

THREE-DIMENSIONAL MODELLING AND INVERSION OF CONTROLLED SOURCE ELECTROMAGNETIC DATA

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Thesis submitted for the degree of Doctor of Philosophy

November 21, 2011

I herewith formally declare that all the contents of this dissertation which are not my own work have been appropriately acknowledged.

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"What you see depends on what you're looking for"
Source Unknown



Abstract

The marine Controlled Source Electromagnetic (CSEM) method is an important and almost self-contained discipline in the toolkit of methods used by geophysicists for probing the earth. It has increasingly attracted attention from industry during the past decade due to its potential in detecting valuable natural resources such as oil and gas.

A method for three-dimensional CSEM modelling in the frequency domain is presented. The electric field is decomposed in primary and secondary components, as this leads to a more stable solution near the source position. The primary field is computed using a resistivity model for which a closed form of solution exists, for example a homogeneous or layered resistivity model. The secondary electric field is computed by discretizing a second order partial differential equation for the electric field, also referred in the literature as the vector Helmholtz equation, using the edge finite element method. A range of methods for the solution of the linear system derived from the edge finite element discretization are investigated. The magnetic field is computed subsequently, from the solution for the electric field, using a local finite difference approximation of Faraday's law and an interpolation method. Tests, that compare the solution obtained using the presented method with the solution computed using alternative codes for 1D and 3D synthetic models, show that the implemented approach is suitable for CSEM forward modelling and is an alternative to existing codes.

An algorithm for 3D inversion of CSEM data in the frequency domain was developed and implemented. The inverse problem is solved using the L-BFGS method and is regularized with a smoothing constraint. The inversion algorithm uses the presented forward modelling scheme for the computation of the field responses and the adjoint field for the computation of the gradient of the misfit function. The presented algorithm was tested for a synthetic example, showing that it is capable of reconstructing a resistivity model which fits the synthetic data and is close to the original resistivity model in the least-squares sense.

Inversion of CSEM data is known to lead to images with low spatial resolution. It is well known that integration with complementary data sets mitigates this problem. It is presented an algorithm for the integration of an acoustic velocity model, which is known *a priori*, in the inversion scheme. The algorithm was tested in a synthetic example and the results demonstrate that the presented methodology is promising for the improvement of resistivity models obtained from CSEM data.

Acknowledgements

I wish to express my gratitude to my supervisors Professor Joanna Morgan and Dr. Lucy MacGregor for all the support, encouragement, advice, guidance, and for giving me the opportunity of being involved in this project.

I also wish to thank Professor Mike Warner for getting me involved in the FULLWAVE III consortium from which I greatly benefitted, from both the personal experience and from the resources available, in particular, the High Performance Computing facilities without which this work would not have been possible.

I am truly thankful to Mr. Adrian Umpleby and Dr. Ivan Štekl for all the discussions which guided me through the intricate process of building up a (very long) computer code, and to Mr. Simon Burbige at the Imperial College HPC facility for his prompt aid and enlightenment for using cx1.

I wish to thank Fundação para a Ciência e Tecnologia (FCT) which supported me financially during the duration of this project, under the POPH-QREN and European Social Fund programs with a research grant (SFRH/BD/40809/2007).

Thanks to Zichen Xue for the long conversations during coffee and lunch breaks, to my colleagues at the next desk Aruna Mannie and Ana Mijic, to Tenice Nangoo, Ahmed Al-Yaqoobi, for all the interesting conversations and to Nikhil Shah and Lluís Guasch for all the passionate discussions about geophysics, inversion, the world in general and for the good time we had attending the SEG annual meeting, at Denver in 2010.

To my parents and sister a special thank you, for all the support and long distance calls which kept me a bit closer during the past three years.

Finally, to Sonia, I am forever indebted for her dedication beyond limits, affection, and encouragement.

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1.1 Introduction to Marine CSEM Methods

Electromagnetic (EM) methods have been widely used to determine the electrical properties of the Earth. Some of the most common applications of electromagnetic methods include, lithospheric studies (O'Reilly & Griffin, 2010), studies of volcanic and seismic hazards (Rikitake, 1950; Muller & Haak, 2004), groundwater prospecting (Benson *et al.*, 1997), exploration for mineral and hydrocarbon resources, defense (Zhdanov & Keller, 1994) and geothermal resource mapping (Zakharova *et al.*, 2007).

It is estimated that 71 % of the surface of the Earth is covered by the ocean, and naturally electromagnetic methods were also developed for use in the exploration of the Earth in the marine environment. Marine electromagnetic methods have a long and rich history, spanning a broad spectrum of applications. It is difficult to establish the exact facts, because early EM applications were mainly used for defense purposes (Drysdale, 1924), consequently some details were kept in secret. In addition, geographical and political constraints led to different approaches and different stages of maturity in the development and application of marine EM, in the former Soviet Union and Western countries (Spiess *et al.*, 1980; Velikhov *et al.*, 1987; Berdichevsky *et al.*, 1989).

One can find references on the use of direct current (DC) methods for shallow marine prospecting as early as 1930's (Schlumberger *et al.*, 1934), nonetheless, this approach had no impact, due to the low economical viability of the marine mineral exploration market at the time, as well as the low effectiveness of the method, as the seawater is less resistive than the sediments and the current flows preferentially through the seawater. The development

of marine Controlled Source Electromagnetic (CSEM) methods had to wait until the end of the 1960's, after electromagnetic methods had reached a good level of maturity in the land environment during the 1950's and 1960's (Kaufman & Keller, 1983). Pioneering work was carried out by Novysh & Fonarev (1966), on the use of electromagnetic methods to explore the Arctic Ocean, and by Cox *et al.* (1971), at the Scripps Institution of Oceanography (SIO), on the use of marine magnetotellurics (MT) to study the electrical conductivity of the oceanic crust. The magnetotelluric field is present everywhere, including the marine environment, and has its origin in the perturbations in the ionosphere, mainly due to the solar wind and thunderstorms (Simpson & Bahr, 2005). Nevertheless, as the seawater is essentially a conductor, the natural electromagnetic field is heavily attenuated, particularly in the high frequency band. For this reason, the need to use a man-made controlled source to compensate for the limited bandwidth and attenuation in the natural EM spectrum became evident (Cox, 1981).

Since its inception, marine CSEM has been utilized to study the oceanic lithosphere for global studies (Spiess *et al.*, 1980; Young & Cox, 1981; Cox, 1981), nonetheless the oil industry was aware of its potential for hydrocarbon exploration (Srnlka, 1986). Despite this early interest, the technique found low applicability for oil and gas prospecting, mainly due to technological limitations and low sensitivity of the recorded signals, as targets were usually located on shallow water environments (Srnlka *et al.*, 2006). It took more than one decade to transform CSEM from an academic discipline into a routinely used technology by the oil industry (Ellingsrud *et al.*, 2002; Darnet *et al.*, 2007), mainly due to the active research at the SIO and the Southampton Oceanography Centre (SOC) (Evans *et al.*, 1991; MacGregor *et al.*, 1998, 2001), and the intense exploration in the Gulf of Mexico using marine MT (Constable *et al.*, 1998; Hoversten *et al.*, 2000). Marine CSEM methods are now a well established technology in the oil industry, and it is possible to anticipate other roles for this exploratory technique in the future, for example in the exploration of gas hydrates (Yuan & Edwards, 2000; Schwalenberg *et al.*, 2010), or metallic deposits at the sea-bottom.

The most widely used marine CSEM acquisition system utilizes a horizontal electric dipole (HED) source towed close to the sea-floor (generally within a few tens of meters). Dipole lengths typically range between 100 and 300 m, and the source generates a high-powered (300-1000 A), low frequency (0.1-0.5 Hz) signal. Generally the source transmits a square waveform signal with multifrequency content (Sinha *et al.*, 1990; Myer *et al.*, 2011), and the electromagnetic field responses are recorded by a set of receivers located at the sea-bottom. Source-receiver offsets can exceed 10 km (MacGregor & Sinha, 2000).

Other variants of the method have been developed over the years, using a transient magnetic dipole (Cheesman *et al.*, 1988), transient electric dipole (Edwards, 1997), frequency domain magnetic dipole (Evans, 2007) and a multi-channel transient electromagnetic system (Ziolkowski, June 2007). In the scope of this thesis it is only considered the horizontal electric

dipole setup.

Marine CSEM methods have been transformed from an academic discipline into a relatively well accepted hydrocarbon exploratory technique. Recent scientific publications show that this technique is likely to go through many changes and innovations in the future and be used for wider applications, for example in time-lapse methods for reservoir monitoring, and be integrated with other geophysical methods. This naturally requires an evolution in the paradigm of instrumentation, survey design, interpretation, modelling and inversion (Constable, 2010).

1.2 Introduction to Electromagnetic Modelling and Inversion

With the increasing number of available data sets in both academia and industry, there is a need to develop effective interpretation workflows. Despite the early existence of mathematical solutions for the three-dimensional forward modelling problem (Raiche, 1974), early analysis of marine CSEM data relied on asymptotic solutions (Bannister, 1968; Kraichman, 1970), due to the lack of computational power. The first 1D available solution was derived for a horizontal electric dipole in a horizontally layered resistivity model, in the frequency domain (Chave & Cox, 1982). Chave and Cox's solution has a closed form, nonetheless, it relies upon the use of digital filtering for numerical integration (Patterson, 1973; Anderson, 1979, 1984).

One-dimensional modelling has been the most widely used technique and still offers a valuable tool, nevertheless, most offshore structures are far more complex than the ones that can be represented by 1D models. The need to represent resistivity models closer to the actual geometry of geological formations led to the development of 2D solutions (also known as 2.5D because the resistivity distribution is 2D and the current density generated by the source is three-dimensional). The 2D solution is obtained by Fourier transforming into the spatial wavenumber domain, a direction along which the resistivity does not change. Unsworth *et al.* (1993) and Li & Key (2007) implemented 2D solutions of the forward modelling problem utilizing finite elements. Two-dimensional solutions for marine CSEM can be calculated rapidly and are computationally inexpensive in comparison to full 3D modelling.

With the substantial increment on computational capabilities, scientists were able to move to full three-dimensional modelling (and inversion). There are fundamentally two strategies to achieve a three-dimensional solution: the use of dyadic Green's functions, and the discretization of electromagnetic field equations in their differential form.

The use of dyadic Green's functions has been extensively used (Avdeev *et al.*, 2002; Hursan & Zhdanov, 2002), mainly due to their high computational efficiency. The representation of complex geometry, however, can be cumbersome and its implementation needs effective storage and solution strategies for dense linear systems.

Alternatively, if it is chosen to discretize the differential form of Maxwell's equations, the magnetic or electric field can be eliminated from the equations, with the choice being purely arbitrary, leading to a second order partial differential equation. Generally the magnetic field is chosen to be eliminated, and the resultant equation is commonly known as the vector Helmholtz equation for the electric field and can be discretized utilizing the finite difference method (FDM) (Newman & Alumbaugh, 1995; Alumbaugh *et al.*, 1996) or the finite integration technique (FIT) (Plessix *et al.*, 2007). Both methods utilize the Yee's cell, which is especially designed for electromagnetic numerical simulation (Yee, 1966).

Other approaches include the decomposition of the electric field in vector and scalar potentials, imposing a gauge condition and enforcing the conservation of current density. Splitting the electric field into components in the active and null spaces of the discrete Maxwell's operator and using gauge conditions, leads to a more stable and strong elliptic system, comparatively to the use of a formulation with components in both spaces (Aruliah *et al.*, 2001; Tyler *et al.*, 2004), at the expense of increasing the number of degrees of freedom in the linear system and requiring the subsequent calculation of the electric and/or magnetic fields, using a numerical approximation for the curl and gradient operators. The equivalent linear system can be discretized with resort to the finite volume method (FVM) (Aruliah *et al.*, 2001; Haber *et al.*, 2000). As pointed out by Aruliah *et al.* (2001) the discretization of the equivalent system of partial differential equations (*i.e.* the unknowns are the scalar and vector potentials) with the finite volume method is accurate as long as variations in conductivity are not extreme. Alternatively, the finite element method with nodal basis functions (FEM) has also been implemented (Badea *et al.*, 2001) and adapted to the marine CSEM forward modelling problem, however, comparisons with analytical solutions showed loss of accuracy for offsets larger than 1 km (King, 2004), limiting its applicability.

The electromagnetic inverse problem aims to estimate a conductivity (or resistivity) distribution that fits the observable data in some sense, depending upon the chosen metric (Parker, 1994). As the relation between the parameters and the observables is nonlinear, the solution for the inverse problem is usually obtained through the use of an optimization scheme, minimizing an objective function.

Solutions for the 1D inverse problem were initially developed, utilizing the frequency-domain 1D solution for the horizontal electric dipole (Constable & Cox, 1996) and Occam's inversion algorithm (Constable *et al.*, 1987). Even though, 1D inversion does not allow geological structures to be represented accurately, its usefulness relies in the fact that approximate models can be obtained rapidly. In addition, different survey parameters such as source-receiver offset, operating frequencies and source orientation can be rapidly tested (Key, 2009).

When geological structures are locally invariant (or less variant) in one direction (for example oceanic mid-ridge), 2D inversion (Unsworth & Oldenburg, 1995) is adequate to aid data interpretation. The main advantage of 2D inversion in general, is the fact that relatively

complex shapes in resistivity models can be represented. Furthermore, the number of parameters usually involved is still small enough to allow the use of a full sensitivities matrix and therefore Gauss-Newton methods (which utilize an approximation of the full Hessian) can be considered in the inversion algorithm, allowing to achieve super-linear convergence (Abubakar *et al.*, 2008a).

In 3D electromagnetic inversion the number of parameters to be estimated is generally very large, hence forming the Hessian and solving the resulting linear system at each tomographic iteration can be computationally expensive. For this reason, Newton and Gauss-Newton methods are generally avoided for 3D inversion. Instead, it is more convenient to consider gradient-type methods (such as the steepest descent method and nonlinear conjugate gradients) or quasi-Newton methods (Newman & Alumbaugh, 1997; Haber, 2005), which only use information from previous iterations, as for example the improved solution and the gradient of the objective function. The non-linear conjugate gradient and quasi-Newton methods have super-linear convergence allowing to achieve convergence significantly faster than the steepest-descent methods, being generally slower than the Gauss-Newton method (Nocedal & Wright, 2006), which converges quadratically. Both quasi-Newton and non-linear conjugate gradient methods, are generally preconditioned with an approximation of the Hessian or its diagonal to improve the convergence rate (Newman & Boggs, 2004; Plessix & Mulder, 2008).

The solution of the inverse problem requires the computation of the sensitivities, that is, the derivative of the field with respect to the model parameters, or the computation of the gradient of the objective function. The sensitivities are generally computed using the reciprocity principle and integrating the field and its adjoint over the support of the respective model parameter (McGillivray *et al.*, 1994). This approach, is also known as the adjoint method and is particularly useful for the computation of the sensitivities matrix. The gradient of the objective function can be computed through the adjoint-state method (Newman & Alumbaugh, 1997; Plessix, 2006; Plessix & Mulder, 2008), which in practice, is equivalent to solving one forward modelling problem. This approach is generally used when Maxwell's equations (or the vector Helmholtz equation) are discretized in the differential form. When using integral equations, it is possible to derive expressions for the direct computation of the Fréchet derivatives using the so called quasi-linear approach (Zhdanov & Hursan, 2000; Golubev & Zhdanov, 2005). This approach has the advantage of not needing an additional forward modelling solution for the calculation of the gradient of the objective function, and the same principle (that is the quasi-linear approximation) is utilized for the computation of the optimal step length (Gribenko & Zhdanov, 2007).

An important aspect of the electromagnetic inverse problem, is that it is ill-posed, thus a solution for the inverse problem does not depend continuously on the data (in practice a small perturbation in the data does not necessarily correspond to a small perturbation in the solution), and the existence and uniqueness of solutions is not guaranteed. This problem

was first tackled by Tikhonov & Arsenin (1977). Regularization theory is a mathematical framework that addresses ill-posed problems. In the context of geophysical non-linear inverse problems, a widely used approach is to minimize stabilized functionals by incorporating constraints, such as smoothing conditions, minimum support of the model parameters, or minimum support of the gradient (Zhdanov, 2002).

Geophysical interpretation and inversion are inherently ambiguous, as different geological structures can have the same signature in the recorded data. The integration of complementary data sets (*e.g.* seismic with electromagnetic and/or gravity data) attempts to mitigate ambiguity in geophysical interpretation and inversion (Lines *et al.*, 1988). Joint inversion provides an automated way of integrating different data sets in one single framework through the use of an optimization scheme, nonetheless there is not a general workflow that can be adopted in all cases (Heincke *et al.*, 2006; Colombo & Stefano, 1996).

An approach for tackling joint inversion schemes is to invert data sets that are sensitive to the same physical parameter (Sasaki, 1989), or using an empirical law which relates disparate physical observations with the same physical parameter (Heincke *et al.*, 2010). Alternatively, one can use information from complementary data sets to add a constraint to the objective function; this approach is commonly known as a structural approach. The fundamental idea behind the structural approach is the assumption that disparate physical parameters change together in the physical space (or if one prefers, they have a similar structure), and the objective function is minimized subject to a measure of structural similarity (Haber & Oldenburg, 1997). In the scope of non-linear inversion, for which the inversion schemes are generally iterative, the structural factor can be determined from *a priori* information obtained through the separate inversion of complementary data sets, or incorporating complementary data sets in the same inversion process and updating the structural term from the approximate model parameters at each iteration. For example, Saunders *et al.* (2005) constrained an inversion of electrical data, utilizing a spatially varying structural constraint term derived from seismic data, which has higher spatial resolution. Gallardo & Meju (2003; 2004) jointly inverted DC and seismic data using the cross gradients of seismic velocity and conductivity as a constraining term, which was updated at each iteration, using the approximated model parameters (both conductivity and velocity). More recently Hu *et al.* (2009a) used cross gradients in the joint inversion of electromagnetic and seismic data in two dimensions, and applied the method on synthetic 2D models, for the cases of surface recorded data and cross-hole tomography.

1.3 Aims of this Thesis

This thesis aims to attain three main objectives:

1. Develop and implement a solver for three-dimensional marine CSEM forward modelling in the frequency domain.
2. Investigate a suitable algorithm for regularized three-dimensional resistivity inversion using the developed forward modelling scheme.
3. Investigate and build an algorithm for three-dimensional inversion of resistivity, constrained with a distribution of acoustic wave velocity, and investigate its effectiveness in improving the structural resolution of the obtained images in comparison to inverting for resistivity alone.

1.4 Description of the Thesis

The second chapter of this thesis is devoted to the development and implementation of a numerical scheme for three-dimensional forward modelling, using the edge finite element method (eFEM).

The chapter includes a review of the fundamental theory of electromagnetism and the decomposition of the electric field in primary and secondary components. The discretization of the vector Helmholtz for the secondary electric field with the edge finite element is derived and the boundary conditions are discussed.

I further investigate the use of a homogeneous and two half-space background models for the calculation of the primary field. The use of the electric field decomposition formulation, requires the solution for the primary field at the centre of all the edges in the regions of the model where there are resistivity (or conductivity) anomalies. Furthermore, when using a two half-space background model it is critical to accelerate the computation of the primary field as it is computationally very intensive due to the need of using adaptive filtering for the calculation of Hankel transforms. Parallelizing over the number of edges is shown to substantially improve the computing times. It is described a method for subsequent computation of the magnetic field using a local finite difference approximation of Faraday's law, and interpolation. The use of the edge finite element method leads to a sparse linear system and both an iterative solver with preconditioning and a direct solver are investigated. Solutions using the eFEM are compared with reference solutions for both electric and magnetic fields.

In the third chapter is investigated an approach for three-dimensional inversion of marine CSEM data. In the first section is presented a short review on inverse problems, and in the second section, non-linear inverse problems are reviewed in the context of geophysical applications, and in the Fourier domain.

As the solution of geophysical non-linear inverse problems relies essentially on optimization techniques, and as generally three-dimensional inverse problems involve the estimation of a large number of unknowns (hundreds of thousand to tens or hundreds of million) the relevant

aspects of deterministic iterative optimization methods are also reviewed in this chapter.

Gradient based methods and Newton-direction based methods are the most widely used optimization methods in large scale inverse problems in the scope of geophysical applications. My first implementation of the inversion algorithm relied on the use of the steepest descent method. The need to make it faster led me to the implementation of the L-BFGS (stands for Low-memory Broyden-Fletcher-Goldfarb-Shanno) algorithm. Both algorithms are described in this thesis, and their performance is compared. Even though the L-BFGS includes in its formulation a methodology to approximate the action of the inverse of the Hessian matrix over the gradient of the parametric functional, it can be significantly improved using preconditioning. The use of a physics-based preconditioner for the approximation of the diagonal of the inverse of the Hessian matrix is reviewed.

Inverse problems are ill-conditioned and unstable, thus the main and relevant aspects of Tikhonov's regularization are reviewed. In the context of non-linear inverse problems, the regularization parameter is adaptive and, for its estimation a *cooling* approach is generally used. In this work I use a method based directly on the decrease of the data misfit between two consecutive iterations, instead of the more commonly used method based upon an artificial mathematical law to decrease the regularization parameter. Only a smoothing regularizer is considered in this work, and a weighted smoothing stabilizer is utilized with a so-called physics-based preconditioner in the solution of the regularized inverse problem.

The gradient of the parametric functional is given by the contributions of the gradient of a data misfit term and of the gradient of the regularization term. Expressions for the explicit computation of the gradient of the misfit term and of the regularization term are derived. The gradient of the misfit term is computed from the reciprocity principle for the electromagnetic field, and an explicit expression is derived for the case of the scattered field formulation (decomposition of the electric field in primary and secondary components). This method is equivalent to alternative methods that only use linear algebra concepts. The proposed methodology requires evaluation of volume integrals over the support of each model parameter, thus the Gauss-Legendre quadrature is reviewed. The numerical integration method is tested and an example comparing the sensitivities for the electric and magnetic fields computed using the adjoint method, with the ones computed using the explicit definition of the Fréchet derivative is presented.

In the last section of the third chapter it is presented an example showing the inversion of a synthetic data set. It is compared the performance of the preconditioned steepest descent method with the one of the L-BFGS method, inverting for one frequency only. It is also presented the inversion for the same model using a data set generated with two different frequencies. This example shows that the proposed inversion scheme is capable of reconstructing a conductivity model which is close to the original model.

In the fourth chapter, it is studied the implementation of an algorithm for constrained

inversion of conductivity using a structural link based upon an *a priori* known velocity model. In the first section of this chapter it is presented a review on the concepts and different approaches available to develop joint inversion and constrained inversion algorithms. It is defined an additive augmented parametric functional using the so called cross-gradient term for the structural constraint of the inversion algorithm. The augmented parametric functional is defined to take into consideration the aforementioned physics-based preconditioner for the inverse of the diagonal of the Hessian matrix.

The augmented functional uses a trade-off parameter to balance the contributions of the data misfit, of the regularization and of the structural constraining term. Two methods are investigated in order to obtain an effective weighting (trade-off) parameter. The performance of each method is investigated through the inversion of a synthetic data set, and it is shown that the structural constraining term improves the inverted models, and only improves spatial resolution to resistivity structures which are correlated with velocity structures.

In the fifth and last chapter, is made a general conclusion of the work developed in this thesis, and the topics relevant for future research are discussed.

1.5 Achievements

1. An original method was developed for 3D marine CSEM forward modelling.
2. Was introduced a weighted smoothing stabilizer, for a consistent formulation of the inverse problem when using a weighted model parameter space (Plessix & Mulder, 2008).
3. Was introduced an alternative approach for the computation of the gradient of the parametric functional (or objective function), within the rationale of decomposing the electric field in primary and secondary components, for the solution of the forward modelling problem.
4. Was introduced an alternative criterion for decreasing the regularization parameter in the non-linear inverse problem, based upon the decrease of data misfit.
5. Was introduced an algorithm for three-dimensional constrained inversion of CSEM data with acoustic velocity. The constrained inverse problem was formulated for a consistent formulation with a weighted model parameter space.
6. Were investigated methods for weighting the structural constraining term.

3D Marine CSEM Modelling with Edge Finite Elements

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Sections of this chapter were submitted for publication in the journal *Geophysics* under the title: *A finite element-multifrontal method for three-dimensional CSEM modeling in the frequency domain*. The manuscript was accepted for publication.

2.1 Background Theory

2.1.1 The Maxwell's equations System

Before introducing Maxwell's equation it is important to specify the response of a material to an external excitation in the context of the electromagnetic field theory. This relation is defined through a set of conditions known as the *constitutive laws*. For our future discussion it is assumed that geological materials are linear, isotropic and without hysteresis, and therefore the following constitutive equations hold (Ward & Hohmann, 1988):

$$\mathbf{D}(\mathbf{r}, \omega) = \varepsilon \mathbf{E}(\mathbf{r}, \omega) \quad (2.1a)$$

$$\mathbf{H}(\mathbf{r}, \omega) = \mu \mathbf{B}(\mathbf{r}, \omega) \quad (2.1b)$$

$$\mathbf{J}_c(\mathbf{r}, \omega) = \sigma \mathbf{E}(\mathbf{r}, \omega) \quad (2.1c)$$

Where $\mathbf{r} = (x, y, z)$ are the spatial coordinates in a three-dimensional space, ω is the angular frequency, $\mathbf{E}(\mathbf{r}, \omega)$ is the electric field, $\mathbf{D}(\mathbf{r}, \omega)$ is the electric displacement field, $\mathbf{B}(\mathbf{r}, \omega)$ is the magnetic induction field, $\mathbf{H}(\mathbf{r}, \omega)$ is the magnetic field, $\mathbf{J}_c(\mathbf{r}, \omega)$ represents the conduction currents, σ is the electrical conductivity, μ is the magnetic permeability and ε is the electric permittivity. Symbols are listed in table A.1. Equation 2.1c is known as Ohm's Law and is particularly important to describe materials that exhibit conductive properties.

