells (Remaki, 2000). The reader is referred to Käser and Dumbser (2006), Dumbser and Käser (2006), Brossier et al. (2008), and Käser and Dumbser (2006).
Etienne et al. (2010) for a detailed description of the DG formulation applied to the elastodynamic equations.

Discretization of Eqs. (2) with the DG method leads to a linear system for each frequency considered:

\[
Au = s,
\]

where \( A \) is the sparse impedance matrix, which is also known as the forward problem operator, and which depends on the frequency, the mesh geometry, the DG interpolation order of each cell, and the physical properties. The right-hand side \( s \) represents the external excitation. The unknown vector \( u \) contains the particle velocity and the stress wavefields in the entire computational domain, and is represented by a local polynomial inside each cell. In the present study, the system of Eqs. (3) is solved with the massively parallel direct solver MUMPS (Amestoy et al., 2006). More details on this algorithm and its performance will be discussed in Section 4.1.

Note that visco-acoustic modelling and inversion can be performed using the elastic algorithm: the fourth and fifth lines of system 2 are not considered in the forward problem; the \( T_2 \) and \( T_3 \) wavefields are forced to zero; and \( V_S \) is set to zero.

### 2.2. Which interpolation?

The theoretical resolution of the FWI is \( \lambda/2 \) if normal-incidence data are recorded, where \( \lambda \) is the local propagated wavelength (Sirgue and Pratt, 2004). A suitable discretization for the inversion mesh should therefore be close to \( \lambda/4 \) to ensure a correct sampling of the medium. Since the physical properties are assumed to be constant inside each cell, a suitable discretization of the forward problem based on the same mesh as that of the inversion should also be close to \( \lambda/4 \) (Sournier et al., 2009a).

DG methods generally take advantage of high orders of interpolation to coarsely discretize the medium and to obtain a high order of accuracy (Käser and Dumbser, 2006; Dumbser and Käser, 2006). In contrast, I will focus here on low interpolation orders for FWI applications because these low orders of interpolation will provide the best compromise between accuracy and computational cost of the forward problem for the discretization imposed by the FWI resolution.

The lowest interpolation order, \( P_0 \) (Brossier et al., 2008), is a possible choice that represents the wavefield by a series of piecewise constant functions inside each cell, and it gives sufficiently accurate solutions for 10–15 cells per wavelength in unstructured triangular meshes. \( P_0 \) interpolation cannot, however, be used on unstructured meshes, where it does not converge to the correct solution, whatever the size of the cell. Moreover, the liquid/solid interface causes some numerical instabilities for structured meshes, and the \( P_0 \) interpolation cannot, therefore, be used in this case. Finally, the \( P_0 \) scheme can be related to the finite volume \( P_0 \) scheme, and is very close to \( O(\Delta x^2) \) FD schemes.

The higher orders of interpolation, \( P_1 \) and \( P_2 \), allow for the use of unstructured meshes, which is an appealing feature for dealing with complex topographies and heterogeneous media, which should require a local adaptation of the mesh size to the local properties (h-adaptive mesh). Sufficiently accurate solutions can be obtained in unstructured meshes with discretization of 10–15 cells per wavelength for \( P_1 \), and three to three and a half cells per wavelength for \( P_2 \). Note that for inversion, \( P_2 \) should be oversampled with four cells per wavelength to correctly sample the medium and mitigate errors in the gradient building (see Section 3.3).

Seismograms computed with the DG \( P_1 \) and DG \( P_2 \) in a homogeneous halfspace are compared with the analytical solution of the Garvin (1956) problem (Figs. 1 and 2). The source is an explosion at depth and the receivers are on the free surface. The comparison is performed in the time-domain, from DG solutions computed in the frequency-domain. To assess the accuracy of the surface wave and of the direct wave, I have here used a discretization of 12 cells and three cells per minimum wavelength in unstructured triangular meshes for \( P_1 \) and \( P_2 \) interpolations, respectively. The comparison between the DG and analytical seismograms shows that sufficiently accurate solutions for both wave types are achieved for these discretizations. For the Garvin test computed in the frequency-domain at 5 Hz, Fig. 3 reviews the accuracy of the three interpolation orders as functions of the mesh size.