The equations of Maxwell constitute the bulk of the analysis of any electromagnetic problem for which the classical field theory holds, and are usually derived and introduced in their explicit form *i.e.* in the spatial-time domain (Jackson, 1998). In the scope of the marine CSEM experiment, data is usually interpreted in terms of amplitude and phase which are obtained using a Fast Fourier Transform (FFT), and inversion of marine CSEM data is generally carried out by inverting for a small number of frequencies, thus requiring the solution of the forward problem only for those same frequencies (MacGregor *et al.*, 2001). For these reasons the space-frequency domain is usually preferred for the development of modeling and inversion codes, and it was also chosen to accomplish the objectives of this thesis.

The Fourier transform and its inverse, are elegant mathematical objects that map the time domain into the frequency domain and the frequency domain into the time domain, respectively, and are reviewed here for a matter of consistency and completeness, reading:

$$\mathbf{U}(\mathbf{r}, \omega) = \mathcal{F}[\hat{\mathbf{U}}] = \int_{-\infty}^{\infty} \hat{\mathbf{U}}(\mathbf{r}, t) e^{-i\omega t} dt \quad (2.2a)$$

$$\hat{\mathbf{U}}(\mathbf{r}, t) = \mathcal{F}^{-1}[\mathbf{U}] = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathbf{U}(\mathbf{r}, \omega) e^{i\omega t} d\omega \quad (2.2b)$$

Where equation 2.2a is the Fourier transform and equation 2.2b its inverse. Vectors $\mathbf{U}$ and $\hat{\mathbf{U}}$ satisfy the usual properties of vector spaces and are integrable in the domain of the Fourier transform pair.

The equations of Maxwell are now introduced in the frequency domain (Ward & Hohmann, 1988):

$$\nabla \cdot \mathbf{D}(\mathbf{r}, \omega) = \rho_c \quad (2.3a)$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}, \omega) = 0 \quad (2.3b)$$

$$\nabla \times \mathbf{E}(\mathbf{r}, \omega) = i\omega\mathbf{B}(\mathbf{r}, \omega) + \mathbf{K}(\mathbf{r}, \omega) \quad (2.3c)$$

$$\nabla \times \mathbf{H}(\mathbf{r}, \omega) = \mathbf{J}(\mathbf{r}, \omega) - i\omega\mathbf{D}(\mathbf{r}, \omega) \quad (2.3d)$$

Where ρ_c is the charge density, and $\mathbf{K}(\mathbf{r}, \omega)$ is the magnetic source. The current density term $\mathbf{J}(\mathbf{r}, \omega)$ includes both the conduction currents $\mathbf{J}_c(\mathbf{r}, \omega)$, expressed by Ohm's Law, and sources of current $\mathbf{J}_s(\mathbf{r}, \omega)$. The second term on the right hand side of Ampère's Law represents the displacement currents. For a matter of simplicity the explicit notation on the dependence of space and frequency will be dropped, and it is assumed that the electromagnetic field depends only on these two variables, unless specified.

The system of Maxwell's equations unifies Gauss's law of electricity (equation 2.3a), Gauss's law of magnetism (equation 2.3b), Faraday's law (equation 2.3c) and Ampère's law (equation 2.3d) in one single fundamental system of equations that describe all electromagnetic phenomena in the context of classical field theory.

With few exceptions, the magnetic permeability of rocks can be considered constant and equal to the magnetic permeability in a vacuum *i.e.* $4\pi \times 10^{-7}$ N/A², and the electric permittivity in geological media, is generally less than 10^{-10} F/m (Zhdanov & Keller, 1994). In addition, marine CSEM surveys are carried out utilizing a source signal with low frequency, usually below 10-20 Hz. For these reasons the displacement currents are negligible and the bulk of current flow is due to conduction as the inequality $\sigma/(\omega\epsilon) \gg 1$ holds. The law of Ampère in the low frequency regime, and for conductive media, is obtained eliminating the displacement currents term and plugging Ohm's law in equation 2.3d:

$$\nabla \times \mathbf{H} = \mathbf{J}_s + \sigma\mathbf{E} \quad (2.4)$$

Following the considerations described above, regarding the electric permittivity and magnetic permeability of geological materials, only the low frequency approximation for the electromagnetic field will be used in scope of this thesis.

2.1.2 Interface conditions for the electromagnetic field

This section reviews the behavior of the electromagnetic field at interfaces of materials with different properties *e.g.* conductivity, magnetic permeability, etc. These interface conditions are derived from Maxwell's equations, the divergence theorem and Stokes's theorem (Marsden, 2003) by choosing appropriate integration domains. These properties are fundamental in the derivation of both analytical and numerical solutions for the equations of Maxwell. A review of a numerical discretization consistent with the electromagnetic field properties is presented in section 2.2.1.

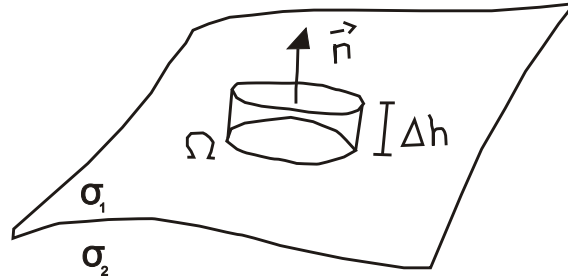


Figure 2.1: Control volume across an interface between different materials.

2.1.2.1 Normal component of the electric field

Integrating the law of conservation of charge $\nabla \cdot \mathbf{J} + \partial \rho_c / \partial t = 0$ (Jackson, 1998), over a test volume Ω , as illustrated in figure 2.1, and using the divergence theorem (Marsden, 2003), yields:

$$\int_{\partial\Omega} \mathbf{J} \cdot d\mathbf{S} = -\frac{\partial}{\partial t} \int_{\Omega} \rho_c dV \quad (2.5)$$

where $\partial\Omega$ is the boundary of Ω . In the limit $\Delta h \rightarrow 0$, all the current enters and leaves the test volume through the top and bottom surfaces, hence substituting Ohm's law in the previous equation, the flux identity (equation 2.5) simplifies to:

$$\int_{\partial\Omega} \mathbf{J} \cdot d\mathbf{S} \approx \int_{\partial\Sigma} \mathbf{J} \cdot d\mathbf{S} \approx \mathbf{J}_1 \cdot \mathbf{n} \Delta s - \mathbf{J}_2 \cdot \mathbf{n} \Delta s = \sigma_1 E_{n1} \Delta s - \sigma_2 E_{n2} \Delta s \quad (2.6)$$

where $\partial\Sigma$ represents the top and bottom boundaries, Δs is the area of the top and bottom boundaries, E_{n1} is the normal component of the electric field at the top boundary and E_{n2} is the normal component of the electric field at the bottom boundary. If a small enough time interval is considered, the quasi-static approximation, $\partial \rho_c / \partial t \approx 0$, holds. Hence we obtain

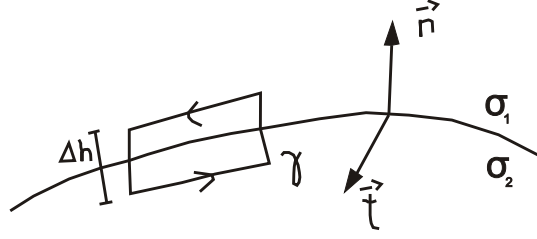


Figure 2.2: Circulation path across an interface between different materials.

the following condition at the interface between the two mediums:

$$\sigma_1 E_{n1} = \sigma_2 E_{n2} \quad (2.7)$$

In conclusion the normal component of the electric field is discontinuous at boundaries between materials with different physical properties.

2.1.2.2 Tangential component of the electric field

To derive the boundary condition for the tangential component of the electric field the integration path γ , is considered, see illustration in figure 2.2. The circulation of the electric field over γ is:

$$C = \int_{\gamma} \mathbf{E} \cdot d\mathbf{r} \quad (2.8)$$

From Stokes's theorem (Marsden, 2003) and substituting Faraday's law (equation 2.3c):

$$\int_{\gamma} \mathbf{E} \cdot d\mathbf{r} = i\omega\mu \int_{\Sigma} \mathbf{H} \cdot d\mathbf{S} \quad (2.9)$$

where Σ is the area enclosed by the integration path γ . In the limit $\Delta h \rightarrow 0$ the right term of equation 2.9 is zero and the left term simplifies to:

$$\int_{\gamma} \mathbf{E} \cdot d\mathbf{r} = \int_{\gamma_1} \mathbf{E} \cdot d\mathbf{r} + \int_{\gamma_2} \mathbf{E} \cdot d\mathbf{r} \quad (2.10)$$

where γ_1 and γ_2 are the integration paths on each side of the interface. By considering a vector, $\mathbf{n}$, normal to the interface and a vector, $\mathbf{t}$, normal to the enclosed surface Σ , the circulation of the electric field over γ is reduced to:

$$\int_{\gamma} \mathbf{E} \cdot d\mathbf{r} = (\mathbf{t} \times \mathbf{n}) \cdot (\mathbf{E}_2 - \mathbf{E}_1) \Delta l = 0 \quad (2.11)$$

Where Δl is the length of the integration path on each side of γ . Thus, the condition at the interface reads:

$$(\mathbf{t} \times \mathbf{n}) \cdot (\mathbf{E}_2 - \mathbf{E}_1) = 0 \quad (2.12)$$

Therefore, the tangential component of the electric field is continuous at interfaces between materials with different physical properties.

2.1.2.3 Normal component of the induction magnetic field

From Gauss's law for magnetism (equation 2.3b) and from the divergence theorem:

$$\int_{\partial\Omega} \mathbf{B} \cdot d\mathbf{S} = 0 \quad (2.13)$$

where Ω is the test volume illustrated in figure 2.1, and $\partial\Omega$ its boundary. In the limit $\Delta h \rightarrow 0$:

$$\int_{\partial\Omega} \mathbf{B} \cdot d\mathbf{S} \approx \mathbf{B}_1 \cdot \mathbf{n} \Delta s - \mathbf{B}_2 \cdot \mathbf{n} \Delta s = 0. \quad (2.14)$$

Where Δs is the area of the top and bottom surfaces. Thus, the normal component of the magnetic induction field is continuous:

$$(\mathbf{B}_1 - \mathbf{B}_2) \cdot \mathbf{n} = 0 \quad (2.15)$$

2.1.2.4 Tangential component of the magnetic field

Similarly for the derivation of the interface condition of the tangential component of the electric field, it is considered the integration path γ , illustrated in figure 2.2. From Ampère's law (equation 2.3d) and Stoke's theorem:

$$\int_{\gamma} \mathbf{H} \cdot d\mathbf{r} = \int_{\Sigma} [\mathbf{J} + i\omega\mathbf{D}] \cdot d\mathbf{S} \quad (2.16)$$

where $\mathbf{J}$ includes both current sources and conduction currents. If we consider a small enough integration path, it is possible to assume that $\mathbf{H}$ is almost constant on both sides of the interface, thus, in the limit $\Delta h \rightarrow 0$, equation 2.16 simplifies to:

$$\int_{\gamma} \mathbf{H} \cdot d\mathbf{r} = (\mathbf{t} \times \mathbf{n}) \cdot (\mathbf{H}_2 - \mathbf{H}_1) \Delta l \quad (2.17)$$

Where Δl is the length of the integration path on both sides of γ . Considering a small enough Δl the right term represents a surface current I_{Σ} , thus the interface condition for the

tangential component of the magnetic field is:

$$(\mathbf{t} \times \mathbf{n}) \cdot (\mathbf{H}_2 - \mathbf{H}_1) = I_\Sigma \quad (2.18)$$

In conclusion the tangential component of the magnetic field is discontinuous at interfaces.

2.1.3 Point sources versus finite length dipoles

A finite length dipole can be represented by the integration of a line of infinitesimal dipoles (or point sources) along a line, and expressions for the solution of the electromagnetic field generated by infinitesimal dipoles in layered media are widely available in the literature (Chave & Cox, 1982; Ward & Hohmann, 1988; Chave, 2009).

Generally in CSEM surveys the source fields are generated by finite length dipoles, thus the point source approximation may not be the most exact representation of a real source.

However, as pointed out by Streich & Becken (2011), the fields generated by a point source and by a 300 m length wire are nearly identical at radii larger than 1 km, thus they are nearly identical in the range of offsets typically used in exploration. In addition, for a configuration utilized for gas hydrates exploration, utilizing a 100 m length wire, the fields are also identical within the range of offsets of practical importance to detect the resistivity anomaly due to the presence of gas hydrates.

Streich & Becken (2011) also stressed the fact that moderate distortions in the source shape can be disregarded when compared with the accuracy of the source orientation. Hence, the point source approximation can be considered a good mathematical representation of real sources, and for the reasons aforementioned only point sources will be considered here.

2.1.4 Decomposition in primary and secondary components

The source term $\hat{\mathbf{J}}_s$, which represents the current density originated by an infinitesimal electric dipole, is given in the time domain by:

$$\hat{\mathbf{J}}_s = \mathbf{P}S(t)\delta(\mathbf{r} - \mathbf{r}_s) \quad (2.19)$$

Where $S(t)$ is the source time function, $\delta(\mathbf{r} - \mathbf{r}_s)$ is the Dirac delta function, $\mathbf{r}_s$ is the position of the source, and $\mathbf{P}$ is the electric dipole moment. In the frequency domain the source term is:

$$\mathbf{J}_s = \mathbf{P}\mathcal{F}[S(t)]\delta(\mathbf{r} - \mathbf{r}_s) \quad (2.20)$$

where $\mathcal{F}[S(t)]$ is the Fourier transform of $S(t)$. In this work, unless specified a normalized electric dipole is used, that is, the source term is divided by $\|\mathbf{P}\|$, and $\mathcal{F}[S(t)] = 1$.

The direct representation of $\mathbf{J}_s$ in a numerical approximation can lead to numerical instabili-

ties and inaccuracy in phase response. A well known remedy for this problem is to decompose the electromagnetic field in primary and secondary components (Newman & Alumbaugh, 1995, 2002):

$$\mathbf{E} = \mathbf{E}_p + \mathbf{E}_s \quad (2.21a)$$

$$\mathbf{H} = \mathbf{H}_p + \mathbf{H}_s \quad (2.21b)$$

$$\sigma = \sigma_p + \Delta\sigma \quad (2.21c)$$

Where $\mathbf{E}_p$ is the primary component of the electric field, $\mathbf{E}_s$ is the secondary component of the electric field, σ_p is the conductivity of the background medium, and $\Delta\sigma$ is the anomalous conductivity. Substituting identities 2.21 into the original form of the equations of Maxwell, we obtain the equivalent law of Faraday and Ampere's laws for the primary field:

$$\nabla \times \mathbf{E}_p = i\omega\mu\mathbf{H}_p \quad (2.22a)$$

$$\nabla \times \mathbf{H}_p = \mathbf{J}_s + \sigma_p\mathbf{E}_p \quad (2.22b)$$

and for the secondary field:

$$\nabla \times \mathbf{E}_s = i\omega\mu\mathbf{H}_s \quad (2.23a)$$

$$\nabla \times \mathbf{H}_s = \Delta\sigma\mathbf{E}_p + \sigma\mathbf{E}_s \quad (2.23b)$$

The primary field is calculated for a simple model with conductivity distribution σ_p , for which a closed form of the solution is known, such as the solution for the electric field generated by an electric dipole in a homogeneous medium (Ward & Hohmann, 1988), or in a horizontally layered medium (Chave & Cox, 1982; Chave, 2009).

Secondary fields are calculated using a numerical approximation method (*e.g.* finite difference method or the finite element method), after calculation of the primary field. The interface conditions derived in section 2.1.2 are naturally valid for the primary and secondary components of the electromagnetic field, as they can be derived from 2.22 and 2.23.

2.1.5 Vector Helmholtz equation for the secondary electric field

Discretizing equations 2.23a and 2.23b with the finite element method, has the inconvenience of requiring a consistent discretization for both magnetic and electric fields (Rodrigue & White, 2001). Furthermore, solving the coupled system of equations for the electromagnetic field in the air leads to a weak coupling, as the conduction term vanishes from Faraday's law. This problem can be addressed by eliminating one of the fields (a choice that is arbitrary) from the partial differential equation system 2.23 (Newman & Alumbaugh, 1995). Eliminating $\mathbf{H}_s$ from 2.23, leads to a second order partial differential equation for the electric field,

also known in the electromagnetic literature as the vector Helmholtz equation for the electric field:

$$\nabla \times \nabla \times \mathbf{E}_s - i\omega\mu\sigma\mathbf{E}_s = i\omega\mu\Delta\sigma\mathbf{E}_p \quad (2.24)$$

Using equation 2.24 has the added advantage of reducing the number of degrees of freedom in the linear system derived from the numerical discretization, in comparison to the use of the first order linear system or the use of potentials (Um *et al.*, 2010a), therefore requiring less computer memory. In the next section the appropriate boundary conditions are discussed in order to achieve a numerical solution for the 3D marine CSEM forward modelling problem.

2.1.6 Boundary conditions

For a complete formulation of the problem and to guarantee the uniqueness of the solution it is required the definition of a boundary condition. A natural boundary condition can be derived from the electric dipole radiation condition at infinite distances from the source, that is, the electromagnetic waves are essentially plane waves, thus only having components orthogonal to the direction of propagation (Jackson, 1998). In practice, computers have limited memory, thus the computational domain has to be truncated.

Since geological materials behave essentially as conductors, it is sensible to assume the absence of electrical insulators at the boundary of the modelling domain, thus the perfect electric conductor (PEC) boundary (Jin, 2010) holds:

$$\mathbf{n} \times \mathbf{E} \big|_{\partial\Omega} = \mathbf{n} \times [\mathbf{E}_p + \mathbf{E}_s] \big|_{\partial\Omega} = \mathbf{0} \quad (2.25a)$$

$$\mathbf{n} \times \mathbf{H} \big|_{\partial\Omega} = \mathbf{n} \times [\mathbf{H}_p + \mathbf{H}_s] \big|_{\partial\Omega} = \mathbf{0} \quad (2.25b)$$

Surface currents at $\partial\Omega$ are assumed to be absent, and $\mathbf{n}$ is the normal to $\partial\Omega$. The truncation of the computational domain with a perfect conductive boundary condition does not cause spurious reflections in the solution, because the amplitude of the electric and magnetic fields decays exponentially in the diffusive regime (Druskin *et al.*, 1999), thus the amplitude values are very small and can be considered zero in practice, but should only be imposed away from the heterogeneous regions of interest in the computational domain (Spichak, 2006). Even though the electric field amplitude does not decay exponentially in the air region, numerical experiments showed that it can be truncated, provided that the grid is severely stretched near the boundary, and provided that the air layer is represented in the model. In practice the amplitude of the primary electric and magnetic fields is very small at $\partial\Omega$, therefore it can be considered zero, thus, the boundary conditions for the secondary components reads:

$$\mathbf{n} \times \mathbf{E}_s \big|_{\partial\Omega} = \mathbf{0} \quad (2.26a)$$

$$\mathbf{n} \times \mathbf{H}_s \big|_{\partial\Omega} = \mathbf{0} \quad (2.26b)$$

Boundary conditions 2.26 will be used to derive a consistent discretization for equation 2.24 in the next section.

The solution for the 3D marine CSEM forward problem was reduced to two auxiliary problems for the electric field, and the magnetic field is subsequently calculated from Faraday's law. The main advantage of this approach is that it avoids numerical instabilities and loss of accuracy due to the direct representation of a point current source. Furthermore, the number of degrees of freedom in the linear system is also greatly reduced. The fact that the magnetic field is not known in the entire computational domain, does not represent an inconvenience since in the context of the marine CSEM experiment, the electromagnetic field is recorded at specific locations (receiver positions), thus it is only important to calculate the magnetic field at those positions, which can be done efficiently by using a local finite difference approximation for Faraday's law and interpolating to the point of interest (Alumbaugh *et al.*, 1996). The method for approximation of the magnetic field is derived in section 2.2.5.

2.2 Numerical solution of the 3D CSEM forward problem

2.2.1 Introduction to Nedelec's edge elements

The discretization of equation 2.24 with finite elements may look deceptively simple. A first approach might be to expand the vector equation 2.24, and discretize for each component separately using a finite element method with nodal basis functions. However, there are two main problems with such an approach. Firstly, the divergence-free condition is not satisfied, and must be explicitly imposed, secondly it does not satisfy the interface conditions for the electric field reviewed in section 2.1.2 (Jin, 2002; Bondeson *et al.*, 2005).

These issues can be effectively addressed if a consistent discretization is utilized for the numerical solution of the vector Helmholtz equation. Nedelec's edge elements (Nedelec, 1980; Jin, 2002; Monk, 2003) are constructed to naturally satisfy the interface conditions for the electromagnetic field. Furthermore, edge elements are divergence-free for first order basis functions, and therefore the numerical solution is free of spurious modes (Jin, 2002). Treating corners and edges at the boundaries can also be cumbersome when nodal basis functions are used, but edge elements provide a natural and efficient way of incorporating them into the discretization. As a consequence of their formulation, edge elements also guarantee that the curl of any vector field expanded using the basis functions of an edge element is square-integrable and therefore they are appropriate for the integration of equation 2.24.

For the implementation of the proposed scheme structured grids were utilized, as they can easily be implemented through the use of a cartesian product of the coordinates in each orthogonal direction in space (Liseikin, 2009; Plessix *et al.*, 2007), thus the computational domain is decomposed using hexahedra. The use of cartesian conforming hexahedra has the

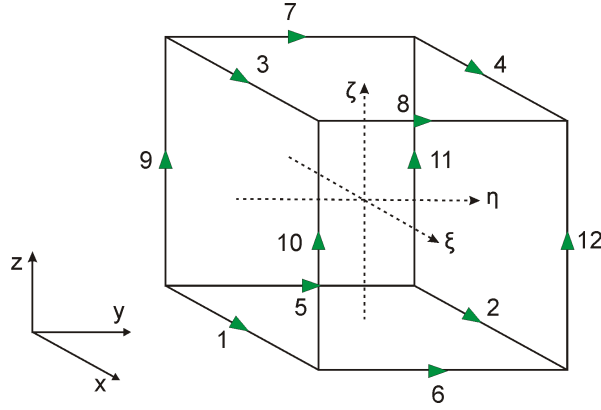


Figure 2.3: Illustration of an arbitrary hexahedron with a local frame of reference, (ξ, η, ζ) , and local numbering of the edges.

main advantage of allowing the implementation of a grid generator without effort, requiring however a suitable grid spacing for a correct sampling of the field. The maximum grid spacing can be determined from the skin depth for a certain resistivity model and frequency $\delta = \sqrt{2/(\omega\mu\sigma)}$ (Plessix *et al.*, 2007). Generally three elements per skin depth are sufficient to guarantee a good sampling. One implication of this scheme, is that complex shapes have to be approximated through stair-casing multiple elements of constant resistivity. However, it does not require averaging schemes for the material properties as in the case of the finite-difference method on a staggered grid (Alumbaugh *et al.*, 1996), which represents an advantage, as it only requires the assignment of the resistivity to each cell.

It is now introduced a piecewise discretization Ω_h , of the computational domain Ω , using a mesh of hexahedral elements Ω^e , such that $\Omega = \cup_{e=1}^{N_e} \Omega^e$ and $\Omega^e \in \Omega_h$. The vector field variables can be approximated over each element using a basis function expansion (Jin, 2002):

$$\mathbf{E}(\mathbf{r}) = \sum_{l=1}^{ne} E_l \mathbf{N}_l(\mathbf{r}) \quad (2.27)$$

where ne is the number of edges in a hexahedron, E_l is the tangential component of the vector field on the l -th edge of the reference hexahedron, and $\mathbf{N}_l$ is the vectorial basis function associated to the l -th edge, thus it has the direction of the reference direction of the l -th edge. Figure 2.3 illustrates a reference hexahedron with a local reference frame (ξ, η, ζ) . A set of first order basis functions over a reference hexahedron are defined by Jin (2002):

$$\mathbf{N}_i = \frac{l_i^e}{8} (1 + \eta_i \eta) (1 + \zeta_i \zeta) \nabla \xi \quad (2.28)$$

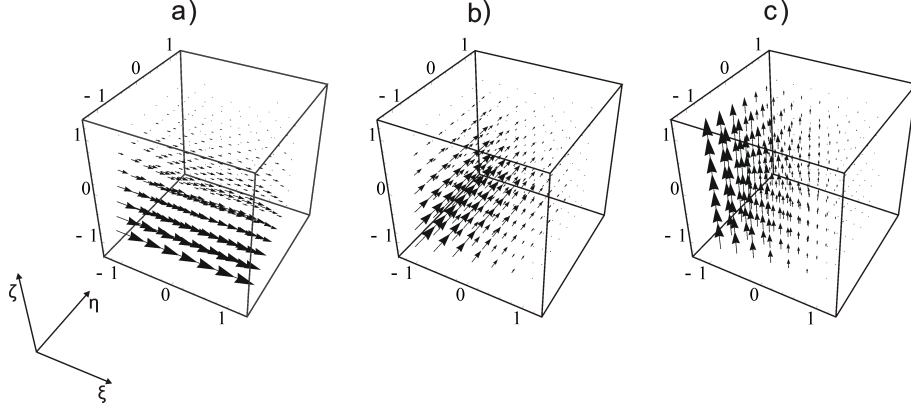


Figure 2.4: Plot of the local basis functions a) $\mathbf{N}_1$, b) $\mathbf{N}_5$ and c) $\mathbf{N}_9$. The maximum magnitude of each basis vector is one at the corresponding edge and decreases to zero in the direction to the opposite edges with the same direction.

where $i \in \{1, \dots, 4\}$, corresponding to the ξ oriented edges.

$$\mathbf{N}_i = \frac{l_i^e}{8}(1 + \xi_i \xi)(1 + \zeta_i \zeta) \nabla \eta \quad (2.29)$$

where $i \in \{5, \dots, 8\}$, corresponding to the η oriented edges, and

$$\mathbf{N}_i = \frac{l_i^e}{8}(1 + \xi_i \xi)(1 + \eta_i \eta) \nabla \zeta \quad (2.30)$$

where $i \in \{9, \dots, 12\}$, corresponding to the ζ oriented edges. l_i^e is the length of the i -th edge on element e . Figure 2.4 shows the plot of the basis functions $\mathbf{N}_1$, $\mathbf{N}_5$ and $\mathbf{N}_9$ on a reference hexahedron. The maximum magnitude of each vector of the basis is one at the corresponding edge, and gradually decreases to zero in the direction of the opposite edges with the same direction (see figure 2.4).

In a cartesian grid, each hexahedron can be mapped to a reference eight node hexahedron, using the parameterization:

$$\begin{aligned} \xi &= \frac{2(x^e - x_c^e)}{l_x^e}, \\ \eta &= \frac{2(y^e - y_c^e)}{l_y^e}, \\ \zeta &= \frac{2(z^e - z_c^e)}{l_z^e} \end{aligned} \quad (2.31)$$

Where, (x^e, y^e, z^e) are the global coordinates of the points in the e -th element, (x_c^e, y_c^e, z_c^e) are the coordinates of the centre of the e -th element, l_x^e, l_y^e, l_z^e are the lengths of the edges of the e -th element in the x, y and z directions, respectively, and $\xi, \eta, \zeta \in [-1, 1]$.

In the next section, a discretization for the numerical approximation of equation 2.24 is derived, using Nedelec's elements over hexahedra.

2.2.2 Discretization of the vector Helmholtz equation with the edge finite element method

In this section a method for the numerical approximation of the secondary electric field is derived. From Galerkin's method (Zienkiewicz & Taylor, 2005; Jin, 2002), the equivalent weak form of the vector Helmholtz equation is:

$$\mathcal{R}_k = \int_{\Omega} \mathbf{N}_k \cdot [\nabla \times \nabla \times \mathbf{E}_s - i\omega\mu\sigma\mathbf{E}_s - i\omega\mu\Delta\sigma\mathbf{E}_p] dV \quad (2.32)$$

Where $\mathcal{R}_k$ is the weighted residual. The computational domain Ω , can be decomposed in a set of hexahedra ($\Omega = \cup_{e=1}^{N_e} \Omega^e$), thus the weak form 2.32 is equivalent to:

$$\mathcal{R}_k = \sum_{e=1}^{N_e} \int_{\Omega^e} \mathbf{N}_k \cdot [\nabla \times \nabla \times \mathbf{E}_s - i\omega\mu\sigma\mathbf{E}_s - i\omega\mu\Delta\sigma\mathbf{E}_p] dV = \sum_{e=1}^{N_e} \mathcal{I}^e \quad (2.33)$$

Using the identity $\nabla \cdot (\mathbf{a} \times \mathbf{b}) = \mathbf{b} \cdot (\nabla \times \mathbf{a}) - \mathbf{a} \cdot (\nabla \times \mathbf{b})$ and the divergence theorem, the integral on each element $\mathcal{I}_e$ is rewritten as:

$$\begin{aligned} \mathcal{I}^e = & \int_{\Omega^e} (\nabla \times \mathbf{N}_k) \cdot (\nabla \times \mathbf{E}_s) dV - \int_{\partial\Omega^e} [\mathbf{N}_k \times (\nabla \times \mathbf{E}_s)] \cdot d\mathbf{S} \\ & - i\omega\mu\sigma \int_{\Omega^e} \mathbf{N}_k \cdot \mathbf{E}_s dV - i\omega\mu\Delta\sigma \int_{\Omega^e} \mathbf{N}_k \cdot \mathbf{E}_p dV \end{aligned} \quad (2.34)$$

From the vector identity $\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = (\mathbf{c} \times \mathbf{a}) \cdot \mathbf{b}$ and the Faraday's for the secondary field (equation 2.23a), the second term of equation 2.34 is rewritten as:

$$\int_{\partial\Omega^e} [\mathbf{N}_k \times (\nabla \times \mathbf{E}_s)] \cdot d\mathbf{S} = -i\omega\mu \int_{\partial\Omega^e} [\mathbf{N}_k \cdot (\mathbf{n} \times \mathbf{H}_s)] dS \quad (2.35)$$

During the assemble of the linear system, all the surface integrals will cancel at the internal surfaces, as each surface is shared by two elements with opposite normal vectors. For the external boundaries the PEC boundary condition is imposed (equation 2.26), thus:

$$\begin{aligned} \mathcal{I}^e = & \int_{\Omega^e} (\nabla \times \mathbf{N}_k) \cdot (\nabla \times \mathbf{E}_s) dV - i\omega\mu\sigma \int_{\Omega^e} \mathbf{N}_k \cdot \mathbf{E}_s dV \\ & - i\omega\mu\Delta\sigma \int_{\Omega^e} \mathbf{N}_k \cdot \mathbf{E}_p dV \end{aligned} \quad (2.36)$$

The element integration is now reduced to the calculation of three volume integrals. Expanding the solution for the secondary electric field with the basis functions $\mathbf{N}_k$, the equivalent

expression for $\mathcal{I}^e$ is:

$$\mathcal{I}^e = \mathcal{K}^e \mathbf{e}_s^e - i\omega\mu\sigma\mathcal{N}^e \mathbf{e}_s^e - i\omega\mu\Delta\sigma\mathcal{N}^e \mathbf{e}_p^e \quad (2.37)$$

where

$$\mathcal{K}_{km}^e = \int_{\Omega^e} (\nabla \times \mathbf{N}_k) \cdot (\nabla \times \mathbf{N}_m) dV \quad (2.38)$$

is a numerical approximation for the curl-curl operator over an element, generally designated as the element stiffness matrix, and

$$\mathcal{N}_{km}^e = \int_{\Omega^e} \mathbf{N}_k \cdot \mathbf{N}_m dV \quad (2.39)$$

is the element mass matrix. Integrals 2.38 and 2.39 can be evaluated with a cubature method or analytically (Smith & Griffiths, 2004; Jin, 2002). For the aims of this thesis I derived analytical expressions for the elements matrices on hexahedra using a computer algebra system (CAS). Substituting 2.37 in equation 2.33, the weighted residual $\mathcal{R}_k$, is:

$$\mathcal{R}_k = \sum_{e=1}^{N_e} [\mathcal{K}^e \mathbf{e}_s^e - i\omega\mu\sigma\mathcal{N}^e \mathbf{e}_s^e - i\omega\mu\Delta\sigma\mathcal{N}^e \mathbf{e}_p^e] \quad (2.40)$$

Equation 2.40 is known as the assemble of the global system of equations. The weighted residual method imposes $\mathcal{R}_k = 0, \forall k$, and therefore 2.40 leads to the equivalent sparse and complex symmetric linear system:

$$\mathcal{A} \mathbf{e}_s = \mathbf{s} \quad (2.41)$$

Where $\mathcal{A}$ is the global matrix resulting from the discretization with finite elements, $\mathbf{e}_s$ is the unknown secondary electric field, and $\mathbf{s}$ is the source term.

2.2.3 Computation of the primary field

The primary field can be calculated using either a homogeneous or a layered background model. For a matter of completeness, solutions in the frequency domain for the electric field generated by an electric dipole in homogeneous and two half-space resistivity models, are reviewed in Appendix C. When using a two half-space background model, one of the half-spaces is always considered non-conductive to represent the air layer, and the electric dipole lies in the conductive half-space. The interface between the two half-spaces matches the air-sea interface. Figure C.1 shows the configuration of the considered two half-space model.

The main advantage of using a homogeneous background model is the fact that the solution can be obtained rapidly and efficiently, even for a large number of discretization points, as shown in table 2.1. However, when an air-layer is included in the resistivity model, the solution for the electric field is not accurate enough, suggesting that the background model

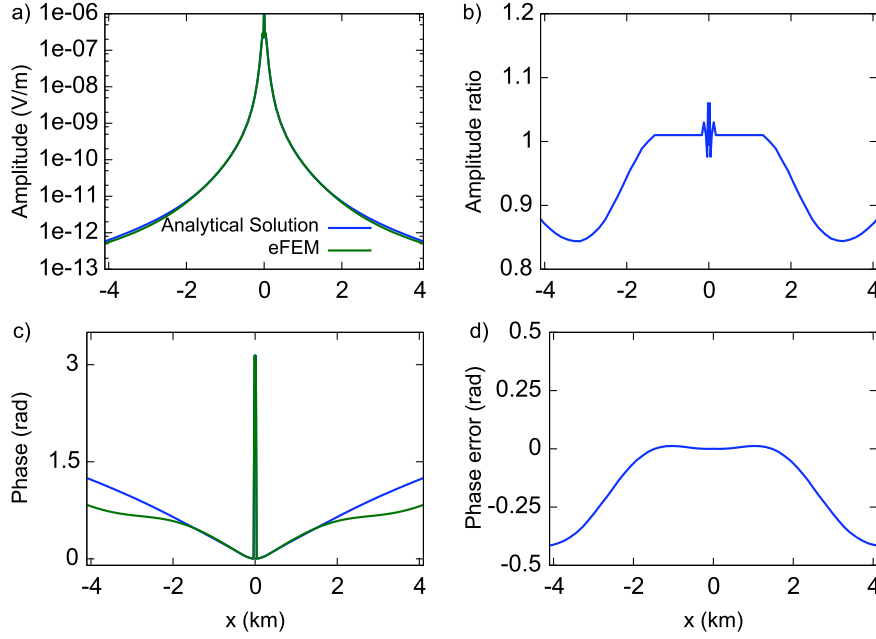


Figure 2.5: Comparison between the 1D analytical solution and the eFEM solution, of the inline electric field (E_x) at receiver line $y = 0$ m, for the resistivity model defined in equation 2.42, using a homogeneous background model; a) amplitude, b) ratio between the amplitudes computed using the 1D and eFEM solutions c) phase, d) difference between the phases computed using the 1D and eFEM solutions.

should also include the representation of the air layer. To support this statement, it is now considered an example for which the edge finite element solution is computed for the same resistivity model, using a homogeneous resistivity background model and a two half-space background model, and the results are compared. It is considered a frame of reference centered at the origin, and the z -direction pointing upwards. The source is a x -oriented electric dipole at $(0, 0, 30)$ m, and the source frequency is 0.1 Hz. The resistivity model is defined by:

$$\rho(z) = \begin{cases} 10^4 \, \Omega\text{m}, & \text{if } z > 1000 \, \text{m} \\ 0.33 \, \Omega\text{m}, & \text{if } 0 < z < 1000 \, \text{m} \\ 1.0 \, \Omega\text{m}, & \text{if } -200 < z < 0 \, \text{m} \\ 10.0 \, \Omega\text{m}, & \text{if } -400 < z < -200 \, \text{m} \\ 1.0 \, \Omega\text{m}, & \text{if } z < -400 \, \text{m} \end{cases} \quad (2.42)$$

It is important to note that the air does not behave as a conductive material. However, for a frequency of 100 Hz, which is above the range of frequencies typically used in CSEM, electrical currents are predominantly conductive currents, for values of resistivity up to $10^7 - 10^8 \, \Omega\text{m}$. Um *et al.* (2010b) showed that $\rho = 10^4 \, \Omega\text{m}$ is an appropriate value for the resistivity of the

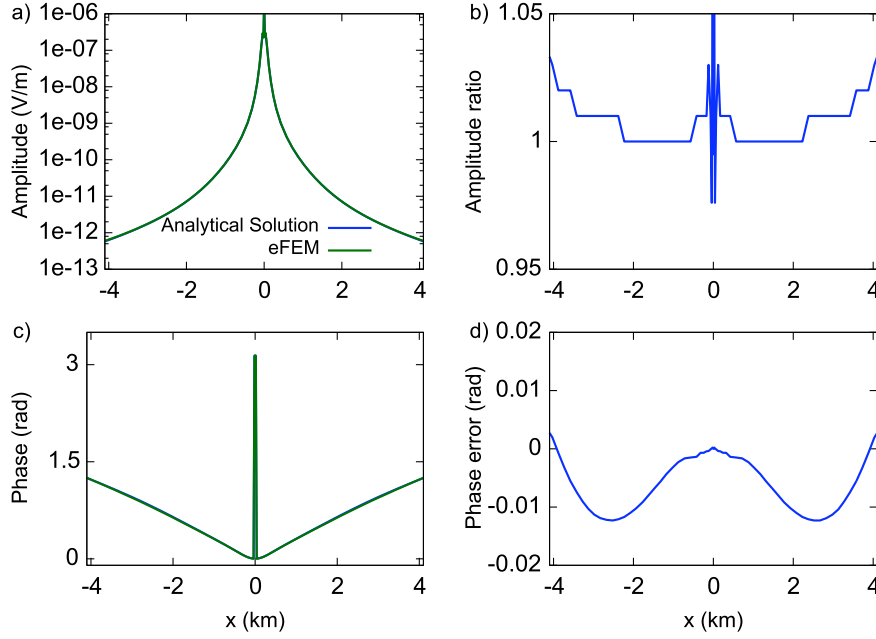


Figure 2.6: Comparison between the 1D analytical solution and the eFEM solution, of the inline electric field (E_x) at receiver line $y = 0$ m, for the resistivity model defined in equation 2.42, using a two half-space background model; a) amplitude, b) ratio between the amplitudes computed using the 1D and eFEM solutions c) phase, d) difference between the phases computed using the 1D and eFEM solutions.

air, in the diffusive regime and in the time domain, guaranteeing that $\sigma \gg \omega\epsilon$ holds, and therefore the displacement currents term can be neglected. This value also led to a good accuracy when used with the presented eFEM scheme, and also regularizes linear system 2.41.

Figure 2.5 compares the amplitude and phase solutions, calculated using the 1D analytical solution (Chave & Cox, 1982) and the edge finite element method (eFEM) with a homogeneous resistivity background, at the receiver line $y = 0$ m. The resistivity of the background resistivity model is the same as the sea-water resistivity, *i.e.* $\rho = 0.33 \Omega\text{m}$. The error increases with offset for both the amplitude and phase (figure 2.5 b,d), and errors can exceed 10 %.

Figure 2.6, compares the amplitude and phase solutions calculated using the 1D solution and the edge finite element method, with a two-half space background conductivity model at the receiver line $y = 0$ m. A very good agreement between solutions can be observed, with error below 5 % (figure 2.6 b,d). Thus, to achieve an accurate solution when using the decomposition of the electric field in primary and secondary components, and when an air layer is included in the resistivity model, an air layer must also be included in the background model.

It is important to note that the 1D code uses a value of $\sigma = 0$ S/m for the conductivity of the air, showing that the chosen value to approximate the resistivity of the air is appropriate.

The main disadvantage of using a two half-space background model is the substantial increase in computational time for the computation of the primary field, in comparison to the use of an homogeneous background, as shown in table 2.1. This increase in computational time is related with the need to compute Hankel transforms through the use of digital filtering (Anderson, 1979), which is computationally very intensive and time consuming.

A possible way to reduce the computational time for the primary field, when using a model with two half spaces, is to resort to parallel computing. In this work, the use of a shared memory paradigm in the parallelization of the primary field computing using openMP (Chapman *et al.*, 2007) has been investigated. As the primary field has to be calculated at the centre of each edge in the grid, a natural way is to parallelize over edges, keeping the digital filtering code serial. To study the acceleration of the calculation of the primary field, the serial implementation for the calculation of the primary field was parallelized. In this section, are presented the results of a test to study the performance of the parallel implementation. For this test is considered a x-oriented electric dipole located at (0,0,25) m, emitting a signal with frequency 1 Hz. The resistivity of the homogeneous domain is $\rho_0 = 0.33 \Omega\text{m}$, and the two half-space model has conductivity $\sigma = 0 \text{ Sm}^{-1}$ for the upper half-space ($z > 1000$ m), and resistivity $\sigma_0 = 0.33 \Omega\text{m}$ for the lower half-space ($z < 1000$ m). The interface between the two half-spaces is at $z = 1000$ m.

Table 2.1, shows the computational times when decomposing the domain $[-3, 3] \times [-3, 3] \times [-3, 1] \text{ km}^3$ with grid sizes of $61 \times 61 \times 31$ and $121 \times 121 \times 61$. All the calculations were done using a computer with two Quad-Core Intel Xeon[®] at 2.8 GHz. $N_{threads}$ is the number of threads, and the ratios are calculated with respect to the time for the solution using a single thread. In practice, there is almost no need to parallelize the computation of the primary field when a homogeneous conductivity background is used, as the computing time is negligible even for a large number of discretization points. The computation time for the primary field, when a two half-space background model is used, was substantially accelerated, and in principle it can be accelerated even further by using processors with a higher number of cores. This aspect could be further explored, using different hardware settings, including a higher number of cores. Alternatively, the task could be parallelized using a distributed memory system with MPI instructions. However, the CSEM forward modelling problem usually requires the solution for multiple sources. For this reason the multisource source solution is obtained by distributing the task over different computational nodes.

In summary, a hybrid model of parallelism was implemented for the calculation of the primary field, threading the calculation for a source in a multi-core architecture and distributing the calculation for several sources over computing nodes in a distributed memory system.

$N_{threads}$	Grid: $61 \times 61 \times 31$		Grid: $121 \times 121 \times 61$	
	Absolute Time / s	Ratio	Absolute Time / s	Ratio
Homogeneous model				
1	0.074	1	0.47	1
2	0.05	1.48	0.26	1.81
4	0.02	3.70	0.12	3.92
8	0.01	7.40	0.07	6.71
Two half-space model				
1	178	1	1139	1
2	91	1.96	582	1.96
4	46	3.87	296	3.85
8	25	7.12	157	7.25

Table 2.1: Scalability study for the calculation of the primary field using a homogenous and a two half-space model. The parallel version is coded with openMP directives.

2.2.4 Solution of the linear system of equations

Three-dimensional CSEM modelling in the frequency domain with the edge finite element method, requires the solution of a symmetric sparse linear system. The solution of large scale linear systems is a key aspect of numerical linear algebra since it has a major impact in the applicability and robustness of numerical solutions of partial differential equations. Linear system 2.41 has special characteristics that need to be taken into account when implementing a solver for its solution. It has been reported that in the low frequency regime, and when representing the air in the model ($\sigma = 0$ S/m) it is particularly difficult to solve the linear system of equations due to its large null space (Weaver *et al.*, 1995; Druskin *et al.*, 1999; Mackie *et al.*, 2007), thus affecting convergence speed of iterative solvers. The use of a small value for the conductivity of the air helps to attenuate this problem.

In three-dimensional applications it is not uncommon to use grids with dimensions larger than $100 \times 100 \times 100$. Thus solutions of linear systems with several million degrees of freedom is common practice. Furthermore, the solution of the marine CSEM forward problem may require the solution for several right hand-sides. For the solution of the inverse problem the computational load increases dramatically, as for each tomographic iteration at least one solution of the forward modelling problem for each source is required, and generally the corresponding adjoint to compute the sensitivities or gradient of the objective function. For example, when gradient or Newton based methods are utilized it is generally required a forward modelling solution, an adjoint solution, and an additional forward modelling solution to estimate the optimal step-length. Consequently, the solution for the linear system must be achieved efficiently.

Krylov subspace techniques (van der Vorst, 2003) are usually preferred for the solution of linear systems derived from the discretization of large-scale 3D problems as the memory storage requirements are relatively modest, and its implementation relies essentially on matrix to vector multiplications. However, when dealing with ill-conditioned linear systems, iterative

solvers may struggle to converge and efficient preconditioning must be used. In the scope of low frequency electromagnetic problems for example, Torquil Smith (1996) introduced the static divergence correction, which corrects the approximate solution of the electric field to a divergence-free electric field solution at each iteration, and Newman & Alumbaugh (2002) introduced the Low Induction Number (LIN) preconditioner which deflates the large null-space associated with the curl operator. These preconditioners were developed in the context of the numerical solution of electromagnetic problems using the FDM with staggered grids. On the other hand, direct solvers are relatively stable when dealing with ill-conditioned linear systems, provided that sufficient arithmetic precision is used in the calculations (Datta, 2010, chap. 4). However, for 3D problems the number of floating point operations and allocated memory is in the order of $\mathcal{O}(N^6)$ and $\mathcal{O}(N^4)$, respectively (Ashcraft & Liu, 1998) (where N is the number of degrees of freedom in the linear system), thus their application in 3D geophysical problems has been traditionally avoided.

Recent advances in numerical factorization algorithms along with the availability of parallel computational resources created the necessary conditions to attract some interest in factorization methods for 3D problems. For example, Ben-Hadj-Ali *et al.* (2008) used a direct solver for 3-D acoustic full-waveform inversion, Oldenburg *et al.* (2008) and Börner *et al.* (2008) utilized direct solvers for transient electromagnetic modelling, and Streich (2009) utilized a direct solver for CSEM modeling in the frequency domain, discretizing Maxwell's equations with the finite difference method over a staggered grid.

A particular aspect of direct solvers, is the fact that solutions for multiple right-hand-sides can be obtained at nearly the expense of one single factorization, if a single linear system represents the entire modelling domain (Abubakar *et al.*, 2008a; Operto *et al.*, 2007). Hence, it was considered worthwhile to investigate the performance of factorization methods in the scope of the this work.

In the next sections the feasibility of both iterative and direct solvers for the solution of the linear system 2.41 is investigated.

2.2.4.1 Iterative Solver - Feasibility study

In this section it is presented a feasibility study on the use of an iterative solver to achieve a solution for the linear system derived from the discretization of equation 2.24 with edge finite elements.

There is not a rule of thumb for the choice of an iterative solver for a particular problem, and it would not be practical to test all the possible Krylov subspace methods with all possible combinations of preconditioners. Choosing an iterative method that delivers the best performance is essentially a trial and error process. A comparative study of the different Krylov subspace methods can be found in Barrett *et al.* (1994). If enough computational ca-

	Grid Dimensions	DOF	Preconditioner	Time / s	N. iterations
Spacing	$121 \times 121 \times 60$	2606219	Jacobi	21956	4689
			ILU(0)	10543	1187
			SGS	3283	385
			SSOR ($\omega = 0.7$)	49180	2404
			SSOR ($\omega = 1.0$)	6398	306
			SSOR ($\omega = 1.5$)	9072	437
Irregular Spacing	$51 \times 51 \times 27$	205326	Jacobi	2859	15479
			ILU(0)	2859	15479
			SGS	1011	1367
			SSOR ($\omega = 0.7$)	3567	2313
			SSOR ($\omega = 1.0$)	7623	4940
			SSOR ($\omega = 1.5$)	-	-

Table 2.2: Comparison between the performance of the different tested preconditioners, discretizing the resistivity model defined in equation 2.42, with regularly and irregularly spaced grids. (-) indicates divergence.

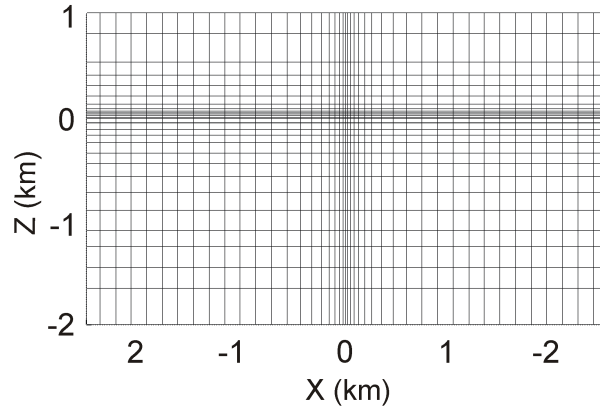


Figure 2.7: Slice of the irregular grid utilized to discretize resistivity model 2.45, at $y = 0$ m.

pabilities are available (as different methods have different requirements in terms of storage and number of matrix to vector multiplications) the main criterion to have in consideration is the properties of the linear system in question. For example, symmetry and positiveness of linear systems are considered when determining which method to choose.

A suitable method for the solution of complex symmetric linear systems is the Bicgstab-2 (der Vorst, 1992). The Bicgstab-2 has already been used in the solution of the CSEM forward modelling problem with the FIT method, which also leads to a complex symmetric linear system (Plessix *et al.*, 2007).

A key aspect of the implementation of an iterative solver is the choice of a preconditioner, as it can dramatically reduce the number of iterations to reach convergence for a solution. The fundamental idea of preconditioning is to transform the original linear system into an

equivalent system (Saad, 2003). For a preconditioner $\mathcal{S}$, the linear system can be left preconditioned:

$$\mathcal{S}^{-1}\mathcal{A}\mathbf{e}_s = \mathcal{S}^{-1}\mathbf{s} \quad (2.43)$$

or right preconditioned:

$$\begin{aligned} \mathcal{A}\mathcal{S}^{-1}\mathbf{u} &= \mathbf{s} \\ \mathbf{e}_s &= \mathcal{S}^{-1}\mathbf{u} \end{aligned} \quad (2.44)$$

The new equivalent system has the same solution as the original, however, its properties are different. If $\mathcal{S} = \mathcal{A}$, the solution would be reached in one iteration. Nonetheless, it is not generally the case that one knows *a priori* the inverse of a matrix, otherwise the whole range of methods for the solution of linear systems would be redundant. However if $\mathcal{S}$ is a good approximation of $\mathcal{A}$ then the number of iterations necessary to reach convergence can reduce substantially. It is important to note that the multiplication of $\mathcal{S}$ by the original system is never explicitly implemented as it would increase significantly the number of operations and memory overhead. The preconditioning of iterative Krylov subspace methods is generally achieved by solving an auxiliary linear system with $\mathcal{S}$ at each iteration (der Vorst, 1992; Saad, 2003).

In this work the performance of the Jacobi, Symmetric Successive Over-Relaxation (SSOR), ILU(0) and Symmetric Gauss Seidel (SGS) preconditioners were all studied. Complete descriptions of these preconditioners can be found in the work of Saad (2003). All the preconditioners were tested using a serial implementation, thus all the presented run times, are with respect to the use of a single central processing unit (cpu).