The \( P_2 \) interpolation provides the best consistency between the discretizations required by the forward problem to compute sufficiently accurate solutions (Figs. 2 and 3) and the spatial resolution of FWI (i.e., the mesh interval corresponding to a quarter of a wavelength), considering my formulation based on constant properties per cell. Higher orders of interpolation would allow one to use coarser meshes for the same level of accuracy, but these coarse meshes would lead to an undersampling of the medium for FWI. Therefore, high orders of interpolation should be applied on unnecessarily fine meshes, at the expense of the computational efficiency, and should, therefore, be rejected for FWI applications. As I will illustrate later, lower orders of interpolation (i.e., \( P_0 \) and \( P_1 \)) can, however, be useful as an alternative to \( P_2 \), depending on the medium properties. Please note that, if heterogeneous properties were considered in cells, higher orders of interpolation could lead to more computationally-efficient modelling engines for FWI. This approach has not been investigated so far.

For computational efficiency, an interesting feature of the DG method is the possibility of mixing the interpolation orders (p-adaptivity), because the degrees of freedom are not shared by
neighbouring cells in the DG formalism. An efficient mix is seen in $P_0$-$P_1$, because both interpolations share the same discretization rule (i.e., 10 cells per wavelength), and therefore, they facilitate the meshing at the transition zones between the $P_0$ and $P_1$ interpolations.

Table 1 summarizes the computational time and memory requirements for the DG method for two simple models, where the $P_0$, $P_1$, $P_0$-$P_1$ and $P_2$ orders of interpolation are used. These have, respectively, a discretization of: 10 cells per minimum wavelength in a structured equilateral mesh; 10 cells per local wavelength in an unstructured $h$-adaptive mesh; 10 cells per local wavelength with a structured/unstructured $hp$-adaptive mesh; and three cells per local wavelength in an unstructured $h$-adaptive mesh. It is worth remembering that these four combinations of interpolation order and discretization give similar accuracies (Fig. 3). Simulations are performed in parallel using 16 processors. The first model is a homogeneous half space, and the second one is a two-layer half space. The first simulation clearly shows that the $P_0$ interpolation on the regular mesh provides the best time and memory performances when the model contains a limited range of velocity. In the second model, the thickness of the upper layer is one tenth of the thickness of the half space, and the velocity in the upper layer is one tenth of the velocity of the lower layer. The upper layer mimics a complex weathering zone in the near surface, which requires a very fine mesh and, therefore, a dramatic increase in the number of cells when regular structured meshes are used (as it should also be with FD). The $P_0$-$P_1$ mesh uses $h$-adaptive unstructured cells ($P_1$) in the upper layer and structured equilateral cells ($P_0$) in the lower layer. In this case, the $P_2$ interpolation on the $h$-adaptive unstructured mesh provides the best time and memory performances, due to the local refinement of the mesh (Table 1). These two extreme canonical cases illustrate how the heterogeneity and the velocity range of the subsurface drive the choice of the mesh type and interpolation order. In the case of a broad velocity bandwidth in the model, $P_2$ interpolation used with $h$-adaptive unstructured meshes should give the best parameterization. In the case of a narrow velocity bandwidth, the $P_0$ or the $P_0$-$P_1$ interpolations should be more relevant. If a flat free surface is present without liquid, the $P_0$ interpolation can be used, while the $P_0$-$P_1$ interpolation should be used when the model contains a liquid/solid interface in a shallow water environment or a complex topography above a shallow weathered layer. For example, a layer of unstructured cells computed with $P_1$ allows discretization of a complex topography or water/solid interface of arbitrary shape, above a $P_3$ regular equilateral mesh, discretizing a more homogeneous medium. The $P_0$-$P_1$ approach is close in spirit to the hybrid FE/FD method proposed by Moczo et al. (1997). We can, however, note that the $P_1$ interpolation used alone never appears to be the optimal choice.

Figs. 4–6 further illustrate the mesh design for three realistic offshore and onshore models. The first represents a velocity model of the Valhall gas field in a shallow-water environment in the North Sea (Munns, 1985). The sea bed is at 70-m depth. The narrow velocity range in most parts of the model requires the use of a regular mesh as much as possible for computational efficiency. To correctly discretize the shallow-water layer, a $p$-adaptivity implemented with a mixed $P_0$-$P_1$ interpolation is chosen: a refined unstructured $P_1$ layer of cells is used for the first 130 m of the subsurface for accurate modelling of the interface waves at the liquid/solid interface, and for accurate positioning of the sources, which are located 5 m below the surface, and of the receivers, which are on the sea bed. The second example represents an onshore foothill model that contains a complex topography, several dipping structures, and a thin weathered layer at the surface (Vp = 700 m/s, Vs = 350 m/s): a dramatic configuration for regular grid-based methods. An $h$-adaptive unstructured mesh that is suitable for the $P_2$ interpolation order was designed for accurate modelling of the free-surface effects of the topography, and for the local adaptation of the cell size to the local wave speeds. The third example corresponds to a crustal-scale model, which represents the Nankai subduction zone, offshore of Japan (Operto et al., 2006). We use a $P_2$ $h$-adaptive unstructured mesh to deal with the broad velocity bandwidth spanned by the crustal model. For FWI applications in such kind of environments, the $hp$-adaptive approach is more relevant. If a flat free surface is present without liquid, the $P_0$ interpolation can be used, while the $P_0$-$P_1$ interpolation should be used when the model contains a liquid/solid interface in a shallow water environment or a complex topography above a shallow weathered layer. For example, a layer of unstructured cells computed with $P_1$ allows discretization of a complex topography or water/solid interface of arbitrary shape, above a $P_3$ regular equilateral mesh, discretizing a more homogeneous medium. The $P_0$-$P_1$ approach is close in spirit to the hybrid FE/FD method proposed by Moczo et al. (1997). We can, however, note that the $P_1$ interpolation used alone never appears to be the optimal choice.

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Fig. 2. Time-domain comparison between DG $P_2$ (solid lines) and analytical (dashed lines) solutions for the Garvin test. The seismograms represent: (a) the horizontal and (b) the vertical components of the particle velocity at the free surface.

Fig. 3. Relative L2 error ($||u_{ex}-u||^2/||u_{ex}||^2$) at the free surface between the analytical solution ($u_{ex}$) and the numerical solutions ($u$) computed with the DG $P_0$, $P_1$, and $P_2$ interpolation orders as a function of the mesh size. The relative L2 error is computed for the 5 Hz frequency, and for the horizontal and vertical geophone components.
strategies just mentioned can be used during the forward modelling. The unstructured mesh is designed before inversion according to the velocity distribution in the starting model. As the velocity model is updated over FWI iterations, a quality control of the mesh can be necessary to check that the discretization criterion of the forward problem is still satisfied. If not, a remeshing can be necessary to locally refine the mesh according to the velocity update. This quality control and the remeshing are not automated so far and require human intervention. The meshing and remeshing steps are performed with Triangle software (Shewchuk, 1996) that allows a local control of cells size.

### Table 1

<table>
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<tr>
<th>Test</th>
<th>Resource</th>
<th>$P_0$</th>
<th>$P_1$</th>
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<th>$P_2$</th>
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<td>136 724</td>
<td>116 363</td>
<td>12 222</td>
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<td>695 795</td>
<td>366 660</td>
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<td>4.1</td>
<td>9.4</td>
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<td>19.80</td>
<td>3.09</td>
<td>4.57</td>
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<td></td>
<td>Time to solve 116 RHS (s)</td>
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<td>28.3</td>
<td>8.1</td>
<td>6.1</td>
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<td>Two-layers</td>
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<td>291 577</td>
<td>247 303</td>
<td>32 664</td>
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<tr>
<td></td>
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<td>4 373 655</td>
<td>2 360 405</td>
<td>979 920</td>
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<td></td>
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<td>109.5</td>
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<td>72.4</td>
<td>30.2</td>
<td>16.2</td>
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</table>

Fig. 4. The synthetic Valhall P-wave velocity model representative of oil and gas shallow water targets, and a close-up of the mesh used for mixed DG $P_0-P_1$ simulations.

Fig. 5. The synthetic IFP/TOTAL Foothill P-wave velocity model representative of onshore targets with complex topographies and weathering zones, and a close-up of the mesh for DG $P_2$ simulations.

Fig. 6. The crustal P-wave velocity model representative of the Japanese Nankai trough, and a close-up of the $h$-adaptive unstructured mesh for DG $P_2$ simulations.

### 3. Inverse problem

#### 3.1. Theory review

We start with a brief review of FWI. A more extensive overview is presented in Virieux and Operto (2009). FWI is an optimization problem that is generally recast as a local non-linear least-squares problem that attempts to minimize the misfit between the recorded and the modelled wavefields (Tarantola, 1987). The inverse problem can be formulated in the frequency-domain (Pratt and Worthington, 1990), and the associated objective function to be minimized is
Algorithm 1. Two-level hierarchical frequency-domain FWI algorithm