The performance of the different preconditioners is compared using the resistivity model:

$$\rho(z) = \begin{cases} 0.33 \text{ } \Omega\text{m}, & \text{if } z > 0 \text{ m} \\ 1.0 \text{ } \Omega\text{m}, & \text{if } -200 < z < 0 \text{ m} \\ 10.0 \text{ } \Omega\text{m}, & \text{if } -400 < z < -200 \text{ m} \\ 1.0 \text{ } \Omega\text{m}, & \text{if } z < -400 \text{ m} \end{cases} \quad (2.45)$$

The source is a x-oriented electric dipole at (0, 0, 30) m with frequency 1 Hz, and the background resistivity model is a homogeneous medium with $\rho = 0.33 \text{ } \Omega\text{m}$. The preconditioners were tested discretizing the resistivity model on a computational domain of $6 \times 6 \times 3 \text{ km}^3$ using a regular grid (50 m grid spacing) and an irregular grid (grid spacing ranging between 25 and 150 m). Figure 2.7, shows a vertical slice of the irregular grid at $y = 0 \text{ m}$. Both grids (regular and irregular) satisfied the Nyquist criterion for a correct spatial sampling (Press *et al.*, 2002) and the tolerance level was set to 10^{-7} .

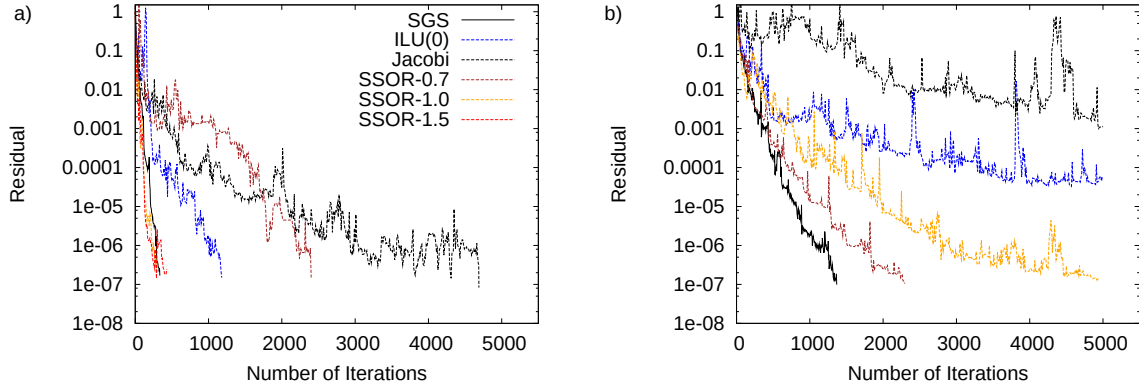


Figure 2.8: Convergence plots for the preconditioners tested, using a) regular grid spacing and b) irregular grid spacing. The SSOR preconditioner with $\omega = 1.5$ diverged for the irregular grid case.

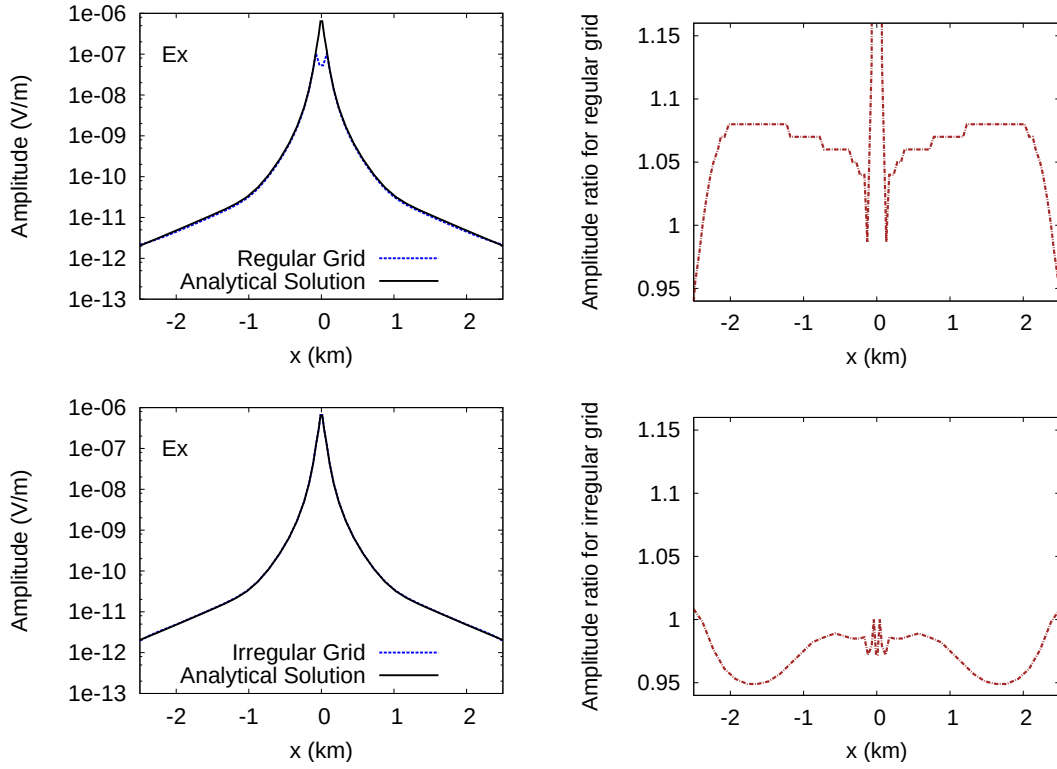


Figure 2.9: Comparison between the eFEM using regular and irregular grids, and the analytical solution (Chave & Cox, 1982), for the inline electric field, using a x-oriented dipole for a signal frequency of 1 Hz.

Table 2.2 summarizes the performance of each one of the preconditioners, in terms of number of iterations and run time, and for both the regularly and irregularly spaced grids. By inspection of figure 2.8 is clear that the SGS and SSOR preconditioners deliver the best results and, for the case of the irregular grid, they are the only ones which allowed a decrease in the residual below the maximum accepted tolerance. In the case of the regular grid, the SSOR preconditioner has a similar performance to the SGS preconditioner. However, SSOR requires tuning the parameter ω , which can differ from linear system to linear system, as shown in this example (in the case of the regular grid, the optimal value is $\omega = 1.5$ and for the case of the irregular grid is $\omega = 0.7$). Thus, the SGS preconditioner has clear advantages in comparison with all the tested alternatives. Although the number of iterations for the case of the irregular grid is higher than for the case of the regular grid, the run time is much higher for the latter as the number of degrees of freedom in the linear system is about an order of magnitude higher. Consequently, the time for matrix to vector multiplications takes longer and the run time per iteration also increases. The use of irregular grids slows down the convergence rate significantly, nonetheless, it allows savings in terms of grid size, and with an order of magnitude fewer degrees of freedom, was obtained a better accuracy for the eFEM solution. Figure 2.9, compares the accuracy of the solution using the regular and the irregular grid. The eFEM solutions were obtained using the SGS preconditioner for both the regular and the irregular grids, and are compared with the 1D analytical solution (Chave & Cox, 1982).

It was shown that the use of a regular grid requires a very fine mesh to cope with the rapid variation of the electric field in the vicinity of the source. Alternatively, an irregularly spaced grid allows to decrease the size of the grid substantially and obtain an accurate solution. However, the number of iterations to attain convergence increases substantially.

A bigger model

From the previous example, one concludes that for the type of finite element used in this work, the grid must be finer near the source to capture the rapid variation of the electric field in its vicinity. The comparison between the run times for a regular grid and irregular grid (for the same preconditioner) are not directly comparable, as the size of the grids is different and therefore the run time for operations, essentially matrix to vector multiplications, is also different. However, it is observed that the use of an irregular grid has a strong impact in the number of iterations necessary to reach convergence for the defined tolerance of 10^{-7} for residuals (table 2.2).

In CSEM data acquisition it is not uncommon to consider source-receiver offsets longer than 10 km (Commer & Newman, 2008). Furthermore, and as aforementioned, it is known that at low frequencies, and particularly when an air-layer is represented in the resistivity

models, the linear system of equations becomes nearly indeterminate (Mackie *et al.*, 2007), affecting the achievement of a solution or its accuracy (Druskin & Knizherman, 1994). In this section are considered two examples, aiming to study how much these two factors affect the attainment of a solution for linear system 2.41, when a more realistic model size is considered. As in the previous section, it is utilized the Bicgstab-2 iterative solver preconditioned with SGS, as this preconditioner led to the best performance in terms of number of iterations and run time to achieve convergence.

In this study, resistivity models 2.45 and 2.42 are discretized with an irregularly spaced grid, finer near the source position (similarly to the grid setting shown in figure 2.7), and with size $135 \times 135 \times 43$. The coarser regions satisfy the Nyquist criterion for appropriate spatial sampling (Press *et al.*, 2002). Resistivity model 2.45 simulates a deep-sea environment for which the air-layer can be ignored, and resistivity model 2.42 simulates an environment for which the air-layer must be considered in the computation. The computational domain for the resistivity model 2.45 is $16.2 \times 16.2 \times 3 \text{ km}^3$, and for the resistivity model 2.42 is $16.2 \times 16.2 \times 14 \text{ km}^3$. Even though both resistivity models are discretized with grids with the same dimensions, the size of the computational domain changes because the air layer is represented with a layer that has a resistivity of $10^4 \Omega\text{m}$ and is 10 km thick. For both models is considered a x-oriented electric dipole emitting a signal at 1 Hz, and located at (0, 0, 30) m. For the deep sea-water example (model 2.45) is considered a homogeneous background model and for the model with a 1000 m thick sea-water layer (model 2.42) it is considered a two-half space background model. Table 2.3 summarizes the dimensions of the grid, number of degrees of freedom of the linear system resultant from the finite element discretization, number of iterations and run time to achieve a solution for a maximum accepted tolerance of 10^{-7} , as in the previous example. Figure 2.10 shows the convergence of the iterative solver for both examples considered in this section.

As expected, the run-time per iteration increased with the size of the linear system as the number of operations also increased. In addition, for the case of the deep sea water model, the number of iterations also increased significantly in comparison with the example with a $51 \times 51 \times 27$ grid. Thus, the number of iterations necessary to reach convergence, for a defined level of tolerance, increases with the size of the problem, that is, the number of degrees of freedom.

As shown in figure 2.10, the number of iterations increased for the case when an air layer is considered in the model. However, one can conclude that the most significant factor affecting the convergence rate is the grid spacing contrast. This result is in agreement with Druskin & Knizherman (1994) who showed that a large contrast in the size of cells leads to ill-conditioned linear systems and an increase in the solution time. When inverting CSEM data for a 3D resistivity model, it is generally required the solution of the forward problem, the adjoint problem, and an extra forward modelling solution to determine the optimal step

	Grid Dimensions	DOF	Time	N. iterations	Allocated memory
Deep sea-water					
(Equation 2.45)	$135 \times 135 \times 43$	2321190	11.3 h	4627	5.74 GB
1000 m thick					
(Equation 2.42)	$135 \times 135 \times 43$	2321190	13.7 h	5655	5.74 GB

Table 2.3: Parameters for the eFEM of the electromagnetic field responses for the resistivity distributions 2.45 and 2.42.

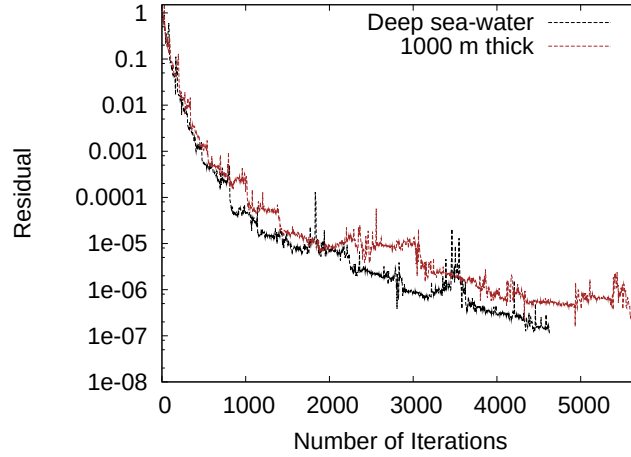


Figure 2.10: Convergence plots using the Bicgstab-2 preconditioned with SGS, for the case of a deep sea-water model and a model with an air layer represented (sea water with 1000 m of depth).

length, for several sources (Commer *et al.*, 2008; Commer & Newman, 2008; Vogel, 2002). Thus, considering the results in this section the use of an iterative solver with the SGS preconditioner can be prohibitive in a practical situation as the convergence for the desired level of tolerance may not be sufficiently fast.

This topic needs further investigation, if an iterative solver is to be considered in a practical solution. Multigrid methods (Trottenberg *et al.*, 2001) is a topic that definitely deserves the attention and probably can offer an efficient preconditioner for the solution of 3D CSEM modelling with edge finite elements. Hiptmair (1998) introduced a geometric multigrid solver and Reitzinger & Schöberl (2002) presented an algebraic multigrid solver for the solution of linear systems derived from the discretization of Maxwell's equations with Nedelec's elements. Even though both works showed a set of numerical experiments in which strong variations of the coefficients of Maxwell's equations were tested, neither studied convergence when grids with large spacing ratios are considered. For these reasons, along with temporal constraints related with the completion of this thesis, the study of a more suitable preconditioner for the solution of the CSEM forward modeling problem with eFEM, had to be considered a topic of future research.

2.2.4.2 Direct Solver - Feasibility study

In contrast to iterative solvers, which attempt to approximate the solution of a linear system by successively constructing a new solution using the approximate result from previous iterations, direct solvers rely on transformations on the matrix entries to obtain an equivalent form which can be used to obtain the solution of the linear system by forward and backward substitution.

Sparse direct solvers commonly involve four main tasks:

1. An ordering stage to obtain a good pivot sequence and analysis. The more important and common algorithms are the minimum degree (Liu, 1985) and the nested dissection methods (Amestoy *et al.*, 1996; Karypis & Kumar, 1998). An optimal ordering can reduce significantly the number of fill-ins in the matrix factors, thus minimizing the amount of needed memory, which is one of the main bottlenecks of factorization algorithms (Germouche *et al.*, 2003).
2. Analysis phase, to determine the data structures necessary to store the factors and intermediate calculations (pivot ordering, partial factorizations for example).
3. Factorization of the system matrix using supernodal left or right looking (Schenk & Gartner, 2004), or a multifrontal method (Liu, 1992) for example.
4. Solution of the linear system by forward and backward substitution using the matrix factors, and iterative refinement to improve the accuracy of the solution.

The implementation of a direct solver can be complex and cumbersome, thus in the scope of this thesis it was used the freely available distribution, Massive Parallel Multifrontal Solver (MUMPS) (Amestoy *et al.*, 2000, 2001). The MUMPS distribution uses a multifrontal method, and is parallelized with openMP and MPI. The implementation in double complex arithmetic was used in this work, because the solution of the linear system 2.41 has a large dynamic range. Further details about the multifrontal method, and MUMPS can be found in the work of Duff *et al.* (1986); Liu (1992); Gould *et al.* (2005) and Davis (2006).

Scalability Study for the Direct Solver

As aforementioned, direct solvers are computationally very intensive and require large amounts of memory. For three-dimensional problems, the allocated memory and number of floating point operations are in the order of $\mathcal{O}(N^4)$ and $\mathcal{O}(N^6)$, respectively (Ashcraft & Liu, 1998), thus requiring parallel computing resources to make realistically-sized problems tractable.

In this section it is studied the scalability of MUMPS in double precision complex arithmetic,

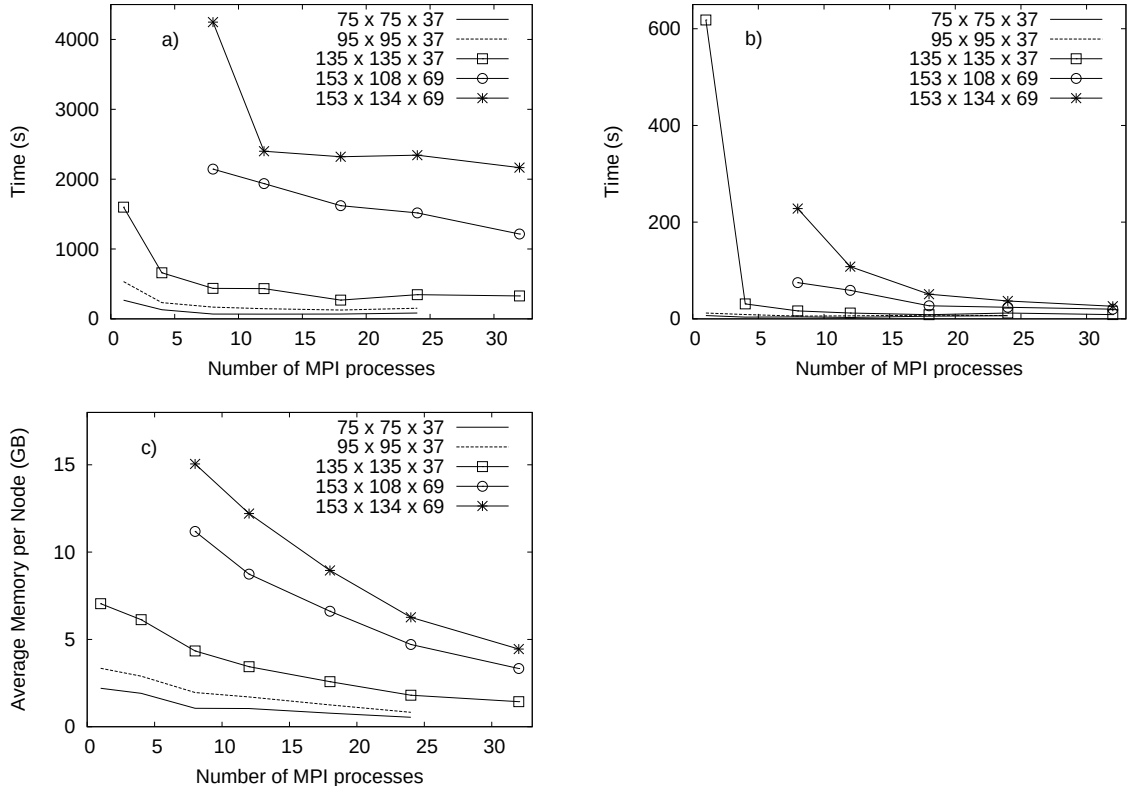


Figure 2.11: Scalability study for the direct solver MUMPS in double complex arithmetic, using a distributed memory system with 8 GB per and 2 Intel Xeon[®] Quad Core per node, interconnected with a Gigabit network. a) Time for factorization, b) Time for back-substitution, c) Memory scalability.

using a cluster with two Xeon[®] Quad-Core processors and up to 23.5 GB per node, interconnected with a Gigabit network. In this work full advantage was taken of the hybrid model of parallelism of MUMPS, that is MUMPS is parallelized with both openMP directives and MPI instructions (Chowdhury & L'Excellent, 2010), as this led to the best performance in terms of run time and memory requirements, and the tasks were distributed up to 32 computer nodes using 32 MPI processes.

For the scalability study, the resistivity model in equation 2.45 was discretized using five grids with different sizes and irregularly spaced, similarly to the grid setting shown in figure 2.7. The source is a x-oriented electric dipole, operating at 1 Hz, and located at (0,0,30) m. Table B.1 in appendix B, summarizes the run times and average amount of memory allocated on each node, for different grid sizes and different number of MPI processes (with eight threads each). Figure 2.11 shows a) the factorization time, b) back-substitution time, and c) average allocated memory per node with the increasing number of computational nodes, illustrating

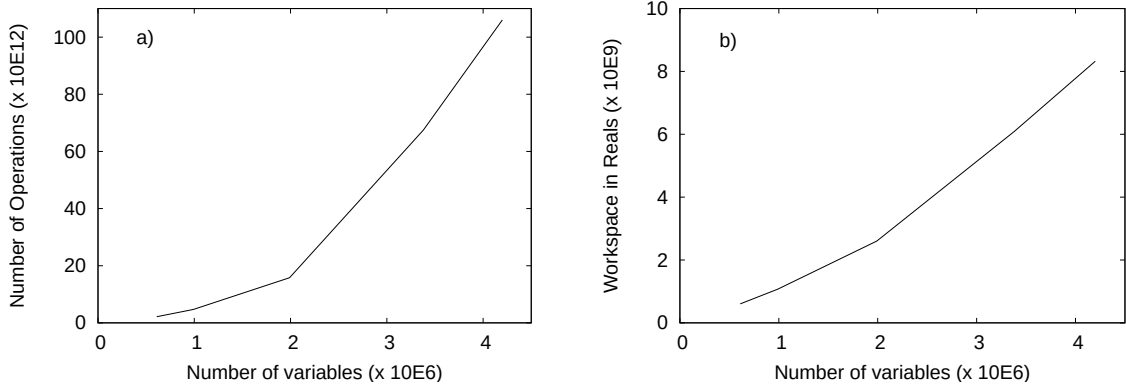


Figure 2.12: Dependence of the a) number of operations and b) workspace with the increasing number of variables in linear system 2.41, in 16 Bytes complex arithmetic.

the data in table B.1. Generally a speedup in the solution time is observed by increasing the number of nodes. Nonetheless, there is a limit (around 12 MPI processes) beyond which is not possible to accelerate the factorization time by adding nodes, as shown in figure 2.11 a), as message passing becomes dominant. Message passing overhead, is also responsible for a slight increase in the run time for the examples with grid size $75 \times 75 \times 37$, $95 \times 95 \times 37$ and $135 \times 135 \times 37$, when the jobs are distributed over a large number of nodes (see table B.1). In addition, figure 2.11 c) shows that the average allocated memory per node decreases with the increasing number of computational nodes, thus preventing the system from running out of memory, which can happen even if the out-of-core option of MUMPS (Agullo *et al.*, 2007) is selected.

Another important aspect of the scalability study is to know how the size of the problem scales with the number of added computer nodes. Figure 2.12 a) and b), shows the dependence of the number of floating point operations and global workspace with the increasing number of degrees of freedom N , for linear system 2.41. As expected from the theoretical relations for three-dimensional problems from Ashcraft & Liu (1998), there is a polynomial relation between both the allocated memory and number of floating point operations with N . Hence, as expected, it is not possible to solve indefinitely bigger problems by increasing the number of computing nodes, utilizing hardware with the same characteristics, and the current state of the art of factorization algorithms.

Even though direct solvers impose limitations regarding the scalability and required amount of memory, it is important to mention that they constitute a viable solution if enough computational capabilities are available. Furthermore, it was shown in this section that solutions for relatively large scale problems can be obtained within an acceptable time window even for large variations in the grid spacing.

The results of this section, demonstrate that the multifrontal solver MUMPS is more reliable than the iterative schemes tested, hence, MUMPS is used to solve the linear system derived from the edge finite element discretization (equation 2.41).

2.2.5 Computation of the magnetic field

After calculating the electric field from the vector Helmholtz equation, the magnetic field can be calculated from a local finite difference approximation of the law of Faraday (2.3c), and interpolating for the point of interest (*e.g.* receiver point) (Newman & Alumbaugh, 1995; Alumbaugh *et al.*, 1996). Using this approach decreases the number of degrees of freedom in the linear system to solve after discretizing Maxwell's equations, being this factor of particular importance as the investigated iterative solver struggles to achieve a timely solution and the direct solver loses scalability rapidly with an increasing number of degrees of freedom. In addition, it also avoids the derivation of a discretization which is consistent simultaneously with the electric and magnetic fields. This approach has been implemented in codes that use the finite difference method over a staggered grid (Weiss, 2005), and was also implemented in this work, combined with the edge finite element method. Its description is included in this thesis for a matter of completeness.

It is assumed that the electric field has been calculated previously and is known at the centre of each edge. For the calculation of the magnetic field at a generic position (x_r, y_z, z_r) , it is considered the region of the computational grid $[x_i, x_{i+1}] \times [y_i, y_{i+2}] \times [z_i, z_{i+2}]$, such that $x_i < x_r < x_{i+1}$, $(y_i + y_{i+1})/2 < y_r < (y_{i+1} + y_{i+2})/2$ and $(z_i + z_{i+1})/2 < z_r < (z_{i+1} + z_{i+2})/2$, as illustrated in figure 2.13.

The x-component of the magnetic field at the centre of each face is calculated using a finite difference approximation of the law of Faraday:

$$\begin{aligned} i\omega\mu H_x &= \frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} \approx \\ &\approx i\omega\mu H_{x;i,j+\frac{1}{2},k+\frac{1}{2}} = \frac{e_{i,j+1,k+\frac{1}{2}} - e_{i,j,k+\frac{1}{2}}}{y_{i,j+1,k+\frac{1}{2}} - y_{i,j,k+\frac{1}{2}}} - \frac{e_{i,j+\frac{1}{2},k+1} - e_{i,j+\frac{1}{2},k}}{z_{i,j+\frac{1}{2},k+1} - z_{i,j+\frac{1}{2},k}} \end{aligned} \quad (2.46)$$

The interpolated x-component of the magnetic field at the point of interest (x_r, y_z, z_r) is:

$$H_x(x_r, y_z, z_r) \approx \frac{1}{i\omega\mu} \sum_{k,j,i=1}^2 \mathcal{W}_{i,j+\frac{1}{2},k+\frac{1}{2}} H_{x;i,j+\frac{1}{2},k+\frac{1}{2}} / \left[\sum_{k,j,i=1}^2 \mathcal{W}_{i,j+\frac{1}{2},k+\frac{1}{2}} \right] \quad (2.47)$$

Where the interpolation weight $\mathcal{W}_{a,b,c}$ is defined by:

$$\mathcal{W}_{a,b,c} = \left| (x_{a,b,c} - x_r)(y_{a,b,c} - y_r)(z_{a,b,c} - z_r) \right| \quad (2.48)$$

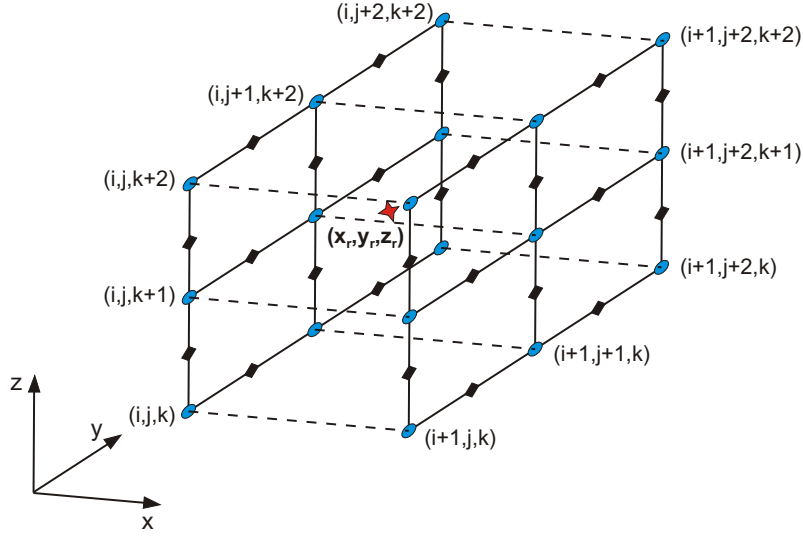


Figure 2.13: Illustration of a small region of interest of the finite element grid, for the calculation of the x-component of the magnetic field at (x_r, y_r, z_r) .

For the y-component of the magnetic field, it is considered the region of the computational grid $[x_i, x_{i+2}] \times [y_i, y_{i+1}] \times [z_i, z_{i+2}]$, such that $(x_i + x_{i+1})/2 < x_r < (x_{i+1} + x_{i+2})/2$, $y_i < y_r < y_{i+1}$ and $(z_i + z_{i+1})/2 < z_r < (z_{i+1} + z_{i+2})/2$. From Faraday's law:

$$\begin{aligned} i\omega\mu H_y &= \frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} \approx \\ &\approx i\omega\mu H_{y;i+\frac{1}{2},j,k+\frac{1}{2}} = \frac{e_{i+\frac{1}{2},j,k+1} - e_{i+\frac{1}{2},j,k}}{z_{i+\frac{1}{2},j,k+1} - z_{i+\frac{1}{2},j,k}} - \frac{e_{i+1,j,k+\frac{1}{2}} - e_{i,j,k+\frac{1}{2}}}{x_{i+1,j,k+\frac{1}{2}} - x_{i,j,k+\frac{1}{2}}} \end{aligned} \quad (2.49)$$

Thus, the interpolated y-component of the magnetic field at (x_r, y_r, z_r) is:

$$H_y(x_r, y_r, z_r) \approx \frac{1}{i\omega\mu} \sum_{k,j,i=1}^2 \mathcal{W}_{i+\frac{1}{2},j,k+\frac{1}{2}} H_{y;i+\frac{1}{2},j,k+\frac{1}{2}} / \left[\sum_{k,j,i=1}^2 \mathcal{W}_{i+\frac{1}{2},j,k+\frac{1}{2}} \right] \quad (2.50)$$

Analogously, for the z-component of the magnetic field, it is considered the region of the grid $[x_i, x_{i+2}] \times [y_i, y_{i+2}] \times [z_i, z_{i+2}]$, such that $(x_i + x_{i+1})/2 < x_r < (x_{i+1} + x_{i+2})/2$, $(y_i + y_{i+1})/2 < y_r < (y_{i+1} + y_{i+2})/2$ and $z_i < z_r < z_{i+1}$. The finite difference approximation of Faraday's law at the centre of each face is:

$$\begin{aligned} i\omega\mu H_z &= \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \approx \\ &\approx i\omega\mu H_{z;i+\frac{1}{2},j+\frac{1}{2},k} = \frac{e_{i+1,j+\frac{1}{2},k} - e_{i,j+\frac{1}{2},k}}{x_{i+1,j+\frac{1}{2},k} - x_{i,j+\frac{1}{2},k}} - \frac{e_{i+\frac{1}{2},j+1,k} - e_{i+\frac{1}{2},j,k}}{y_{i+\frac{1}{2},j+1,k} - y_{i+\frac{1}{2},j,k}} \end{aligned} \quad (2.51)$$

And the interpolated z-component at the point of interest is:

$$H_z(x_r, y_z, z_r) \approx \frac{1}{i\omega\mu} \sum_{k,j,i=1}^2 \mathcal{W}_{i+\frac{1}{2},j+\frac{1}{2},k} H_{z;i+\frac{1}{2},j+\frac{1}{2},k} / \left[\sum_{k,j,i=1}^2 \mathcal{W}_{i+\frac{1}{2},j+\frac{1}{2},k} \right] \quad (2.52)$$

Equations 2.47-2.52 allow to calculate the three-components of the magnetic field efficiently after the total electric field is obtained from the eFEM approximation. In section 2.2.6 are presented examples that show this method is reliable even near the source position, where the electric field changes rapidly and the mesh size is very small.

2.2.6 Synthetic model examples

Thin resistive layer model

In this section the eFEM solution is validated by considering the resistivity model in figure 2.14. The model responses obtained through the use of the proposed finite element scheme are compared with the model responses calculated using a 1-D code based on Chave and Cox's (1982) method of solution for 1-D models.

It is considered a frame of reference with the z-axis origin at the sea-floor level and pointing upwards. The source is a x-oriented electric dipole with a frequency of 0.25 Hz and located at (0, 0, 30) m. The model was discretized with a $141 \times 103 \times 51$ irregular mesh, representing a computational domain of $20 \times 16.4 \times 7.0$ km³ and approximately 2.2×10^6 degrees of freedom. Near the source position the grid is made finer to capture the rapid variation in the electric field in space, as the chosen finite element basis is of first order. The grid spacing ranges between 10 and 200 m in the horizontal direction, and between 10 and 500 m in the vertical direction. The growth ratio between adjacent elements is based on the edge length in each direction, and it is chosen to be not higher than 1.5, as this value led to the best compromise between accuracy of the solution and size of the grid. Figure 2.15 shows a vertical slice of the grid used to compute the electric and magnetic field responses, using the edge finite element scheme and the resistivity model illustrated in figure 2.14. The background resistivity model is homogeneous and has the same resistivity as the sea-water (0.3125 Ω m).

The solution of the resulting linear system was distributed over 10 nodes with 8 cores each, totalizing 80 processing units. The factorization and back-substitution took 575 s and 12 s, respectively. Each node allocated 6.1 GB of memory on average.

Figures 2.16 to 2.21 show the comparison between the eFEM solution and the 1D solution (Chave & Cox, 1982) for the three components of the electric and magnetic fields, and respective amplitude ratios and phase differences. The phase was plotted unwrapped in all figures.

The amplitude ratio and phase difference plots 2.16-2.21, show that the error is generally be-

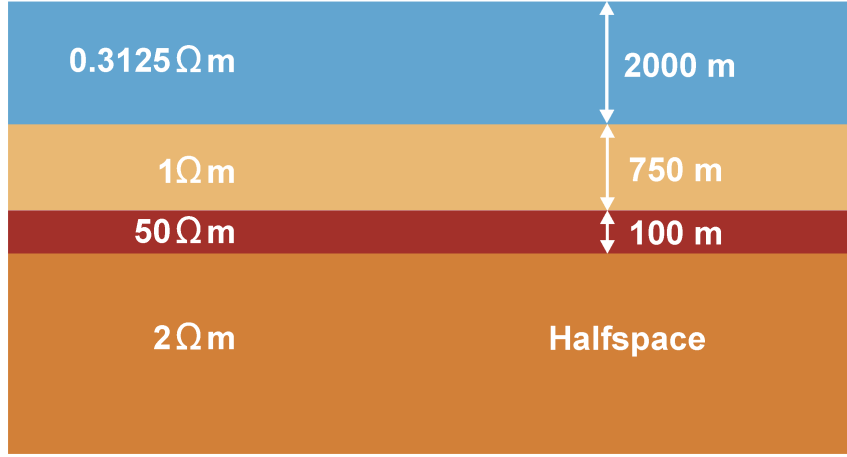


Figure 2.14: Illustration of the 1D model used for comparison of the finite element solution with the one obtained from Chave and Cox's (1982) method.

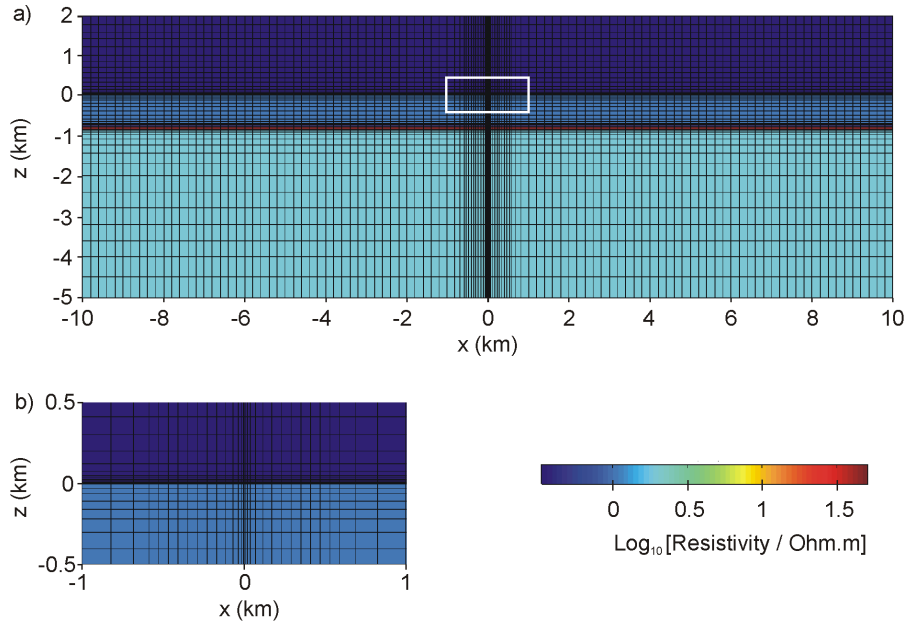


Figure 2.15: Slice of grid used for the discretization of the resistivity model showed in figure 2.14, (a) in the plane $y = 0 \text{ m}$, and (b) excerpt of the grid in the vicinity of the source, corresponding to the area delimited by the white rectangle in a).

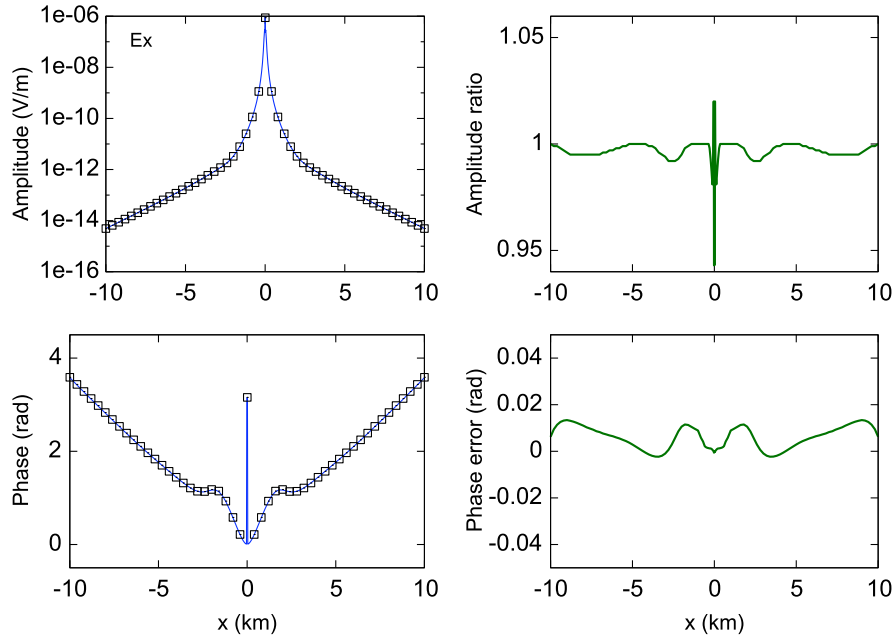


Figure 2.16: Comparison between the eFEM (solid line) and 1D solutions (open squares) for the x-component of the electric field, for the resistivity model illustrated in figure 2.14, along the receiver line $y = 0$ m. The phase is unwrapped and the source frequency is 0.25 Hz. The plots on the right side show the respective amplitude ratios and phase differences.

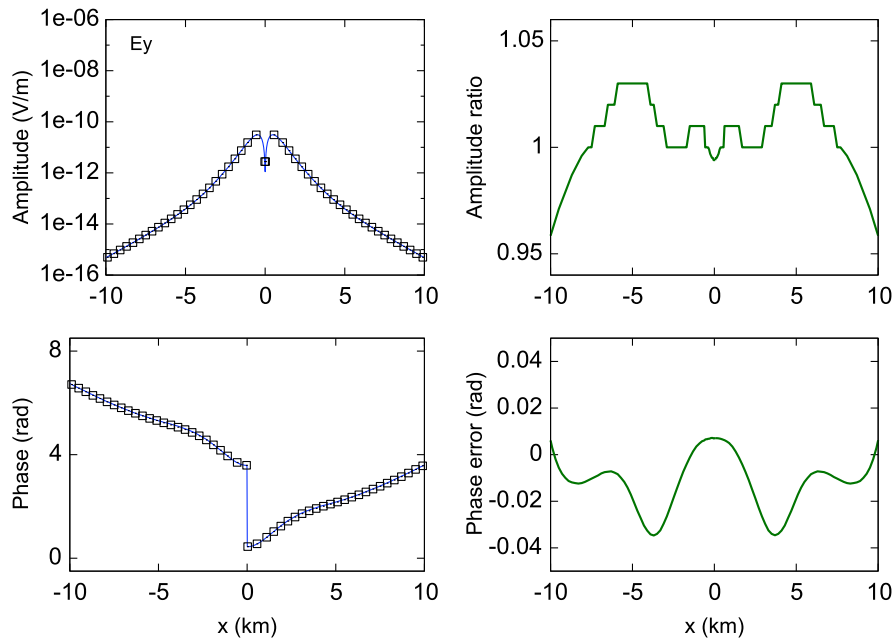


Figure 2.17: Comparison between the eFEM (solid line) and 1D solutions (open squares) for the y-component of the electric field, for the resistivity model illustrated in figure 2.14, along the receiver line $y = 1000$ m. The phase is unwrapped and the source frequency is 0.25 Hz. The plots on the right side show the respective amplitude ratios and phase differences.

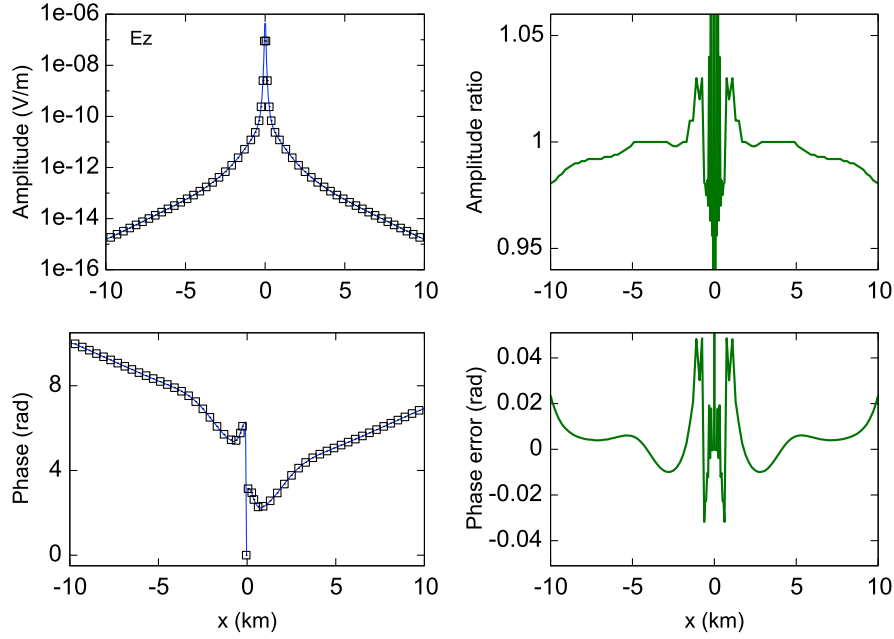


Figure 2.18: Comparison between the eFEM (solid line) and 1D solutions (open squares) for the z -component of the electric field, for the resistivity model illustrated in figure 2.14, along the receiver line $y = 0$ m. The phase is unwrapped and the source frequency is 0.25 Hz. The plots on the right side show the respective amplitude ratios and phase differences.

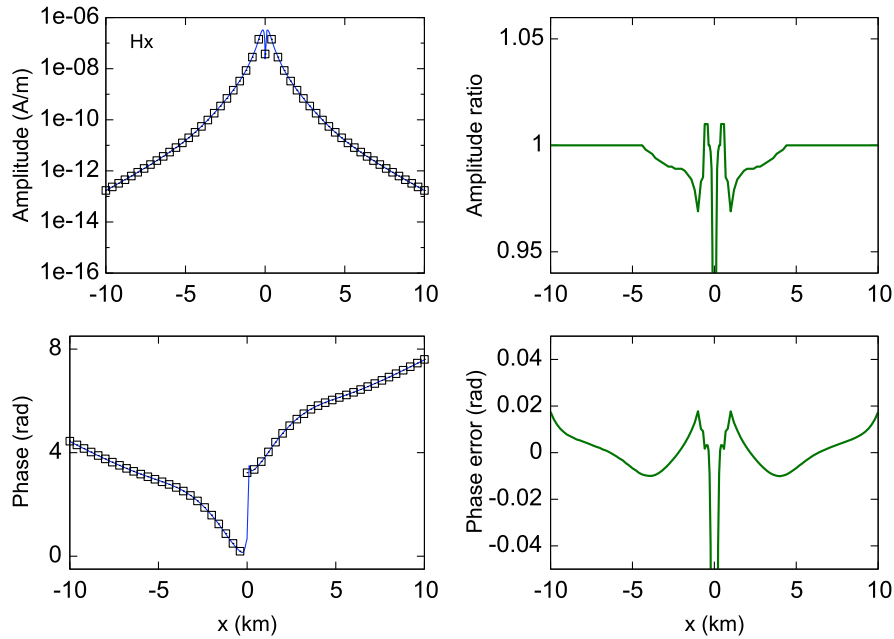


Figure 2.19: Comparison between the eFEM (solid line) and 1D solutions (open squares) for the x -component of the magnetic field, for the resistivity model illustrated in figure 2.14, along the receiver line $y = 260$ m. The phase is unwrapped and the source frequency is 0.25 Hz. The plots on the right side show the respective amplitude ratios and phase differences.

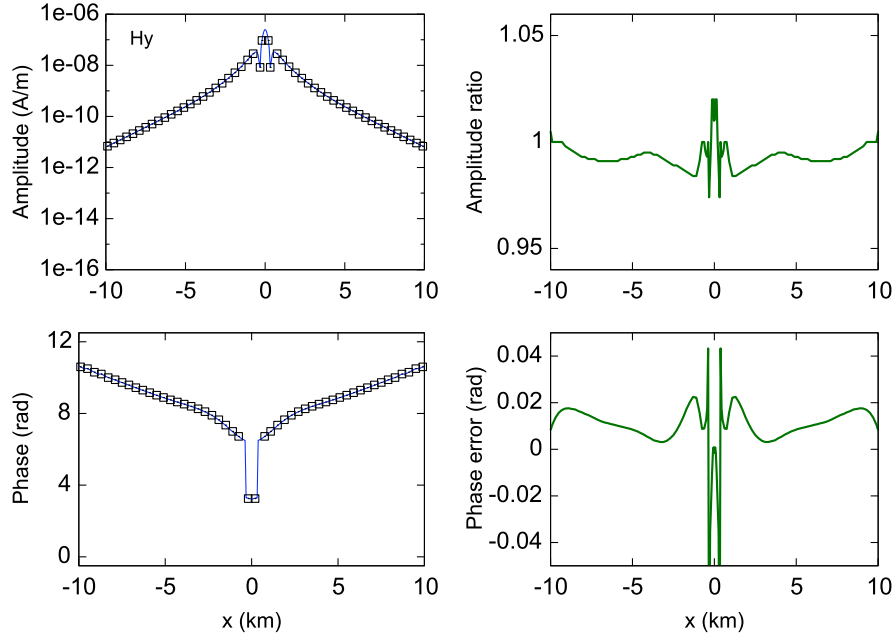


Figure 2.20: Comparison between the eFEM (solid line) and 1D solutions (open squares) for the y-component of the magnetic field, for the resistivity model illustrated in figure 2.14, along the receiver line $y = 350$ m. The phase is unwrapped and the source frequency is 0.25 Hz. The plots on the right side show the respective amplitude ratios and phase differences.

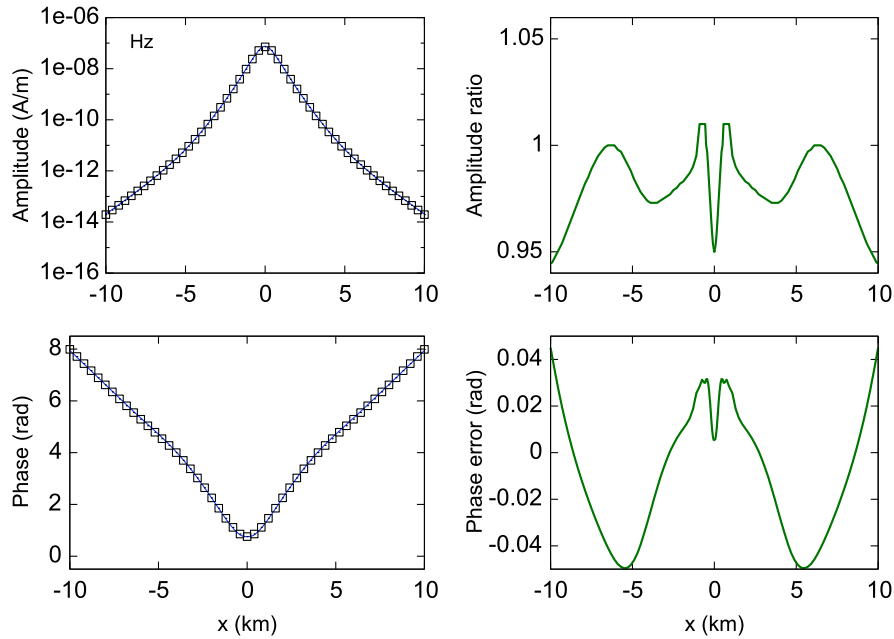


Figure 2.21: Comparison between the eFEM (solid line) and 1D solutions (open squares) for the z-component of the magnetic field, for the resistivity model illustrated in figure 2.14, along the receiver line $y = 500$ m. The phase is unwrapped and the source frequency is 0.25 Hz. The plots on the right side show the respective amplitude ratios and phase differences.

low 5%, and increases towards the boundary of the modelling domain. The relatively larger errors observed in the vicinity of the source position are mainly controlled by two factors. First, the sea-bottom is close to the source position, thus the primary field changes rapidly in a region of anomalous resistivity, and consequently the secondary field also has a strong spatial variation in the vicinity of the source. Second, it is used a first order finite element basis which has difficulty in capturing the strong spatial variation of the electric field in this region of the model. From the computational point of view we can consider the accuracy of the solution to be very good for both the electric and magnetic fields. In addition, as shown in section 2.2.5, the magnetic field is calculated from the numerical solution for the electric field using an interpolator and a local finite difference approximation of Faraday's law (equation 2.3c). Figures 2.19-2.21 show that this approach is suitable for the calculation of the magnetic field, as the magnitude of the error is small and below 5%. It is remarkable that the scheme for the numerical approximation of the magnetic field is stable near the source position, where the electric field changes very rapidly and the grid spacing is small, thus expected to be prone to present problems with stability and accuracy.

In the context of application to inversion of marine CSEM data, we still can consider a very good level of accuracy as any real data set with 5% of uncertainty is considered a good quality data set (Behrens, 2005). In the case of an experiment where repeatability is required, as in the case of time-lapse reservoir monitoring, measurement repeatability should be better than 5% (Orange *et al.*, 2009). However as Orange *et al.* stated, there are several factors which can produce discrepancies larger than 5%, such as near-surface inhomogeneities, bad representation of the ocean conductivity and inaccuracy in the position of sources and receivers. Thus, the level of accuracy obtained with the proposed methodology can be considered good in the framework of the available technology for CSEM data acquisition. For the reasons stated above, I consider that there is a very good agreement between the solution obtained with the edge finite element and the 1D solutions. In addition, considering the level of accuracy, the proposed methodology is suitable for applications to aid real data interpretation and inversion.

Three-dimensional model

It is now shown a three-dimensional resistivity model example which includes an air layer. The eFEM solutions are compared with the ones obtained using an integral equation solution code developed by the CEMI consortium (Hursan & Zhdanov, 2002; Zhdanov *et al.*, 2006). As in the model in the previous section, it is considered a frame of reference with the z-origin at the sea-floor level, all z positive values above the sea-floor and all z-negative values below the sea-floor. Figure 2.22 shows a representation of the 3-D model (truncated at the air-sea interface). The seawater column is 1000 m thick.

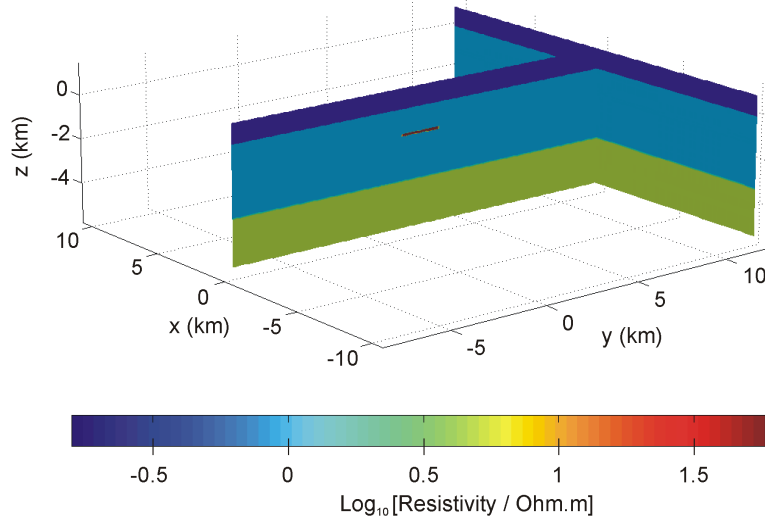


Figure 2.22: Three dimensional resistivity model. The sea-water is 1000 m thick. The air is not represented in the figure, but is included in the resistivity model. The color bar represents the Log_{10} of the resistivity.