1: \( \text{for } ig = 1 \text{ to } ng \text{ do} \)
2: \( \text{for } id = 1 \text{ to } nd \text{ do} \)
3: \( \text{while (NOT convergence AND } n < n_{\text{max}}) \text{ do} \)
4: \( \text{for } if = 1 \text{ to } nf \text{ do} \)
5: \( \text{Compute incident wavefields } u \text{ from sources} \)
6: \( \text{Compute residual vectors } \Delta d \text{ and cost function } C \)
7: \( \text{Compute back-propagated wavefields } w \)
8: \( \text{Build gradient vector } g^{(n)} \text{ (with Algorithm 2)} \)
9: \( \text{end for} \)
10: \( \text{Compute perturbation vector } \Delta m^{(n)} \text{ (with Algorithm 3)} \)
11: \( \text{Define optimal step length } \alpha^{(n)} \text{ by parabola fitting} \)
12: \( \text{Update model } m^{(n+1)} = m^{(n)} + \alpha^{(n)} \Delta m^{(n)} \)
13: \( \text{end while} \)
14: \( \text{end for} \)
15: \( \text{end for} \)

This algorithm was applied successfully for imaging the elastic parameters of onshore and offshore synthetic data in Brossier et al. (2009a, b).

3.3. Gradient computation

The gradient computation with the adjoint-state method is described formally by Eq. (7). For computational time and memory use efficiency, some adaptations and approximations can be applied to compute the gradient vector.

Let me first introduce several notations. The matrix \( A_1 \) denotes the impedance matrix resulting from the discretization of the first-order velocity/stress formulation of the elastodynamic equations (Eq. (2)). The matrix \( A_2 \) denotes the impedance matrix resulting from the discretization of the second-order velocity formulation of the elastodynamic equations. This matrix can be derived from the first-order velocity/stress system through a parsimonious formulation (Luo and Schuster, 1990), as developed in Brossier et al. (2008)
for DG $P_0$. Note, however, that building the $A_2$ matrix through the parsimonious formulation is more complicated for higher order of interpolation, particularly when $p$- adaptivity is used. This complexity drove me to perform the forward problem with the first-order matrix $A_1$. Subscript $p_k$ denotes the $k$ order of interpolation used during forward problem modelling. The projection matrix $P_{p_k}$ interpolates a $p_k$ wavefields vector at the barycentre of each cell, giving a $p_k$-representation of fields. Finally the restriction operator $P_k$ allows one to extract only the velocity components from a velocity/ stress wavefield vector.

Considering these notations, Eq. (7) can be rewritten as

$$G_m = - \sum_{\theta = 1}^{nf} \sum_{i=1}^{ni} \partial_i \left\{ u_{p_k} \frac{\partial A_1^T}{\partial m_l} T_{p_k} \right\}$$

(9)

Because the first-order velocity/stress and the second-order velocity systems are theoretically equivalent for the computing of the velocity wavefields, Eq. (9) can be rewritten, without approximation, as

$$G_m = - \sum_{\theta = 1}^{nf} \sum_{i=1}^{ni} \partial_i \left\{ u_{p_k} P_{p_k} \frac{\partial A_2^T}{\partial m_l} P_{p_k} T_{p_k} \right\} = - \sum_{\theta = 1}^{nf} \sum_{i=1}^{ni} \partial_i \left\{ u_{p_k} \frac{\partial A_2^T}{\partial m_l} T_{V/p_k} \right\}$$

(10)

This expression allows one to compute the gradient $\nabla$ considering only the velocity wavefields ($u_{p_k}$, $T_V$), the stress wavefields are therefore not required. Since the incident and adjoint wavefields are stored in core-memory for all the sources in the algorithm, a reduction of the memory storage of the wavefields by a factor two and a half is obtained keeping only velocity wavefields.

Since the matrix $A_2$ is difficult to build for $P_1$ and $P_2$ interpolation orders, Eq. (10) is not used in practice. Instead, we perform the modelling with the first-order velocity–stress matrix $A_1$, as mentioned above and extract the modelled data $d_{calc}$ at receiver positions (either, the pressure or the particle velocities depending whether the hydrophone or the geophone components are inverted) for each source before deleting the stress wavefields for gradient computation. Second, we use a $P_0$ radiation pattern matrix $\partial A_2/\partial m_l$ instead of a $P_k$ one, because the second-order impedance matrix $A_2$ is easier to build. The $P_0$ representation of the radiation pattern requires to project the $P_k$ incident and the $P_k$ adjoint velocity wavefields onto the $P_0$ mesh. This projection step leads to an additional saving of memory and computational time compared to that achieved with Eq. (10).