In this example it is used a flat sea-floor, in order to ensure that the same geometry is used in both the finite element and integral equation solutions. The effective representation of bathymetry will be considered in future work, as the use of the proposed scheme requires stair-casing multiple elements of constant resistivity to approximate complex shapes.

It is considered a electric-dipole source oriented in the x-direction, represented by a point source in the frequency domain, at $(0, 0, 5)$ m, and are presented solutions for two frequencies that are in the range of frequencies typically used in the CSEM experiment: 1 Hz and 0.1 Hz. It is considered a two half-space background model for both frequencies.

To compute the model responses for a frequency of 1 Hz the model was discretized using a $148 \times 150 \times 65$ irregularly spaced grid (ranging between 10 and 150 m), finer near the source position as in the previous example, representing a computational domain of $20 \times 20 \times 15.5$ km³ and approximately 4.29×10^6 degrees of freedom in double complex arithmetic. The air was represented with a 10 km thick and 10^4 Ωm resistivity layer.

Figure 2.23, shows the response of the electric field in terms of amplitude and phase for a source frequency of 1 Hz. The amplitude and phase values for the x-component are plotted along the receiver line $y = 0$ m, and the y-component values are plotted along the receiver line $x = 500$ m. Figure 2.24, shows the response of the magnetic field for a source with 1 Hz. The amplitude and phase values for the x-component are plotted along the receiver line $y =$

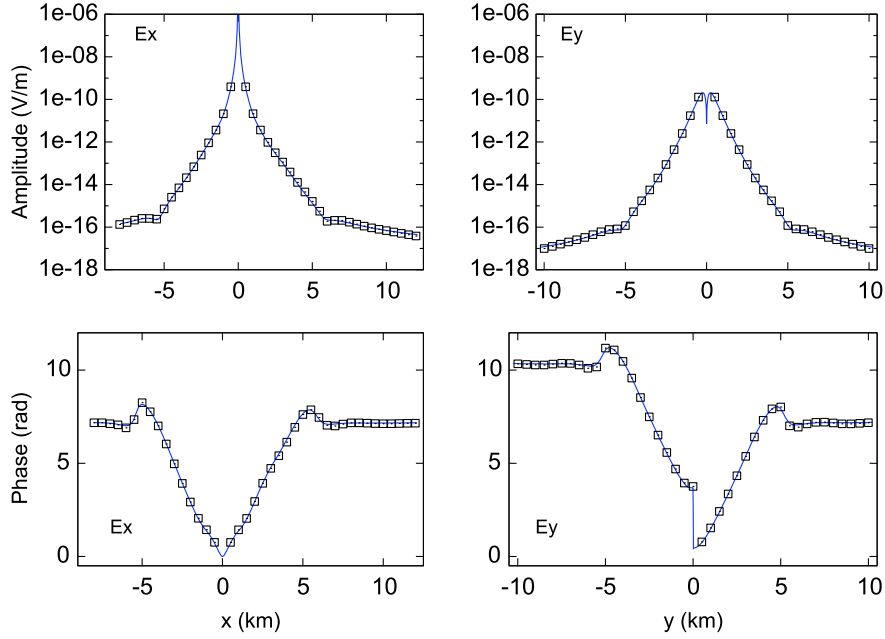


Figure 2.23: Comparison of the electric field responses for the model in figure 2.22 calculated using the finite element method (line) and the integral equation method (open squares). The phase is unwrapped and the frequency is 1 Hz. The field values for the x-component are y-components are plotted along the receiver lines $y = 0$ m and $x = 500$ m, respectively.

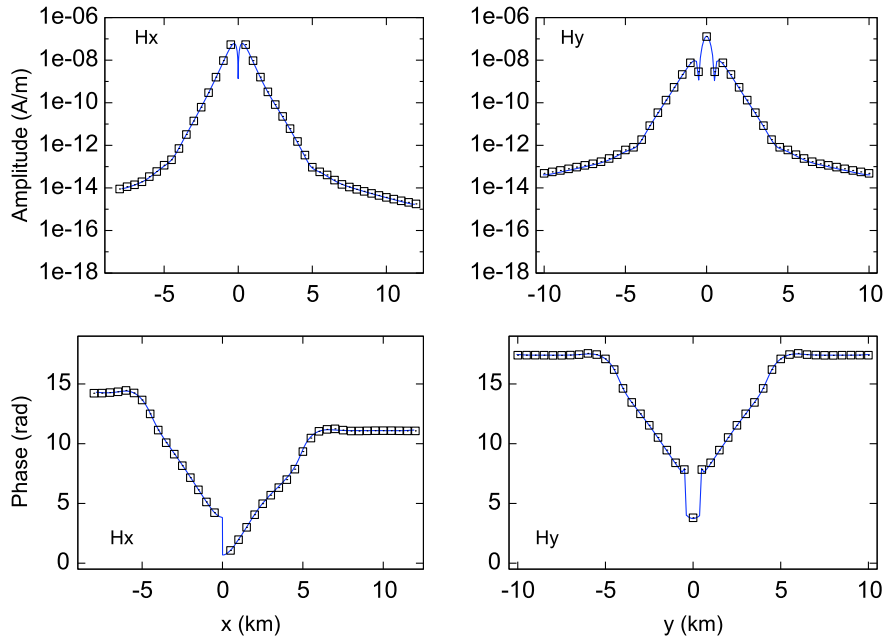


Figure 2.24: Comparison of the magnetic field responses for the model in figure 2.22 calculated using the finite element method (line) and the integral equation method (open squares). The phase is unwrapped and the frequency is 1 Hz. The field values for the x-component and y-component are plotted along the receiver lines $y = 500$ m and $x = 500$ m, respectively.

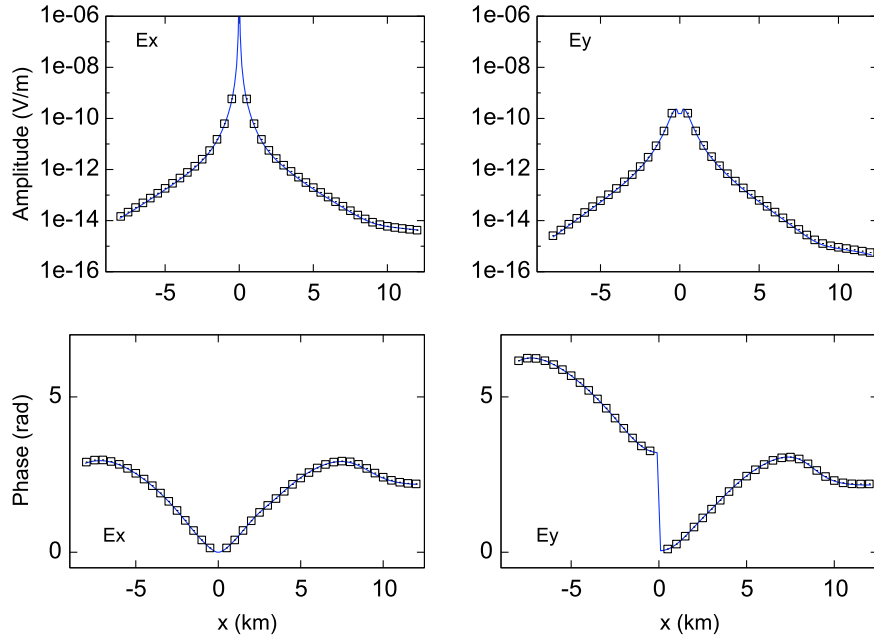


Figure 2.25: Comparison of the electric field responses for the model in figure 2.22 calculated using the finite element method (line) and the integral equation method (open squares). The phase is unwrapped and the frequency is 0.1 Hz. The x-component is plotted along the receiver line $y = 0$ m, and the y-component is plotted along the receiver line $y = 500$ m.

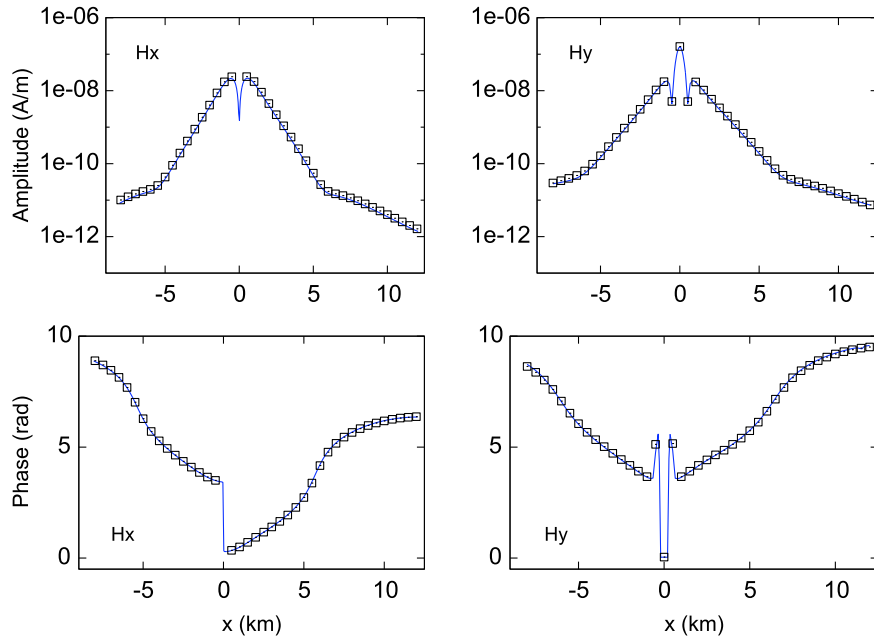


Figure 2.26: Comparison of the magnetic field responses for the model in figure 2.22 calculated using the finite element method (line) and the integral equation method (open squares). The phase is unwrapped and the frequency is 0.1 Hz. The x-component is plotted along the receiver line $y = 1000$ m, and the y-component is plotted along the receiver line $y = 500$ m.

500 m, and for the y component are plotted along the receiver line $x = 500$ m. The phase is plotted unwrapped for both components of the electric and magnetic fields.

For a frequency of 0.1 Hz the model was discretized with a $153 \times 108 \times 69$ irregularly spaced grid representing a computational domain of $23 \times 16 \times 20.6$ km³ and approximately 3.39×10^6 degrees of freedom in double complex arithmetic. The air was represented with a 10 km thick and 10^4 Ω m resistive layer. The grid spacing ranges between 10 and 250 m. The Nyquist criterion is satisfied in the coarser regions of the grid allowing to have less degrees of freedom comparatively to the grid utilized for 1 Hz.

Figure 2.25 shows the response of the electric field for an electric dipole x-oriented and with frequency of 0.1 Hz. The amplitude and phase values for the x-component are plotted along the receiver line $y = 0$ m, and the y-component values are plotted along the receiver line $y = 500$ m. Figure 2.26 shows the response of the magnetic field for an electric dipole oriented in the x direction and with a frequency of 0.1 Hz. The x-component values are plotted along the receiver line $y = 1000$ m whereas the y-component values are plotted along the receiver line $y = 500$ m. The phase is plotted unwrapped for both components of the electric and magnetic fields.

Figures 2.23-2.26 show that there is a very good agreement between the solutions obtained using finite elements and the integral equation method, for both magnetic and electric fields, and for both frequencies.

2.3 Conclusions

In this chapter a method for the solution of the marine CSEM forward modelling problem with the edge finite element method was presented.

As the source presents a singularity at the origin, the electric field is decomposed in primary and secondary components, allowing to remove the singularity from the numerical solution. The primary field can be calculated using a homogeneous or layered background model. It was shown that, when an air layer is represented in the model, it must also be represented in the background model. Its representation in the background model is achieved using a two half-space model. However, the use of layered background models, or two-half space models in particular, requires the calculation of Hankel transforms which is very computationally intensive. As the primary field needs to be calculated at the centre of each edge, the computation of the primary field is parallelized over the edges with openMP directives, keeping the adaptive filtering code serial. Results showed that this approach led to a very good speedup and the computation time of the primary field per source was substantially reduced.

Numerical tests with the presented eFEM scheme, showed that to provide a good level of accuracy using a regularly spaced mesh requires a very fine mesh. Alternatively, a coarser

mesh that satisfies the Nyquist sampling theorem can be used, however, it must be finer near the source position to capture the rapid variation of the electric field in its vicinity.

For a computational domain with the same dimensions, it was shown that the use of a finer grid near the source position, means that an accurate solution can be achieved with significantly less storage needs (in terms of grid dimensions and size of the linear system to solve) than when using a regularly spaced grid.

Several preconditioners were tested to determine which one could provide efficient convergence rates. The Symmetric Gauss-Seidel (SGS) preconditioner showed significant improvements in comparison with the GS, ILU(0) and SSOR preconditioners. The use of an irregularly spaced grid proved to be problematic leading to a significant slowing down of the convergence rate as shown in section 2.2.4.1. Results also showed, that for a large scale model, the practical application of an iterative solver preconditioned with SGS could be prohibitively slow, particularly if a solution must be achieved for a large number of right-hand sides. A parallel implementation of the tested iterative solvers was not tested, as for a larger number of right-hand sides, the needed computational resources will increase dramatically. Thus a more effective preconditioner must be found in order to achieve iterative solutions effectively. The development of preconditioners is an important and active topic of research, and it was not possible to test all preconditioners in the time available. However, for a good scalability of the solver and particularly in three-dimensional problems, it is preferable to use an iterative method, thus further investigation would be useful in the future.

On the other hand, direct solvers scale poorly with the size of the problem and require large computational resources to make relatively large scale problems manageable, but have the advantage of allowing a solution for multiple right hand sides. Nevertheless, it is important to note that, for a multi-source solution the grid needs to be refined near each source position, therefore limiting the size of the problem that can be considered with current hardware and in the current paradigm of factorization algorithms. It was shown that eFEM solutions can be obtained with both iterative and direct solvers. However, for the attainment of the goals of this thesis the direct solver was used as it proved to be more reliable.

A method was implemented for subsequent calculation of the magnetic field, using a finite difference approximation of Faraday's law and an interpolator (Alumbaugh *et al.*, 1996). This technique had already proved useful and effective when combined with the use of the finite difference method scheme for marine CSEM forward modelling, for which grids with constant spacing (or small variation) are generally utilized. In the case of the edge finite element, when using first order basis functions, the grid needs to be finer near the source position where the electric field also changes rapidly, therefore potentially leading to instabilities in the approximation of the magnetic field. It was shown that, even in such conditions, the approach is stable and reliable.

Comparisons with analytical solutions showed errors below 5% which indicate a very good

level of accuracy between solutions for both the electric and magnetic fields. Furthermore, comparisons between eFEM solutions and the integral equation method also showed a very good agreement between the solutions, allowing the conclusion that the proposed method is an alternative to existing marine CSEM forward modelling algorithms, and thus will be used to attain the remaining objectives of this work.

An Approach for 3D CSEM Inversion

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3.1 Introduction to inverse problems

Inverse problems aim to estimate information from a physical system from measurements of some observable at some points (not necessarily at the boundary) of that system. Physical laws are formulated within the rationale *cause-effect*. The solution of an inverse problem is by opposition the *cause* recovered from the *effect*.

The usefulness of finding the solution of an inverse problem relies on the fact that it allows estimates of physical parameters which are not directly observable. For example, estimating

the velocity distribution of the Earth's subsurface from measured travel times is a typical example of an inverse problem. More examples can be found in many different scientific fields, such as medical imaging, remote sensing, statistics or nuclear physics, just to list a few.

Inverse problems are typically ill-posed problems, i.e. at least one of the following condition is not satisfied, accordingly to Hadamard (1902):

1. Existence of solution.
2. Uniqueness of solution.
3. Stability of the solution.

From the geophysical applications point of view, the solution for the inverse problem should exist in some sense, as the problem is being solved for a practical situation. However, the model (or the forward modelling operator) might not represent all the phenomena from which the data depends, that is, the model is approximate, and in addition, data is frequently affected by noise, thus the existence of a solution is not guaranteed. The problem of non uniqueness is well known among practitioners as different models can explain the same measurements, or if one prefers, the same data. Measurements are usually carried out sparsely at the surface of the Earth, or in a very restricted portion of the domain (as in the case of recordings in a borehole), and are always affected by noise. In addition, there is no guarantee of having independent measurements, i.e. that each measurement adds information that cannot be added by any combination of the remaining measurements. Thus, generally the information to reconstruct the model parameters is insufficient, and for that reason the solution is non-unique. Another important issue is the non-continuous dependence of the data. Under such conditions, a small perturbation in the data may create large changes in the model parameters, thus the solution is unstable. This problem is generally mitigated through the use of additional constraints in the inversion procedure, also known as *regularization* of the inverse problem (Zhdanov, 2002).

Before moving further it is important to define some concepts, as sometimes practitioners of inverse problems refer to the same mathematical or physical quantity differently. In this work, the term *model* is used to describe a conceptualization of the physical system and is represented by $\mathbf{G}$. The model is assumed to depend on one or a set of physical parameters, which will be represented through the text by $\mathbf{m}$, such that $\mathbf{G} = \mathbf{G}(\mathbf{m})$, and it is assumed that there is a relation between the model parameters and the data, $\mathbf{d}$:

$$\mathbf{G}(\mathbf{m}) = \mathbf{d} \tag{3.1}$$

Geophysicists generally prefer to use the term *forward modelling operator* to refer to $\mathbf{G}(\mathbf{m})$, and this will also be the term used in this text.

Deriving an exact inverse operator for $\mathbf{G}(\mathbf{m})$, such that $\mathbf{G}^{-1}(\mathbf{d}) = \mathbf{m}$ is a continuous function of $\mathbf{d}$, may not be possible, as such an operator has an infinitely large number of degrees of freedom and generally we only have available a finite amount of input data. In addition, the exact solution of inverse problems is generally unstable and only applicable to very particular problems, thus is of very limited practical relevance, hence geophysical inverse problems are generally solved recasting the continuous formulation to an equivalent discrete form (Parker, 1994; Snieder & Trampert, 1999).

Inverse problems generally fall into two main categories: linear and non-linear. What determines the linearity or non-linearity of the inverse problem is in fact the dependence of the forward modelling operator from the model parameters. If this dependence is linear, the inverse problem is also linear, on the other hand, if the dependence of the forward problem operator from the model parameters is non-linear, then the inverse problem is non-linear. For the case of linear problems, $\mathbf{m}$ is separable from the forward modelling operator, thus equation 3.1 is transformed into:

$$\mathbf{G}\mathbf{m} = \mathbf{d} \quad (3.2)$$

Hence the solution of the linear inverse problem is obtained through the solution of a linear system. Linear systems derived from linear inverse problems are generally rank-deficient and ill-conditioned, thus appropriate methodologies are necessary to achieve a solution. A systematic and comprehensive overview of methods for the solution of linear inverse problems can be found in Aster *et al.* (2005).

The three-dimensional CSEM inverse problem is a non-linear problem, as $\mathbf{G}$ does not depend linearly from $\mathbf{m}$. In the next sections are reviewed the principal techniques for the solution of non-linear inverse problems. Even though these concepts are presented in the context of electromagnetic inversion, they are completely general and can be applied in a straight-forward way to other geophysical inverse problems such as seismic wave inversion for example. This section is a very short introduction to inverse problems. Further details can be found in Zhdanov (2002), Vogel (2002), Aster *et al.* (2005) and Tarantola (2005).

3.2 An overview of the non-linear inverse problem

The solution of the non-linear inverse problem is generally obtained by recasting 3.1 in an optimization problem, by defining a parametric functional of the form:

$$\min f(\mathbf{m}) = \frac{1}{2} [\mathcal{D}(\mathbf{G}(\mathbf{m}) - \mathbf{d})]^T [\mathcal{D}(\mathbf{G}(\mathbf{m}) - \mathbf{d})^*] + \frac{1}{2} \lambda \mathcal{R}(\mathbf{m}) = \frac{1}{2} \Delta \mathbf{d}^T \Delta \mathbf{d}^* + \frac{1}{2} \lambda \mathcal{R}(\mathbf{m}) \quad (3.3)$$

Where $\mathcal{D}$ is a weighting matrix, λ is the regularization parameter and $\Delta \mathbf{d}$ is the vector of weighted data residuals. Equation 3.3 is also referred to as cost function or objective function. Mathematical symbols are listed in table A.1. The first term represents a measure of the misfit between the observations and the predicted model responses and the second term is the so-called regularization term which aims to stabilize the solution. The regularization term $\mathcal{R}(\mathbf{m})$, can assume many forms depending on which type of constraint is desirable. This term generally has a strong impact on the smoothness or roughness of the estimated model (Zhdanov, 2002; Aster *et al.*, 2005). This issue, including the estimation of the regularization parameter (λ) is further discussed in section 3.4. The asterisk denotes complex conjugation. Generally it is assumed that the noise present in the observations is uncorrelated and Gaussian, thus the weighting matrix $\mathcal{D}$ is diagonal, and it can have assigned to the members in the main diagonal, the standard deviation (Farquharson & Oldenburg, 2004; Aster *et al.*, 2005), or the inverse of the amplitudes of the field observations (Gribenko & Zhdanov, 2007).

There are essentially two approaches for the solution of 3.3: probabilistic methods and deterministic methods. The choice of which method to use relies fundamentally on the approach adopted to obtain the forward modelling solution. Probabilistic methods attempt to quantify the probability of a certain model being the solution of the inverse problem, depending naturally on its consistency with the geological structures and on explaining the observations, that is, the synthetic data *fits* in some sense the observed data (Tarantola, 2005). When implementing such methods it is necessary to use a good random number generator (Press *et al.*, 2002) and generally it is required the estimation of millions of states of the system, or, if one prefers, millions of forward modelling solutions (Sen & Stoffa, 1995). Thus, their use is prohibitive when the forward modelling solution is obtained with the finite difference method or the finite element method, as a solution for the inverse problem can not be achieved in a practical time window. Deterministic methods on the other hand, are iterative (for the case of non-linear inverse problems) and rely on the use of an initial guess of the optimal model parameters, which is improved at each iteration, until the optimal solution for the model parameters is found. Deterministic methods require the estimation of derivatives of the parametric functional with respect to the model parameters. Generally, optimal solutions are attained within a few hundreds of iterations, however, the number of iterations that are necessary to achieve an optimal solution is highly variable and depends on the type of the problem, initial guess, conditioning and stabilization. For example, an inappropriate starting model can make the algorithm to search for a solution in a basin of attraction which is not the one of the global minimum. In addition, deterministic methods are local and consequently susceptible of being trapped in a local minimum (Plessix, 2006). In this work only deterministic local methods based on the use of the gradient of 3.3 are considered, and the relevant theory for its implementation is described in the next sections.

The most widespread approaches for the solution of the non-linear inverse problem use

gradient-based methods, such as steepest descent or non-linear conjugate gradients, or Newton-based methods, such as quasi-Newton methods or Gauss-Newton methods. These methods generally require the solution of three forward modelling problems in each tomographic iteration. That is, forward modelling solutions are required to calculate the data misfit, the search direction, and to determine the optimal search parameter.

A particularly interesting approach is that, when integral equations are used, the sensitivities and optimal step length can be calculated using the quasi-analytical approximation (Zhdanov & Hursan, 2000), reducing the number of forward modelling solutions per tomographic iteration to one (Golubev & Zhdanov, 2005; Gribenko & Zhdanov, 2007), therefore reducing significantly the computing time.

The contrast source inversion (CSI) method reformulates the forward modelling problem in terms of the scattered field (*e.g.*, acoustic pressure, electromagnetic field, etc.) and a contrast function of the physical parameter to be estimated. The inverse problem is formulated in an optimization problem to reconstruct the contrast-function and the contrast-source (van den Berg & Kleinman, 1997). The particular formulation of the CSI method avoids the solution of the forward modelling problem at each iteration, requiring only the estimation of the gradient and the optimal line search parameter. The estimation of the optimal line search parameter can also be circumvented by using the multiplicative cost function (van den Berg *et al.*, 1999) instead of the more widely used additive cost function 3.3. The CSI has been applied in a wide range of imaging problems using both the integral equation method and the finite difference method (Abubakar *et al.*, 2008b, 2011b).

As the three-dimensional CSEM inverse problem may require the estimation of several millions of parameters, and the forward modelling solution is obtained with the finite element method, the only feasible option is the use of iterative optimization methods. Section 3.3 provides a short reviewed of the most relevant aspects of iterative optimization methods for the attainment of the objectives of this work.

3.3 A short review on iterative optimization methods

The solution of the inverse problem, was reformulated to find a set of model parameters that fits the data in the sense of 3.3, thus requiring the solution of an optimization problem. Optimization algorithms generate a sequence of approximations $\mathbf{m}_k$, until a solution is found or any other stopping criteria is satisfied. At iteration k , the algorithm searches for a new solution $\mathbf{m}_{k+1}$, such that the value of f decreases, that is $f(\mathbf{m}_{k+1}) < f(\mathbf{m}_k)$, using information about the objective function f and possibly from previous iterations, $\mathbf{m}_0, \mathbf{m}_1, \dots, \mathbf{m}_{k-1}$ (Nocedal & Wright, 2006).

There are essentially two approaches to move to a new iteration: *Line search* and *Trust region* methods. *Line search* methods determine a direction $\mathbf{p}_k$, and search in this direction

for a new iterate $\mathbf{m}_{k+1}$ for which the functional value decreases, such that $\mathbf{m}_{k+1} = \mathbf{m}_k + \alpha_k \mathbf{p}_k$. The factor α_k is known as the step length and is determined from:

$$\min_{\alpha_k > 0} f(\mathbf{m}_k + \alpha_k \mathbf{p}_k) \quad (3.4)$$

It is important to note that it is sufficient to determine the step-length approximately and that the minimization problem 3.4 is never solved exactly as this is expensive (Kelley, 1995; Nocedal & Wright, 2006). This problem will be revisited later in the text.