This leads to the following approximate expression of the gradient:

$$G_m = - \sum_{\theta = 1}^{nf} \sum_{i=1}^{ni} \partial_i \left\{ u_{p_k} P_{p_k} \frac{\partial A_2^T}{\partial m_l} P_{p_k} P_{V/p_k} T_{V/p_k} \right\}$$

$$= - \sum_{\theta = 1}^{nf} \sum_{i=1}^{ni} \partial_i \left\{ u_{p_k} \frac{\partial A_2^T}{\partial m_l} T_{V/p_k} \right\}$$

(11)

The approximation of the gradient, resulting from the $P_0$ projection of the $P_k$ incident and adjoint wavefields and from the $P_0$ radiation pattern matrix on coarse mesh, can be justified by the fact that the gradient computation does not need to be discretized with the same order of accuracy as the impedance matrix used in the forward problem (Sourbier et al., 2009b). This approximation allows one to save a factor of three and six, both in computational time to build the gradient and in core-memory to store the velocity wavefields, when the forward problem is solved with DG $P_1$ and $P_2$, respectively. This approximation introduces, however, some errors in the gradient. In the unfavourable case of $P_0$ interpolation and coarse meshes of four cells per wavelength, these errors have been estimated to be less than nine percents on individual sensitivity kernels, which affects marginally the inversion results in the framework of iterative FWI. Please note, however, that only the incident and adjoint wavefields are $P_0$ projected for gradient building. The data residual $Ad$ is computed without approximation using the $k$ interpolation order before the $P_k$ modelling of the adjoint wavefield.

Finally, the gradient vector is computed through Eq. (11) with Algorithm 2.

**Algorithm 2.** Algorithm of gradient computation

1: for $m = 1$ to $m_{dis}$ do
2: Compute $\partial A_2^T/\partial m_l$ through full vector/sparse matrix product routine
3: for $is = 1$ to $ns$ do
4: Compute $\beta \leftarrow (\partial A_2^T/\partial m_l)u_{V/p_k}$ through full vector/sparse matrix product routine
5: Compute $G_m \leftarrow G_m - \partial (\beta \cdot T_{V/p_k})$ with sparse vector/full vector dot product routine
6: end for
7: end for

3.4. L-BFGS and multi-parameter inversion

FWI is generally solved with the steepest-descent or conjugate-gradient methods, preconditioned by a diagonal approximation of the Hessian (Pratt et al., 1998; Operto et al., 2006; Shin et al., 2001). Limited-memory, quasi-Newton methods, such as the limited-memory Broyden–Fletcher–Goldfarb–Shanno (L-BFGS) method (Nocedal, 1980), can, however, provide an efficient alternative to classic steepest-descent or conjugate-gradient methods for FWI problems (Epanomeritakis et al., 2008; Symes, 2008; Brossier et al., 2009a).

The Hessian matrix allows for: correction of the gradient from the geometrical amplitude spreading of the incident and adjoint wavefields; improvement of the imaging resolution by correctly deconvolving the gradient from limited-bandwidth effects, taking into account the off-diagonal terms of the Hessian; suitable scaling of the model perturbation vector for different parameter classes; and accounting for double scattering effects (Pratt et al., 1998; Nocedal and Wright, 1999). L-BFGS provides an approximation of the inverse $H$ of the Hessian matrix from few gradient and model difference vectors, stored from previous iterations. Moreover, the double-loop recursive algorithm designed by Nocedal (1980) does not explicitly build and store $H^{-1}$, but directly computes the perturbation vector $\Delta m_l = -H^{-1}G_m$ with additions, differences and inner products of vectors. A diagonal approximation of the inverse Hessian computed from the diagonal terms of the approximate Hessian (Pratt et al., 1998; Operto et al., 2006) or pseudo-Hessian (Shin et al., 2001), can be provided to the L-BFGS algorithm for a better and faster estimation of $H^{-1}G_m$.

In the framework of the inversion of multiple classes of parameter with different units and amplitudes (for example, reconstruction of wave speeds, density, attenuation factors), the L-BFGS algorithm requires some normalizations for consistent dimensionless computation of the model perturbation vector. Algorithms 3 and 4 review the computation of the perturbation model with appropriate normalizations that account for the different classes of parameters in the L-BFGS algorithm (Nocedal, 1980, modified following Gratton (personal communication)). The normalization of the gradient, the diagonal Hessian, and the perturbation model are performed according to a characteristic value $m_{dis}$ that is defined for each parameter class, taken as the mean of the initial model of each parameter class. This normalization is
equivalent to the computation of the gradient and the diagonal Hessian for normalized parameters \( m_i/m_0 \), where \( i \) denotes the parameter class.