Alternatively *trust region* methods, search for a new iterate within a pre-defined distance from $\mathbf{m}_k$, or trust region. If there is no sufficient decrease in f then it is concluded that the trust region is too large, and a new search is started after reducing the trust region. Otherwise a new iteration is found, and the previous steps are repeated until a solution of the optimization problem is found or no progress is made. The well known Levenberg-Marquardt (Levenberg, 1944; Marquardt, 1963) algorithm is a trust region method.

In summary, line search methods determine a search direction and then an optimal distance for updating the solution, whereas trust region methods use a pre-defined region in the space of model parameters where is assumed to exist an iterate that will decrease the value of the functional by a certain quantity, and then determine the direction along which the approximate solution is updated.

In the context of this thesis there are no particular reasons to choose one method or the other, as the theoretical framework of both approaches can be adopted to solve optimization problems 3.3. Nonetheless, line search methods are the chosen strategy for this work, as the mathematical theory is very mature at this stage and they have been traditionally and successfully applied in many geophysical inverse problems.

In conclusion, the use of local methods for the solution of non-linear optimization problems, requires the determination of a search direction and estimation of an optimal step length. In the next two sections these two topics are reviewed.

3.3.1 Determination of the search direction

In this section is reviewed an approach to determine the search direction. Expanding 3.3 in a second order Taylor's series (Marsden, 2003) in the neighborhood of $\mathbf{m}_k$ yields:

$$f(\mathbf{m}_{k+1}) = f(\mathbf{m}_k) + \nabla_m f(\mathbf{m}_k) \Delta \mathbf{m} + \frac{1}{2} \Delta \mathbf{m}^T \mathcal{H}(\mathbf{m}_k) \Delta \mathbf{m} + \mathcal{O}(\Delta \mathbf{m}^3) \quad (3.5)$$

Where $k = 0, 1, \dots$, $\Delta \mathbf{m} = \mathbf{m}_{k+1} - \mathbf{m}_k$, $\mathcal{H}(\mathbf{m}_k)$ is the Hessian of the objective function at $\mathbf{m}_k$, and $\mathcal{O}(\Delta \mathbf{m}^3)$ is the truncation error. We are searching for a model parameter update, $\mathbf{m}_{k+1} = \mathbf{m}_k + \alpha_k \mathbf{p}_k$, thus the search direction $\mathbf{p}_k$ and the model update $\Delta \mathbf{m}$ have the same direction, differing in magnitude by a factor α_k .

The direction of fastest decrease is given by the vector that minimizes the value of $f(\mathbf{m}_{k+1})$ for a first order approximation (Nocedal & Wright, 2006):

$$\mathbf{p}_k = -\nabla_m f(\mathbf{m}_k) / \|\nabla_m f(\mathbf{m}_k)\|_2 \quad (3.6)$$

The Newton direction is constructed by using a Taylor's expansion for the gradient of f (Aster *et al.*, 2005; Nocedal & Wright, 2006):

$$\nabla f(\mathbf{m}_{k+1}) = \nabla f(\mathbf{m}_k) + \mathcal{H}(\mathbf{m}_k)\Delta\mathbf{m} + \mathcal{O}(\Delta\mathbf{m}^2) \quad (3.7)$$

If $\mathbf{m}_{k+1}$ is a minimizer then $\nabla f(\mathbf{m}_{k+1}) = \mathbf{0}$, hence:

$$\mathcal{H}(\mathbf{m}_k)\Delta\mathbf{m} = -\nabla_m f(\mathbf{m}_k) \quad (3.8)$$

As $\mathbf{p}_k$ and $\Delta\mathbf{m}$ have the same direction, one can conclude that the Newton search direction is given explicitly by (Kelley, 1995; Nocedal & Wright, 2006):

$$\mathbf{p}_k = -\mathcal{H}_k^{-1}(\mathbf{m}_k)\nabla_m f_k(\mathbf{m}_k) \quad (3.9)$$

It is worth noting that gradient methods are outperformed by methods that use the Newton direction as the latter uses a quadratic model of the cost function (Kelley, 1995; Nocedal & Wright, 2006). However, Newton-based methods require the computation of the Hessian, which must be positive definite, and can require the solution of a linear system at each tomographic iteration, as in the case of the Gauss-Newton method. Thus they are computationally more demanding than gradient based methods. In this work is utilized the L-BFGS method which minimizes the computational burden of these two factors.

3.3.2 Determination of the step-length

The determination of the optimal step length α_k lies at the heart of many optimization procedures, and should allow for a considerable decrease of the functional f . Identifying α_k exactly requires the solution of the minimization problem 3.4. Nonetheless, such an approach can be computationally very expensive, possibly requiring a large number of evaluations of the objective function along the search direction $\mathbf{p}_k$. Thus generally its determination is done by an inexact line search method. Here is presented a short review on an inexact line search approach and necessary conditions to achieve a sufficient reduction in the functional, as this is a fundamental aspect of the non-linear optimization methods applied in this work. To ensure that a chosen step length is appropriate, it is sufficient to meet the following

conditions (Nocedal & Wright, 2006; Kelley, 1995):

$$f(\mathbf{m}_k + \alpha_k \mathbf{p}_k) \leq f(\mathbf{m}_k) + \delta_1 \alpha_k \nabla f(\mathbf{m}_k)^T \mathbf{p}_k \quad (3.10a)$$

$$\nabla f(\mathbf{m}_k + \alpha_k \mathbf{p}_k)^T \mathbf{p}_k \geq \delta_2 \nabla f(\mathbf{m}_k)^T \mathbf{p}_k \quad (3.10b)$$

$$0 < \delta_1 < \delta_2 < 1$$

Inequalities 3.10 are known as the *Wolfe conditions*, and 3.10a is also known as the *Armijo condition*. The Armijo condition ensures that a sufficient decrease in the functional is attained at each iteration. For a better understanding of Wolfe conditions it is convenient to use the following parameterization of the functional 3.3:

$$\begin{aligned} \phi(\alpha) &= f(\mathbf{m}_k + \alpha \mathbf{p}_k) \\ \alpha &> 0 \end{aligned} \quad (3.11)$$

Thus the following identity holds:

$$\phi(\alpha) = f(\mathbf{m}_k + \alpha \mathbf{p}_k) = f(\mathbf{m}_k) + \alpha \nabla f(\mathbf{m}_k)^T \mathbf{p}_k \quad (3.12)$$

and the Wolfe conditions can be recast:

$$\phi(\alpha) \leq \phi(0) + \delta_1 \alpha \phi'(0) \quad (3.13a)$$

$$\phi'(\alpha_k) \geq \delta_2 \phi'(0) \quad (3.13b)$$

Where $\phi'(x) = d\phi/d\alpha|_{\alpha=x}$. Thus, the first condition imposes the regions of the functional along the direction $\mathbf{p}_k$ for which it is acceptable to move. The second condition makes sure that the line search stops if the curvature only changes slightly, or if it is positive.

Generally only the Armijo rule is utilized. Thus, if a chosen α_0 produces a sufficient decrease, the new iteration is accepted. Otherwise, the interval $[0, \alpha_0]$ contains step-lengths that satisfy condition 3.10a, thus an acceptable step length can be found by interpolation (Nocedal & Wright, 2006). In the interval $[0, \alpha_0]$, the following identities hold:

$$\phi(0) = f(\mathbf{m}_k) \quad (3.14a)$$

$$\phi'(0) = \nabla f(\mathbf{m}_k)^T \mathbf{p}_k < 0 \quad (3.14b)$$

$$\phi(\alpha_0) = \phi(0) + \alpha_0 \phi'(0) \quad (3.14c)$$

To determine an appropriate step length, equation 3.11 is approximated with a second order polynomial:

$$\phi(\alpha) = a + b\alpha + c\alpha^2 \quad (3.15)$$

and the coefficients a , b and c , are determined from conditions 3.14, hence:

$$\phi(\alpha) = \phi(0) + \phi'(0)\alpha + \left[\frac{\phi(\alpha_0) - \phi(0) - \phi'(0)\alpha_0}{\alpha_0^2} \right] \alpha^2 \quad (3.16)$$

Thus the optimal step-length is determined at the minimum of 3.16 in the interval $[0, \alpha_0]$, that is, the point α_1 for which $\phi'(\alpha_1) = 0$, thus:

$$\alpha_1 = -\frac{\phi'(0)\alpha_0^2}{2(\phi(\alpha_0) - \phi(0) - \phi'(0)\alpha_0)} \quad (3.17)$$

If α_1 does not produce sufficient decrease, then a third-order polynomial is constructed, utilizing information from $\phi(0)$, $\phi'(0)$, $\phi(\alpha_0)$ and $\phi(\alpha_1)$. Thus the parametric equation 3.11 is approximated by:

$$\phi(\alpha) = a + b\alpha + c\alpha^2 + d\alpha^3 \quad (3.18)$$

From conditions, 3.14, $a = \phi(0)$ and $b = \phi'(0)$, and the remaining coefficients are determined by the solution of the linear system:

$$\begin{pmatrix} \alpha_1^2 & \alpha_1^3 \\ \alpha_0^2 & \alpha_0^3 \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} \phi(\alpha_1) - \phi(0) - \phi'(0)\alpha_1 \\ \phi(\alpha_0) - \phi(0) - \phi'(0)\alpha_0 \end{pmatrix} \quad (3.19)$$

After determining the coefficients c and d , the minimum of 3.18 in the interval $[0, \alpha_0]$ is determined by setting its derivative to zero, yielding:

$$\alpha_2 = \frac{-c + \sqrt{c^2 - 3d\phi'(0)}}{3d} \quad (3.20)$$

It is important to note that the minimization problem with the third-order polynomial has two mathematical solutions, nonetheless 3.20 is the only one that can be positive, as it is required a positive value for α .

The line search method reviewed in this section, was implemented in the inversion algorithms developed in this thesis.

An extensive and more fundamental description of line search methods can be found in Nocedal & Wright (2006) and Kelley (1995). In the next sections some of most important methods for the solution of the optimization problem 3.3, are reviewed.

3.3.3 Solution of the optimization problem

3.3.3.1 Steepest descent method

The steepest descent method, only requires the direction of the gradient of the functional in model parameter space, and each new iterate is obtained from the previous one by the

update formula (Kelley, 1995):

$$\mathbf{m}_{k+1} = \mathbf{m}_k - \alpha_k \nabla_m f(\mathbf{m}_k) \quad (3.21)$$

Algorithm 1 describes the steepest descent algorithm as generally presented in the literature and as implemented here in a Fortran 90 code. The maximum number of iterations k_{max} is defined by the user and ε_1 and ε_2 are the threshold tolerances for the norm of the gradient and for the objective function, respectively.

At each iteration an appropriate step-length α_k , is estimated from the values of functional and of the gradient, and a new iteration is found if the Armijo condition (expression 3.10a) is satisfied.

The steepest descent method, is remarkable for its simplicity and low demand of computational capabilities because it requires essentially the storage of the gradient vector and the storage of two vectors with the approximated model parameters of the current and next iterations. Nonetheless, it suffers from slow convergence when the curvature of the functional to be minimized changes significantly with direction and, when it approaches the minimum of the functional. The non-linear conjugate gradient method or quasi-Newton methods are a suitable alternative as they generally offer faster convergence than the gradient descent method, but are slightly more expensive in computational terms.

Algorithm 1 Steepest descent algorithm

```

Set  $\mathbf{m}_0$ 
Evaluate  $\nabla f_0$ 
 $k \leftarrow 0$ 
while ( $\|\nabla_m f\| > \varepsilon_1; f > \varepsilon_2; k < k_{max}$ ) do
  Set  $\alpha_k$ 
   $p_0 \leftarrow -\nabla f_0$ 
   $\mathbf{m}_{k+1} = \mathbf{m}_k + \alpha_k p_k$ 
  Check Armijo Condition
  Compute  $\nabla f_{k+1}$ 
   $k \leftarrow k + 1$ 
end while

```

3.3.3.2 L-BFGS method

The use of the Hessian in iterative optimization schemes improves significantly the convergence rate, as it uses a second order approximation of the parametric functional. Nonetheless the Hessian matrix is dense, thus its storage or manipulation during calculations may be impractical for large scale problems in which millions of parameters are estimated. Quasi-Newton methods try to circumvent this problem approximating the Hessian of the objective function by measuring changes in the gradient at each iteration. The Limited-Memory

Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) algorithm (Liu & Nocedal, 1989) uses a recursive formula to estimate an approximate inverse of the Hessian by using a pre-determined small number of approximated solutions in the previous iterations and respective gradients. As mentioned before, the Newton direction for the updating of the model parameters at iteration k is:

$$\mathbf{m}_{k+1} = \mathbf{m}_k + \alpha_k \mathbf{p}_k = \mathbf{m}_k - \alpha_k \mathcal{H}_k^{-1}(\mathbf{m}_k) \nabla_m f(\mathbf{m}_k) \quad (3.22)$$

From expression 3.22 it is evident that only the action of $\mathcal{H}_k^{-1}$ over $\nabla_m f_k$, is necessary, allowing a substantial saving in computer storage. A recursive expression for updating the action of the inverse of the Hessian over the gradient of the objective function can be derived from (Nocedal & Wright, 2006):

$$\mathcal{H}_{k+1}^{-1} = \mathcal{V}_k \mathcal{H}_k^{-1} \mathcal{V}_k + \tau_k \mathbf{s}_k \mathbf{s}_k^T \quad (3.23)$$

and,

$$\begin{aligned} \tau_k &= \frac{1}{\mathbf{y}_k^T \mathbf{s}_k} \\ \mathcal{V}_k &= \mathcal{I} - \tau_k \mathbf{y}_k \mathbf{s}_k^T \\ \mathbf{s}_k &= \mathbf{m}_{k+1} - \mathbf{m}_k \\ \mathbf{y}_k &= \nabla_m f_{k+1} - \nabla_m f_k \end{aligned} \quad (3.24)$$

Algorithm 2 describes the L-BFGS method as it is generally presented in the literature, and implemented here in a Fortran 90 code. Again k_{max} is the maximum number of iterations defined by the user and ε_1 and ε_2 are the threshold tolerances for the gradient and the objective function, respectively.

When using the L-BFGS method it is sensible to consider the unit step-length ($\alpha_k = 1$), as the search direction is close to the Newton direction. The action of the inverse of the Hessian matrix over the gradient is computed at each iteration using the recursive update expression based on expressions 3.23 and 3.24.

For the first w iterations, the L-BFGS method behaves as a preconditioned steepest-descent method, as the inverse of the Hessian is being updated at each iteration utilizing an identity matrix scaled by γ_k . The low memory BFGS method, is more costly, in terms of number of computing operations and memory requirements in comparison to the steepest descent method, as it requires updating the Hessian matrix at each iteration and the storage of the vector pairs $\mathbf{y}_k$ and $\mathbf{s}_k$ from the previous w iterations. Therefore the memory requirements increase with the size of the model. However, it is important to note that is only necessary to store a small number of vector pairs, making this method very efficient in terms of the

Algorithm 2 L-BFGS algorithm

```

Set  $\mathbf{m}_0$ 
Evaluate  $f_0$  and  $\nabla f_0$ 
Set number of vector pairs to store  $w$ 
 $\mathcal{H}_0^{-1} = \mathcal{I} / \|\nabla f_0\|$ 
 $k \leftarrow 0$ 
while ( $\|\nabla_m f\| > \varepsilon_1; f > \varepsilon_2; k < k_{max}$ ) do
   $\mathbf{p}_k \leftarrow -\mathcal{H}_k^{-1} \nabla f_k$ 
   $\alpha_0 \leftarrow 1$ 
   $\mathbf{m}_{k+1} = \mathbf{m}_k + \alpha_k \mathbf{p}_k$ 
  Check Armijo Condition
   $\mathbf{s}_k = \mathbf{m}_{k+1} - \mathbf{m}_k$ 
  Evaluate  $\nabla f_{k+1}$ 
   $\mathbf{y}_k = \nabla f_{k+1} - \nabla f_k$ 
  if  $k > w$  then
    Discard  $\mathbf{y}_{k-l}$  and  $\mathbf{s}_{k-l}$ 
  end if
  Store  $\mathbf{s}_k$  and  $\mathbf{y}_k$ 
   $\gamma_{k+1} = \mathbf{s}_k^T \mathbf{y}_k / \mathbf{y}_k^T \mathbf{y}_k$ 
  if  $k > w$  then
    Update the inverse of the Hessian  $\mathcal{H}_{k+1}^{-1}$ , using  $\mathcal{H}_k^{-1} = \gamma_{k+1} \mathcal{I}$  and 3.23
  else
     $\mathcal{H}_{k+1}^{-1} = \gamma_{k+1} \mathcal{I}$ 
  end if
   $k \leftarrow k + 1$ 
end while

```

trade-off between computing requirements and improved convergence speed.

Methods that only use information from the gradient of the objective function can be further improved by using a preconditioner to improve the direction of the gradient. This topic will be further explored in section 3.8.

3.4 Regularization

Inverse problems are *ill-posed* and therefore are unstable. This problem was initially tackled by Tikhonov & Arsenin (1977) leading to the development of an almost self-contained mathematical discipline named *regularization theory*. The main concept at the heart of the regularization theory, is replacing the original ill-posed problem by an approximate well-posed problem depending on the parameter λ , and the solution of the new well-posed problem tends to the true solution when $\lambda \rightarrow 0$ (Zhdanov, 2002).

The main approach used to stabilize the solution of the inverse problem is to include additional constraints in the objective function, and there are essentially two approaches:

the additive cost function (as in equation 3.3) or the multiplicative cost function (van den Berg *et al.*, 1999). The first is the most widely used formulation in the geophysical community, whereas the latter, despite not so commonly used, has recently gained more attention and has been applied to both electromagnetic and seismic imaging problems (Abubakar *et al.*, 2009; Hu *et al.*, 2009b; Liang *et al.*, 2010).

The regularization term $\mathcal{R}(\mathbf{m})$, can assume many forms depending on the desired characteristics of the estimated model. Some of the most common stabilizers are, the minimum norm for the model, minimum norm of the gradient, minimum norm of the Laplacian (or smoothness constraint) and total variation. A comprehensive explanation and discussion on the advantages and disadvantages of the different types of stabilizers can be found in Zhdanov (2002) and Vogel (2002). In this work it was chosen a smoothing constraint, by discretizing the Laplacian operator using a finite difference approximation, which is sparse (Press *et al.*, 2002). This operator penalizes solutions which are rough in the second derivative (Aster *et al.*, 2005). Due to its particular characteristic of leading to smooth models, this stabilizer may fail to represent geological features where the physical properties change rapidly. Nonetheless, it has been successfully implemented in many inversion schemes (Constable *et al.*, 1987; Zhdanov & Fang, 1996), including the inversion of CSEM field data (Commer *et al.*, 2008; Commer & Newman, 2008). The chosen norm is the L_2 norm to keep consistency with the residual term (first term of 3.1), which is also quadratic. The regularization term is represented by:

$$\mathcal{R}(\mathbf{m}) = \|\mathcal{L}\mathbf{m}\|_2^2 \quad (3.25)$$

Where $\mathcal{L}$ is the finite difference approximation of the Laplacian operator (Press *et al.*, 2002). One crucial aspect of regularized non-linear inversion is the estimation of the regularization parameter λ . When using the multiplicative cost function, the regularization parameter is estimated automatically (van den Berg *et al.*, 1999). In the case of using an additive cost function, this parameter must be estimated and there are several strategies depending if the inverse problem is linear or non-linear. In the case of the linear inverse problem the estimation of λ does not represent a major obstacle. For example, if the solution is obtained with the Singular Values Decomposition (SVD) the solution can simply be regularized by neglecting the vectors of the decomposition that correspond to null singular values (Hansen, 2010). Alternatively, the linear inverse problem can be solved for several regularization parameters and the dependence of the norm of the data misfit with the norm of the regularization term plotted on a *log-log* scale, resulting in a "L-shape" curve. This approach is called the *L-curve criterion*. This behavior is expected as the regularization is penalizing some measure of the model variation, therefore this term decreases with increasing λ and the norm of the data misfit increases with decreasing λ (Aster *et al.*, 2005). By inspection of the so-called L-curve it is possible to determine the model that simultaneously fits the data and minimizes the

constraint term (Hansen, 1994).

In the case of non-linear inverse problems such an approach is impractical as it would require several estimates of the regularization parameter at each iteration, increasing substantially the computational load in terms of run time and storage requirements. An effective approach is to use a *cooling* method (Newman & Hoversten, 2000; Gribenko & Zhdanov, 2007; Farquharson & Oldenburg, 2004) to determine the regularization parameter. The cooling approach consists in choosing a large number for the regularization parameter at the first iteration, and use a defined mathematical law to decrease this number at each tomographic iteration (Gribenko & Zhdanov, 2007):

$$\begin{aligned}\lambda_n &= \lambda_0 a^{n-1} \\ n &= 1, 2, \dots \text{ and } 0 < a < 1\end{aligned}\tag{3.26}$$

The process continues until the misfit is below the pre-defined threshold.

In the developed inversion algorithm I implemented a slightly different cooling approach, and is based upon the fact that, for large values of the regularization parameter, the algorithm will be essentially minimizing the stabilizing component, and that when the values of the regularization parameter are small the inversion algorithm will be essentially fitting the model responses to the observations. For example, if the regularization parameter is very large and kept constant during the inversion scheme, there is a point beyond which one can still observe a decrease in the value of the functional, but the data misfit is increasing. This suggests that the regularization parameter can be decreased by taking into account the improvement in data misfit.

The cooling approach introduced here, starts with a large value for the regularization parameter, and decreases it accordingly to the conditions expressed in algorithm 3. This algorithm presents an alternative to decrease the regularization parameter based on the decrease of the data misfit in relation to the previous iteration. The regularization parameter decreases by a

Algorithm 3 *Cooling* approach for the regularization parameter

ϑ_{old} Data misfit (RMS) in the previous iteration
 ϑ_{new} Data misfit (RMS) in the current iteration
 λ_{old} Regularization parameter in the previous iteration
 λ_{new} Regularization parameter in the current iteration
 χ *Cooling* factor
 δ Threshold parameter to control decrease of the data misfit
if $\vartheta_{new} > \delta \vartheta_{old}$ **then**
 $\lambda_{new} = \chi \lambda_{old}$
else
 $\lambda_{new} = \lambda_{old}$
end if

factor χ if the data misfit does not decrease by at least a pre-defined fraction of the previous level of the data misfit in the previous iteration. I can speculate that this approach could be used with other stabilizers, however, the temporal constraint related with the completion of this thesis dictated that only the smoothing stabilizer was explored in the presented inversion scheme.

3.5 Re-parameterization of the model parameters

The solution of the minimization problem does not necessarily lead to physically meaningful solutions. For example, the estimated discrete distribution of conductivity (or resistivity) may contain negative values. In addition, it is known that the conductivity of geological formations can change by several orders of magnitude, leading to an ill-scaled problem. The re-parametrization of the inverse problem is a well known strategy to overcome these two problems (Newman & Alumbaugh, 1997), by defining the k -th model parameter (corresponding to the k -th cell) as:

$$m_k = \log_{10}(\sigma_k) \quad (3.27)$$

Thus the conductivity (or resistivity) is constrained to positive values and the inverse problem is better scaled. The relation between the partial derivatives with respect to m_k and σ_k is obtained from the chain rule, yielding:

$$\frac{\partial g_i}{\partial m_k} = \frac{\partial g_i}{\partial \sigma_k} \frac{\partial \sigma_k}{\partial m_k} = \sigma_k \ln(10) \frac{\partial g_i}{\partial \sigma_k} \quad (3.28)$$

Where $g_i = [\mathbf{G}(\mathbf{m})]_i$, is the computed model response for the i -th observation. In the next sections is reviewed the necessary theory to compute the sensitivities of the electromagnetic field using the reciprocity theorem.

3.6 Computation of the sensitivities

3.6.1 Numerical computation of the Fréchet derivative using an explicit method

When analytical expressions are not available for the calculation of Fréchet derivatives, which almost always happens, sensitivities must be calculated numerically. A first approach is to use the sensitivity-equation method, consisting in differencing the forward model operator with respect to a model parameter and solve the boundary value problem. Hence the Fréchet derivative is explicitly computed using (Parker, 1994):

$$\frac{\partial g_i}{\partial \sigma_k} = \lim_{\delta \sigma_k \rightarrow 0} \frac{g_i(\sigma_1, \sigma_2, \dots, \sigma_k + \delta \sigma_k, \dots, \sigma_{N_m}) - g_i(\sigma_1, \sigma_2, \dots, \sigma_k, \dots, \sigma_{N_m})}{\delta \sigma_k} \quad (3.29)$$

One can find applications of this approach in electromagnetic inverse problems in Jupp & Vozoff (1976) for example. The main drawback of this route, is that it requires as many forward modelling solutions as number of parameters to estimate, thus it can be cumbersome even for a few tens of parameters (McGillivray *et al.*, 1994) and completely impractical for three-dimensional problems. Nonetheless, the explicit computation of the Fréchet derivative is useful to benchmark alternative and more efficient methods.

3.6.2 Calculation of the sensitivities by the adjoint method

The adjoint method allows to obtain the sensitivities with significantly less computational effort, in comparison to the sensitivity-equation approach presented in the previous section. There are essentially two approaches when deriving expressions for the adjoint solutions of the electromagnetic sensitivities. Perhaps the more widely used by the electromagnetic geophysical community is the one introduced by McGillivray *et al.* (1994). This approach consists of considering a time-harmonic Maxwell system and an auxiliary Maxwell system, or the so called adjoint Maxwell system. Both systems are derived with respect to the conductivity and a reciprocity relation is obtained, involving the electric field and the adjoint electric field. An alternative approach consists of perturbing Maxwell's equations, and using the reciprocity relations for the dyadic Green's functions (Chew, 1999) to derive expressions for the sensitivities of the electromagnetic field (Abubakar *et al.*, 2008a).