**Algorithm 3.** Perturbation computation: outer part

1. if \( n = 1 \) then
2. Compute diagonal of pseudo-Hessian \( B_0 \) (Shin et al., 2001)
3. for \( l = 1 \) to \( n_{\text{parameter, class}} \) do
4. Normalize diagonal of Hessian \( B_{m, m} = B_{m, m} m_0^2 \)
5. end for
6. Apply damping to the diagonal of Hessian (Levenberg–Marquardt method) \( B_0 = B_0 + \alpha I \)
7. end if
8. for \( l = 1 \) to \( n_{\text{parameter, class}} \) do
9. Normalize gradient \( \tilde{\eta}_m^{(n)} = \tilde{\sigma}_m^{(n)} m_0 \)
10. end for
11. Compute \( \tilde{\eta}^{(n)} = B_0^{-1} \tilde{\sigma}^{(n)} \)
12. if \( n > k \) then
13. Discard the vector pair \( (y_{n-k-1}, s_{n-k-1}) \)
14. end if
15. if \( n > 1 \) then
16. Compute and store \( s_{n-1} = m^{(n)} - m^{(n-1)} \)
17. Compute and store \( y_{n-1} = \tilde{D}^{(n)} - \tilde{D}^{(n-1)} \)
18. end if
19. Compute \( \delta m^{(n)} \) with Algorithm 4
20. for \( l = 1 \) to \( n_{\text{parameter, class}} \) do
21. Denormalize perturbation vector \( \delta m^{(n)} = \tilde{\delta} m^{(n)} m_0 \)
22. end for

**Algorithm 4.** Perturbation computation: L-BFGS algorithm (Nocedal and Wright, 1999, p. 178), modified following Gratton

1. \( q \leftarrow \tilde{D}^{(n)} \)
2. for \( i = n - 1 \) to \( n - k \) do
3. \( \rho_i \leftarrow \sqrt{y_i/s_i} \)
4. \( z_i \leftarrow \rho_i z_i q \)
5. \( q \leftarrow q - z_i y_i \)
6. end for
7. \( \gamma_n \leftarrow \rho_n y_n^{(n)} \)
8. \( r \leftarrow \gamma_n q \)
9. for \( i = n - k \) to \( n - 1 \) do
10. \( \beta \leftarrow \rho_i y_i r \)
11. \( r \leftarrow r + s_i (z_i - \beta) \)
12. end for
13. \( \hat{\delta} m^{(n)} = -r \)

Fig. 7 shows the FWI results in a canonical configuration: 113 horizontal point force sources are located all around the target each 50 m, and each source wavefield is recorded by 112 two-component geophones all around the target each 50 m. Absorbing boundary conditions are used on the four sides of the domain to simulate an infinite medium. The true models contain one circular heterogeneous of 200 m diameter at different locations for each of the five parameters: P-wave and S-wave velocities (\( V_P \) and \( V_S \)), density (\( \rho \)), and P-wave and S-wave quality factors (\( Q_P \) and \( Q_S \)) (Fig. 7). Table 2 summarizes the background and heterogeneity values for each parameter. The inversion is performed for 10 frequencies between 4 and 13 Hz each 1 Hz, starting from homogeneous background models. The inverted parameters are \( \lambda \), \( \mu \) (the Lamé parameters), \( \mu_0 \), \( Q_P \), and \( Q_S \), to deliberately invert parameters with contrasted amplitudes (\( Q_P \) and \( Q_S \) \( \sim 10^4 \) \( \sim 10^6 \) while \( \lambda \) and \( \mu \) \( \sim 10^8 \) \( \sim 10^9 \)). Despite these differences, the normalization procedure allows for a correct estimation of the Hessian through L-BFGS, and allows for a convergence towards acceptable models without any need for heuristic weighting of each parameter class. Note that the weighting provided by the inverse Hessian estimation does not require the performing of extra forward problems, whereas the subspace method of Sambridge et al. (1991), which is generally used in multi-parameter inversions, requires the performing of one extra forward problem per parameter class to estimate the steplength. Note, however, that in Fig. 7 there are some coupling effects between some parameters that result from the physics of the diffraction pattern of each parameter class, and not from the choice of the optimization method.

The algorithm allows one to reconstruct one quality factor for each wave type (\( Q_P \) and \( Q_S \)). A non-dispersive attenuation model is currently used for both modelling and inversion. A dispersive model, as the Kolsky–Futterman model (Kolsky, 1956; Futterman, 1962), could, however, be taken into account without extra computational cost. Note, however, that reliable reconstruction of attenuation factors from seismic data is a difficult task that strongly depends on acquisition geometry (Mulder and Hak, 2009). A detailed analysis of the ability of my algorithm to reconstruct attenuation is beyond the scope of this paper.

The reader can refer to Brossier et al. (2009a, b) for realistic applications of that strategy to onshore and offshore synthetic data from the imaging of P-wave and S-wave velocity models.

**4. Parallelization and performance**

To tackle imaging of realistically sized targets, the computationally demanding FWI method needs to be implemented in parallel to exploit multiple CPU facilities, also with a large amount of available core-memory, compared to sequential execution.

**4.1. Forward problem**

The forward problem of FWI, as the resolution of the linear system of Eq. (3) for multiple sources (right-hand-side (RHS)), is performed with the massively parallel direct solver MUMPS (Amestoy et al., 2006), which performs a LU decomposition of the matrix \( A \), based on a multi-frontal approach (Duff and Reid, 1983). The parallelization allows for the speeding up of the factorization by more than one order of magnitude, compared to sequential execution, and for the distribution of the LU factors in the core-memory over all of the processors ( Sourbier et al., 2009b), which makes this quite efficient for solving large problems without intensive I/O resources. The MUMPS software is based on message passing interface (MPI) standards for applications with distributed memory architectures. The workflow of the MUMPS algorithm can be summarized as: (1) analysis of the \( A \) matrix pattern (note that unknowns are treated independently in the current version of the algorithm, without taking advantage of the block structure provided by elements), followed by reordering of the matrix to limit the fill-in during factorization. The analysis step is performed sequentially on the master processor with the current MUMPS version (but does not modify the workflow if done in parallel); (2) parallel factorization of the \( A \) matrix with dynamic pivoting; (3) parallel forward and backward substitutions to obtain solution vectors \( u \) from RHS vectors \( b \).
of the sparse matrix are therefore not suitable for the application of the projection operator because the MUMPS strategy is to optimize LU decomposition with accurate dynamic pivoting and reduced fill in. The distribution is therefore not suitable for the application of the projection operator $P_N P_V$ to the local in-core solutions (i.e., the solutions at the different nodes for one wavefield of a triangular cell are not systematically stored in-core on the same processor). To overcome this limitation, the solutions are re-ordered following well-balanced mesh partitioning, performed with the METIS software (Karypis and Kumar, 1999). The MUMPS-distributed solutions are mapped to the METIS decomposition with MPI point-to-point communications, before the application of operator $P_N P_V$. This mapping/projection step represents about 25% of the MUMPS substitution time. The forward and back-propagated wavefields are stored in the in-core memory for all sources. The gradient and the diagonal of the Hessian are therefore efficiently computed in parallel with local in-core wavefields for the local subdomain associated with each process, before being centralized on the master processor for perturbation-model building. Of note, the assembly and storage of the sparse $A$ matrix are performed by the master process, as the storage of the mesh-related tables, the wavefield solutions at the receiver positions for computing the objective function, and the composite residual sources for adjoint-wavefield computation. To avoid prohibitive memory allocation on the master processor, the master process is not involved in the factorization and substitution/projection steps, the wavefield storage, and the gradient/Hessian computation.

### 4.3. Two parallelism levels

The scalability of parallel direct solvers is intrinsically limited because of the large amount of communications between the MPI processes, and the memory overhead generated by the number of MPI process involved in the factorization (Sourbier et al., 2009b). Therefore, the single parallelization level with MPI cannot be adapted for large-scale applications. A second parallelism level, based on multi-threading, can, however, be efficiently implemented on multi-core architectures. The main computationally demanding parallel tasks of the FWI algorithm are the forward problem resolutions (factorization and substitutions/projection) and the building of the gradient and diagonal Hessian.

The MUMPS solver uses the Basic Linear Algebra Subroutines (BLAS) library mainly for level 2 and 3 operations (matrix/vector, and matrix/matrix operations). Several BLAS libraries are available in multi-thread distributions, which allow an efficient low-level of parallelization for multi-core architectures with shared memory.

The gradient and diagonal Hessian computations have several nested loops embedded (Algorithm 2). In addition to the MPI-based domain-decomposition parallelism, the outer loop over the local model parameters can be easily parallelized with shared-memory thread technology (as with standard OpenMP) to speed up the loop on the available computing-cores without duplicating or exchanging data.

An alternative to classical parallelization using one MPI process per computing-core is, therefore, to run one MPI process on $n$ computing-cores that share the same memory (physically on the same node), and to launch $n$ shared-memory threads per MPI-process during the BLAS operations, and the gradient and diagonal Hessian computations. These two levels of parallelism can mitigate the memory overhead of the factorization, the network usage for intensive communications, and the computational time for LU factors.

A third level of parallelism could also be implemented over frequencies and/or time-damping factors (Shin and Min, 2006). This third level of parallelism has, however, not been investigated in the current algorithm.
4.4. Performance

Simulations are performed on a distributed-memory architecture composed of 18 nodes, each of which includes two quad-core 2.7 GHz Opteron processors with 64 GB of shared memory. The nodes are interconnected by an Infiniband ConnectX network. This cluster is located at Geoazur Institute, and it provides 144 computing-cores and 1.125 TB of memory.

A first test corresponds to a middle-scale application that is focused on the elastic Valhall model (Fig. 4). A 1 042 720-cell mesh was designed with the Triangle software (Shewchuk, 1996). The mesh is composed of a thin unstructured layer on top for \( P_t \) interpolation, and a large zone of equilateral structured triangles for \( P_h \) in depth. This mesh allows frequencies of up to 7 Hz to be modelled in the elastic case. The substitution/projection phase is performed for 315 RHSs, corresponding to 315 explosive sources. Fig. 8 shows the evolution of the computational times and the memory usage for the main inversion steps as a function of the number of computing-cores, using one- and two-level parallelism.

We clearly see a decrease in the computational time when the computing-cores number increases, although the efficiency is limited by the intrinsic scalability of the MUMPS direct solver. The best trade-off between performance and computational resources is obtained with 24 computing-cores, with one MPI-process per computing-core used. When two levels of parallelism are used with shared-memory threads, the in-core memory required by the factorization decreases, an appealing feature if the memory available is limited. However, the memory saving is at the expense of the computational time, particularly for the substitution/projection step. Here, I postulate that for this middle-scale application, the speed-up provided by the multi-thread computation is not significant with respect to the time overheads due to thread launching, leading to a limited time performance for this application.

A second test focuses on a large-scale elastic crustal model (Fig. 6). An \( h \)-adaptive unstructured mesh was designed with Triangle for DG \( P_t \) modelling up to 6.5 Hz, leading to 528 080 cells. To mimic the SFJ-OBS experiment (Operto et al., 2006), 93 sources were considered, corresponding to 93 ocean-bottom seismometers, for the substitution/projection phase. Fig. 8 summarises the computational times and memory usage for this test. Note that the time for gradient building is negligible compared to that of the MUMPS steps, due to the small number of RHSs and the cell number in the mesh. For this large-scale application that requires a large amount of distributed memory to store the 200 GB of LU factors, shared-memory-threads technology is the alternative choice to the one-level parallelism, to minimize the number of MPI processes, and therefore the memory overheads during LU factorization. The data obtained with multiple threads show that both the computational time for the factorization and the substitution/projection steps can be decreased, while saving a significant amount of core memory.

The results of these two applications suggest that the two-level parallelism over MPI processes and shared-memory threads that are embedded in my FWI algorithm provide an efficient and flexible tool to tackle realistic size target imaging. Depending on the computing facilities available and the size of the case study, a judicious combination of the two levels of parallelism can be found for optimal performances in terms of computational time and core-memory usage.

5. Conclusion

A massively parallel algorithm was developed to perform frequency-domain full-waveform modelling and inversion for imaging 2D visco-elastic media. The forward problem of inversion, as the resolution of the elastodynamics equation in the frequency-domain, is solved using a low-order finite element discontinuous Galerkin method. This
allows for complex topographies and high velocity-contrasts to be taken into account, and to use unstructured h-adaptive triangular meshes combined with p-adaptive interpolations. The linear system, resulting from this discretization is solved with the parallel MUMPS direct solver, allowing the LU factors to be stored in a distributed form over the processors. The wavefield solutions are also stored in a distributed form, following mesh partitioning for a well-balanced workload over the processors. The inverse problem of the FWI is solved with a non-linear local optimization scheme. The implementation of the gradient of the objective function has been optimized for computational time and memory saving. A quasi-Newton L-BFGS optimization has been implemented to estimate the inverse of the Hessian matrix at a negligible computational cost, improving the reconstruction of several classes of parameter (P-wave and S-wave speeds, density, and attenuation factors $Q_P$ and $Q_S$). A two-parallelism level through MPI-processes and shared-memory threads has been implemented for optimal use of the computational time and core-memory resources, which will depend on the computer facilities.

This FWI algorithm will be used to tackle the imaging of realistically sized targets at various scales, from near-surface geotechnical applications to crustal-scale exploration. Ongoing studies include the extension to anisotropic (vertically transverse isotropic) media and the adaptation to teleseismic configurations for lithospheric imaging.

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References


Fig. 9. Computational time and memory use for the main inversion tasks for a large-scale application, as a function of the number of computing-cores, and the parallel strategy, as indicated.