It is important to note that albeit McGillivray *et al.* (1994) and Abubakar *et al.* (2008a) used different mathematical routes, equivalent expressions were obtained. In this section it is reviewed the calculation of the sensitivities as presented in Abubakar *et al.* (2008a). In appendix D are reviewed the basic properties of the electromagnetic dyadic Green's functions and of the reciprocity relations for the electromagnetic field. As reviewed in chapter 2, the Maxwell problem for an electric dipole source is described by:

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) - i\omega\mu\sigma\mathbf{E}(\mathbf{r}) = i\omega\mu\mathbf{J}(\mathbf{r}) \quad (3.30)$$

The electromagnetic field is considered to have a time-harmonic dependence, and the conductivity only depends on the spatial coordinate, $\mathbf{r}$. It is assumed that a perturbation in electrical conductivity $\delta\sigma$, induces a perturbation in the electric field, such that:

$$\nabla \times \nabla \times \tilde{\mathbf{E}}(\mathbf{r}) - i\omega\mu[\sigma + \delta\sigma]\tilde{\mathbf{E}}(\mathbf{r}) = i\omega\mu\mathbf{J}(\mathbf{r}) \quad (3.31)$$

and $\delta\mathbf{E}(\mathbf{r}) = \tilde{\mathbf{E}}(\mathbf{r}) - \mathbf{E}(\mathbf{r})$. Subtracting 3.31 from 3.30 yields:

$$\nabla \times \nabla \times \delta\mathbf{E}(\mathbf{r}) - i\omega\mu\delta\sigma\mathbf{E}(\mathbf{r}) = i\omega\mu\delta\sigma\tilde{\mathbf{E}}(\mathbf{r}) \quad (3.32)$$

The dyadic Green's function for the electric field due to a current density source satisfies (Chew, 1999):

$$\nabla \times \nabla \times \mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}') - i\omega\mu\sigma\mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}') = i\omega\mu\mathbf{I}\delta(\mathbf{r} - \mathbf{r}') \quad (3.33)$$

Thus, the solution of equation 3.31 reads:

$$\delta\mathbf{E}(\mathbf{r}) = \int_{\mathcal{V}_k} d\mathbf{r}' \delta\sigma \mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}') \cdot \tilde{\mathbf{E}}(\mathbf{r}') \quad (3.34)$$

Where $\mathcal{V}_k$ is the support of $\delta\sigma$. The support of a function f , in a three-dimensional space, is given by:

$$Sup(f) = \{(x, y, z) \mid f(x, y, z) \neq 0\} \quad (3.35)$$

Thus, $\mathcal{V}_k$ is the region of space occupied by the k -th inversion cell. Both terms will be used through out the text with the same meaning. As shown in Appendix D $[\mathcal{G}^{EJ}(\mathbf{r}', \mathbf{r})]^T = \mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}')$, hence:

$$\delta\mathbf{E}(\mathbf{r}) = \int_{\mathcal{V}_k} d\mathbf{r}' \delta\sigma \tilde{\mathbf{E}}(\mathbf{r}') \cdot \mathcal{G}^{EJ}(\mathbf{r}', \mathbf{r}) \quad (3.36)$$

It is now convenient to analyze equation 3.36 in terms of components. From the definition of the dyadic Green's functions (equation D.8), it is evident that the m -th column of $\mathcal{G}^{EJ}(\mathbf{r}', \mathbf{r}_R)$ is the electric field at $\mathbf{r}'$, generated by a point current source at $\mathbf{r}_R$ oriented in the m -th direction, this being the only component contributing to the m -th component of $\delta\mathbf{E}(\mathbf{r}_R)$. Thus, defining $\mathbf{E}_J^\dagger(\mathbf{r})$ as the electric field due to a point current source at $\mathbf{r}_R$, oriented in the m -th direction, we have:

$$\delta E_m(\mathbf{r}_R) = \int_{\mathcal{V}_k} d\mathbf{r}' \delta\sigma \tilde{\mathbf{E}}(\mathbf{r}') \cdot \mathbf{E}_J^\dagger(\mathbf{r}') \quad (3.37)$$

The conductivity anomaly $\delta\sigma$ is constant in its support $\mathcal{V}_k$, thus:

$$\frac{\delta E_m}{\delta\sigma_k}(\mathbf{r}_R) = \int_{\mathcal{V}_k} d\mathbf{r}' \tilde{\mathbf{E}}(\mathbf{r}') \cdot \mathbf{E}_J^\dagger(\mathbf{r}') \quad (3.38)$$

Where σ_k represents the conductivity with support $\mathcal{V}_k$. Finally, when $\delta\sigma_k \rightarrow 0$, $\tilde{\mathbf{E}} \rightarrow \mathbf{E}$, hence:

$$\lim_{\delta\sigma_k \rightarrow 0} \frac{\delta E_m}{\delta\sigma_k}(\mathbf{r}_R) = \frac{\partial E_m}{\partial\sigma_k}(\mathbf{r}_R) = \int_{\mathcal{V}_k} d\mathbf{r}' \mathbf{E}(\mathbf{r}') \cdot \mathbf{E}_J^\dagger(\mathbf{r}') \quad (3.39)$$

It is now reviewed the theory for the computation of the sensitivities of the magnetic field. In this case, it is considered a magnetic dipole in the receiver position, and the following identities hold (from Faraday's law):

$$\delta\mathbf{H}(\mathbf{r}) = \frac{1}{i\omega\mu} \nabla \times \delta\mathbf{E}(\mathbf{r}) \quad (3.40)$$

and

$$\mathcal{G}^{HJ}(\mathbf{r}, \mathbf{r}') = \frac{1}{i\omega\mu} \nabla \times \mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}') \quad (3.41)$$

Substituting equations 3.36 and 3.41, in equation 3.40, yields:

$$\begin{aligned} \delta\mathbf{H}(\mathbf{r}) &= \frac{1}{i\omega\mu} \nabla \times \delta\mathbf{E} = \frac{1}{i\omega\mu} \nabla \times \int_{\mathcal{V}_k} d\mathbf{r}' \delta\sigma \mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}') \cdot \tilde{\mathbf{E}}(\mathbf{r}') = \\ &= \frac{1}{i\omega\mu} \int_{\mathcal{V}_k} d\mathbf{r}' \delta\sigma [\nabla \times \mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}')] \cdot \tilde{\mathbf{E}}(\mathbf{r}') = \\ &= \int_{\mathcal{V}_k} d\mathbf{r}' \delta\sigma \mathcal{G}^{HJ}(\mathbf{r}, \mathbf{r}') \cdot \tilde{\mathbf{E}}(\mathbf{r}') \end{aligned} \quad (3.42)$$

As demonstrated in appendix D, $\mathcal{G}^{HJ}(\mathbf{r}, \mathbf{r}') = -[\mathcal{G}^{EK}(\mathbf{r}', \mathbf{r})]^T$, thus:

$$\begin{aligned} \delta\mathbf{H}(\mathbf{r}) &= - \int_{\mathcal{V}_k} d\mathbf{r}' \delta\sigma [\mathcal{G}^{EK}(\mathbf{r}', \mathbf{r})]^T \cdot \tilde{\mathbf{E}}(\mathbf{r}') = \\ &= - \int_{\mathcal{V}_k} d\mathbf{r}' \delta\sigma \tilde{\mathbf{E}}(\mathbf{r}') \cdot \mathcal{G}^{EK}(\mathbf{r}', \mathbf{r}) \end{aligned} \quad (3.43)$$

Following the same rationale as before, the m -th column of $\mathcal{G}^{EK}(\mathbf{r}', \mathbf{r}_R)$ is the electric field at $\mathbf{r}'$ due to a point magnetic dipole at $\mathbf{r}_R$. Defining $\mathbf{E}_K^\dagger(\mathbf{r}') = \mathcal{G}_{\bullet, m}^{EK}(\mathbf{r}', \mathbf{r}_R)$ yields:

$$\delta H_m(\mathbf{r}_R) = - \int_{\mathcal{V}_k} d\mathbf{r}' \delta\sigma \tilde{\mathbf{E}}(\mathbf{r}') \cdot \mathbf{E}_K^\dagger(\mathbf{r}') \quad (3.44)$$

As the conductivity anomaly is constant in its support:

$$\frac{\delta H_m}{\delta\sigma_k}(\mathbf{r}_R) = - \int_{\mathcal{V}_k} d\mathbf{r}' \tilde{\mathbf{E}}(\mathbf{r}') \cdot \mathbf{E}_K^\dagger(\mathbf{r}') \quad (3.45)$$

And taking the limit $\delta\sigma_k \rightarrow 0$:

$$\lim_{\delta\sigma_k \rightarrow 0} \frac{\delta H_m}{\delta\sigma_k}(\mathbf{r}_R) = \frac{\partial H_m}{\partial\sigma_k}(\mathbf{r}_R) = - \int_{\mathcal{V}_k} d\mathbf{r}' \mathbf{E}(\mathbf{r}') \cdot \mathbf{E}_K^\dagger(\mathbf{r}') \quad (3.46)$$

From equations 3.39 and 3.46 one can conclude that the calculation of the sensitivities using the adjoint method, as reviewed here and as introduced by (McGillivray *et al.*, 1994), requires the integration over a "small volume" in space corresponding to the support of each model parameter that is to be estimated from the inversion scheme. Thus, this approach is not entirely independent of the number of parameters. However, it is important to point out that the integration over the support of each model parameter is obtained numerically, which can be done rapidly and without significant computational effort. This numerical integration approach for the calculation of the sensitivities is further addressed in section 3.6.2.1. As

pointed out by (McGillivray *et al.*, 1994), the use of the presented approach requires the solution for the adjoint field for each receiver point. This can be expensive for three dimensional problems.

However, the inversion algorithm implemented in this thesis only relies on the use of the gradient of the functional. I will demonstrate that, by using the afore derived expressions, it is possible to achieve a solution for the gradient that requires only one extra linear system solution per source (and per frequency) for the calculation of the adjoint field, and the computation of the primary field for each receiver position using an appropriate source. As the background model does not change during the inversion, the primary field only needs to be computed once. Therefore this approach can be considered as similarly computationally expensive as the schemes presented by Newman & Alumbaugh (1997) and Plessix & Mulder (2008), if the computational cost for the numerical integration in 3.39 and 3.46, and the computational cost for the calculation of the primary field for each receiver, are disregarded. Naturally, a question arises as to what is the advantage of using such an approach for the calculation of the gradient if there are already alternatives which are efficient, not requiring the integration over the support of each model parameter, and do not require the computation of the primary field at each receiver position. The answer is that, during this work it was found that a sharp source term in 2.41 produces numerical instabilities in the solution, thus the use of the alternative adjoint solutions as presented by Newman & Alumbaugh (1997) and Plessix & Mulder (2008) would not be reliable when using the presented edge finite element scheme for the solution of the 3D CSEM forward modelling problem.

The presented approach for the calculation of the gradient proved to be reliable, thus avoiding the mentioned numerical instability. This topic is further developed in section 3.7.

3.6.2.1 Numerical integration of the expressions for the sensitivity

For the computation of integrals 3.39 and 3.46 it is assumed that both the electric and the adjoint electric fields are known at the edges of the finite element grid, and it is used the numerical integration method of Gauss-Legendre (Press *et al.*, 2002). In this section, it is briefly reviewed the Gauss-Legendre integration method utilizing hexahedra and in the scope of the finite element. Expressions for the explicit numerical computation of 3.39 and 3.46 are derived.

The integral of a function over an arbitrary volume is approximated by (Smith & Griffiths, 2004):

$$\int_{\mathcal{V}} f(x, y, z) dx dy dz = \int_{\tilde{\mathcal{V}}} f(\xi, \eta, \zeta) |\det(\tilde{\mathcal{J}}(\xi, \eta, \zeta))| d\xi d\eta d\zeta = \sum_{i=1}^{N_{ip}} W_i f(\xi_i, \eta_i, \zeta_i) |\det(\tilde{\mathcal{J}}(\xi_i, \eta_i, \zeta_i))| \quad (3.47)$$

Where (ξ_i, η_i, ζ_i) is the coordinate of the i -th integration point, W_i is the integration weight corresponding to the i -th integration point, N_{ip} is the number of integration points, and $\tilde{\mathcal{J}}(\xi, \eta, \zeta)$ is the Jacobian of the mapping $\tilde{\mathcal{V}} \rightarrow \mathcal{V}$ (Smith & Griffiths, 2004). The numerical integration domain is a reference cube $\tilde{\mathcal{V}} = [-1, 1]^3$. Numerical experiments, showed that eight integration points are enough to obtain a good accuracy in this case. Table 3.1 lists the coordinates of the integration points and respective associated weights, for the Gauss-Legendre integration formulae (rightmost term of equation 3.47) over a cube using eight integration points.

Expression 3.47 establishes a rule for numerical integration. The conductivity is constant on each element, thus the physical domain corresponding to a finite element is a natural support for the numerical integration. However, as the forward modelling grid is stretched in the vicinity of each source and receiver to take full advantage of one single factorization of the linear system 2.41, I decided to use a different grid for the estimation of the model parameters to avoid the unnecessary estimation of parameters in the regions of the space that are over-sampled as a result of the forward modelling grid stretching. However, I considered an inversion grid conformal with the forward modelling grid, that is, the faces and nodes of the inversion grid and of the forward modelling grid match. Hence the support of the k -th model parameter $\mathcal{V}_k$ (or the k -th inversion cell) can be a finite element, or a combination of neighboring finite elements. Figure 3.1 illustrates the construction of an arbitrary inversion cell. Naturally, due to the additive property of the integral, if a model parameter $\mathcal{V}_k = \cup_{e=1}^{N_k} \Omega_{h(e)}$, where N_k is the number of elements in $\mathcal{V}_k$, then the integration over $\mathcal{V}_k$ is:

$$\int_{\mathcal{V}_k} f(x, y, z) dx dy dz = \sum_{e=1}^{N_k} \int_{\Omega_{h(e)}} f(x, y, z) dx dy dz \quad (3.48)$$

Where $h(e)$ is some parametrization that maps the e -th element of $\mathcal{V}_k$ into the global numbering of the element. Thus, the numerical computation of the sensitivities only requires evaluating 3.39 and 3.46 for all finite elements at the region of interest. Generally for the case of marine CSEM this includes all the region below the sea-bottom. In addition, a parametrization that maps one finite element or a set of neighboring elements to a defined inversion cell, is also necessary.

As the coordinates of each node of the modelling grid are known and therefore are also known the coordinates of each node of each element, it is possible to define a mapping between the global coordinate system (x, y, z) , and the local coordinate system (ξ_i, η_i, ζ_i) of each finite element. This mapping can be established using a defined nodal basis function for each element. Finite elements that use this attribute are known as *isoparametric elements* (Zienkiewicz & Taylor, 2005). This approach is very convenient for numerical integration in finite element schemes. It is important to note that this approach could have been used

(ξ_i, η_i, ζ_i)	W_i
$(1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$	1
$(1/\sqrt{3}, 1/\sqrt{3}, -1/\sqrt{3})$	1
$(1/\sqrt{3}, -1/\sqrt{3}, 1/\sqrt{3})$	1
$(1/\sqrt{3}, -1/\sqrt{3}, -1/\sqrt{3})$	1
$(-1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$	1
$(-1/\sqrt{3}, -1/\sqrt{3}, 1/\sqrt{3})$	1
$(-1/\sqrt{3}, 1/\sqrt{3}, -1/\sqrt{3})$	1
$(-1/\sqrt{3}, -1/\sqrt{3}, -1/\sqrt{3})$	1

Table 3.1: Coordinates and integration weights for the eight-point Gauss-Legendre integration over a reference cube.

to achieve the numerical solution of the forward modelling using the edge finite element. However, such an approach was not considered, as exact expressions for the integrals using the first order basis over a hexahedron are easily obtained using a computer algebra system, thus the isoparametric approach is unnecessary for the particular case considered in the second chapter. It is now defined the coordinate transformation:

$$[\mathbf{x}] = [\mathbf{x}_c] [\mathbf{N}] \quad (3.49)$$

Where $[\mathbf{N}] = [N_1, N_2, \dots, N_8]^T$, $[\mathbf{x}] = [x \ y \ z]^T$ are the global coordinates for points at $\mathcal{V}$, and each column of $[\mathbf{x}_c]$ contains the coordinate of each node of the reference hexahedron. The interpolation functions for an eight node hexahedron are defined as (Smith & Griffiths, 2004; Zienkiewicz & Taylor, 2005):

$$N_j = \frac{1}{8}(1 + \xi_j \xi)(1 + \eta_j \eta)(1 + \zeta_j \zeta) \quad (3.50)$$

where (ξ_j, η_j, ζ_j) is the local coordinate of the j -th node of the reference hexahedron. The determinant in equation 3.47 requires the computation of the local Jacobian matrix, which by definition is formed by the partial derivative of each global coordinate with respect to each local coordinate. Using equation 3.49 is obtained the identity:

$$\tilde{\mathcal{J}}(\xi, \eta, \zeta) = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} & \frac{\partial x}{\partial \zeta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} & \frac{\partial y}{\partial \zeta} \\ \frac{\partial z}{\partial \xi} & \frac{\partial z}{\partial \eta} & \frac{\partial z}{\partial \zeta} \end{bmatrix} = [\mathbf{x}_c] \begin{bmatrix} \frac{\partial [\mathbf{N}]}{\partial \xi} & \frac{\partial [\mathbf{N}]}{\partial \eta} & \frac{\partial [\mathbf{N}]}{\partial \zeta} \end{bmatrix} \quad (3.51)$$

Once the local Jacobian matrix $\tilde{\mathcal{J}}$, is obtained for each element, the computation of the determinant is straightforward. It is important to note that these computations are very fast

because the Jacobian matrix is a 3×3 matrix.

As the electric and adjoint electric fields are only known at the edges of the finite element grid, and the interpolation points are inside $\tilde{\mathcal{V}}$, expression 2.27 is used for the interpolation of the electric and adjoint electric field values into the integration points. Thus expressions 3.39 and 3.46 are approximated by:

$$\frac{\partial E_m}{\partial \sigma_k} \approx \sum_{i=1}^{N_{ip}} W_i \mathbf{E}(\xi_i, \eta_i, \zeta_i) \cdot \mathbf{E}_J^\dagger(\xi_i, \eta_i, \zeta_i) |\det(\tilde{\mathcal{J}}(\xi_i, \eta_i, \zeta_i))| \quad (3.52a)$$

$$\frac{\partial H_m}{\partial \sigma_k} \approx - \sum_{i=1}^{N_{ip}} W_i \mathbf{E}(\xi_i, \eta_i, \zeta_i) \cdot \mathbf{E}_K^\dagger(\xi_i, \eta_i, \zeta_i) |\det(\tilde{\mathcal{J}}(\xi_i, \eta_i, \zeta_i))| \quad (3.52b)$$

Expressions 3.52 are general and can be used for any polyhedra. In addition, the support of each model parameter does not need to be necessarily a finite element in the forward modeling grid.

In this section was presented a scheme for the numerical computation of 3.39 and 3.46 using a Gauss-Lobatto scheme, combined with concepts generally used in isoparametric finite element schemes. By using this approach, it is possible to consider a grid for the inversion which is decoupled from the forward modelling grid, avoiding the estimation of redundant model parameters due to the forward modelling grid stretching in the vicinity of sources and receivers. For the implementation of the presented approach was considered an inversion grid conformal with the forward modelling grid. It is possible to extend the presented method to the case of an inversion grid which is not conformal with the forward modelling grid, at the cost of increasing the computational complexity of the code. This topic will be considered in future research.

3.6.3 Comparison between the direct computation of the Fréchet derivative and the adjoint solution

In this section, the adjoint solutions for the sensitivities of the electric and magnetic fields, computed using the numerical integration expressions 3.52a and 3.52b are compared with those obtained using the Fréchet derivative 3.29.

To make this comparison, it is used a resistivity model consisting of a block with resistivity $1.0 \, \Omega\text{m}$ embedded in a homogeneous medium with resistivity $0.33 \, \Omega\text{m}$, as illustrated in figure 3.2. The source is a 1 Hz, x-oriented electric dipole located at $(0,0,30)$ m, and a series of receiver points were placed at $z = 5$ m and equally spaced in x and y directions as illustrated in figure 3.2. The z-axis is pointing upwards. For the calculation of the sensitivities using 3.29, the conductivity of the embedded block was perturbed by $0.01 \, \Omega\text{m}$. Figure 3.3 shows a map of the ratio between the real and imaginary part of the sensitivities computed using the Fréchet

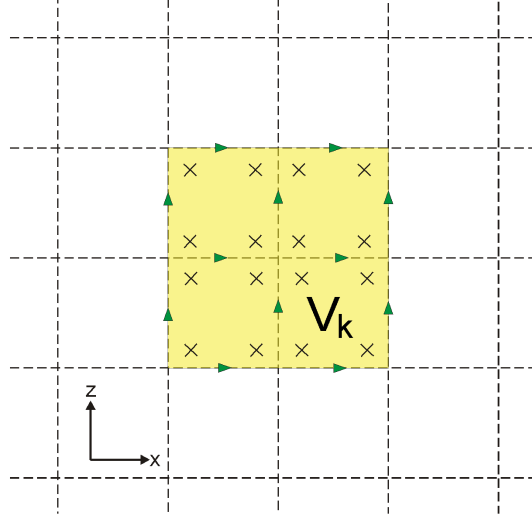


Figure 3.1: Vertical slice of the finite element mesh and the inversion cell $\mathcal{V}_k$. The green arrows represent the electric field discretized at the edges of the finite element mesh, and the crosses represent the projection of the integration points (ξ_i, η_i, ζ_i) , at the face of the respective elements.

derivative and the sensitivities computed using the adjoint solution, for all the components of the electromagnetic field. It can be observed that the ratio between the sensitivities computed using the two distinct methods is generally close to 1, with a maximum discrepancy of around 50 %. Furthermore, as observed in figure 3.3 all the ratio values are positive, showing that the sensitivities are being estimated with the correct signal. This aspect is critical for adequate model updates for each tomographic iteration.

It is important to note that this ratio should not be interpreted as an error estimator, but as an indicator on how close the solutions are, as both methods have associated errors, and most likely the finite difference approximation 3.29 produces inaccurate results, due to an inadequate choice of the perturbation factor or accumulation of the errors associated with the calculation of the electric field for the original and the perturbed resistivity models. In conclusion, the presented methodology for the numerical integration of 3.39 and 3.46, resulted in an excellent agreement with the results obtained using the Fréchet derivative, showing that it is adequate for computation of sensitivities in terms of both accuracy and computational requirements.

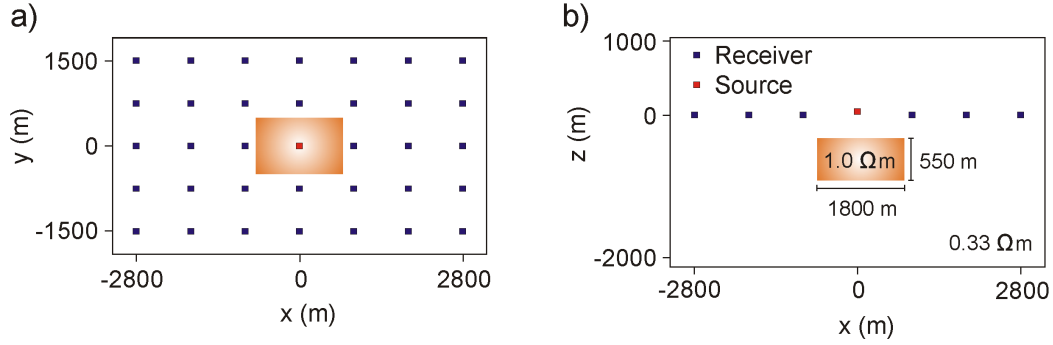


Figure 3.2: Illustration of the configuration utilized for the comparison between the sensitivities computed using the adjoint solution and the Fréchet derivative; a) horizontal slice of the model, showing the position of the source and receivers, b) vertical slice at $y = 0$ m.

3.7 Gradient of the functional

The gradient of the parametric functional 3.3, is given by:

$$\nabla_m f = \nabla_m f_D + \lambda \nabla_m f_R \quad (3.53)$$

Where $f_D = \frac{1}{2} \Delta \mathbf{d}^T \Delta \mathbf{d}^*$, and $f_R = \frac{1}{2} \mathcal{R}(\mathbf{m})$. One can identify two distinct terms contributing to the gradient of the objective function: the gradient of the data misfit term $\nabla_m f_D$, and the gradient of the regularization term $\nabla_m f_R$. From 3.3 and 3.25 the gradient of the objective function is given explicitly by:

$$\nabla_m f(\mathbf{m}) = \Re [\mathcal{J}^T(\mathbf{m}) \Delta \mathbf{d}^*] + \lambda \mathcal{L}^T \mathcal{L} \mathbf{m} \quad (3.54)$$

For a problem with N_m unknown parameters, and a data set with dimension N_D , the Jacobian matrix has dimension $[N_D, N_m]$, and is given by:

$$\mathcal{J}_{i,k} = \frac{\partial [\mathbf{G}(\mathbf{m})]_i}{\partial m_k} \quad (3.55)$$

The Jacobian matrix is also known as the *sensitivities matrix*. The element $[\mathbf{G}(\mathbf{m})]_i / \partial m_k$ of the Jacobian is the Fréchet derivative, and links changes in data with changes in the model parameters (Parker, 1994; McGillivray & Oldenburg, 1990).

An explicit Hessian for expression 3.3 can also be derived, yielding:

$$\mathcal{H}(\mathbf{m}) = \Re [\mathcal{J}^T(\mathbf{m}) \mathcal{J}^*(\mathbf{m}) + \mathcal{B}(\mathbf{m})] + \lambda \mathcal{L}^T \mathcal{L} \quad (3.56)$$

Where $\mathcal{B}_{i,j} = \sum_{k=1}^{N_m} \left[\frac{\partial^2}{\partial m_i \partial m_j} \Delta \mathbf{d}_k \right] \Delta \mathbf{d}_k^*$, thus involving only second order derivatives. This term is generally neglected from the equations leading to the Gauss-Newton method (Aster

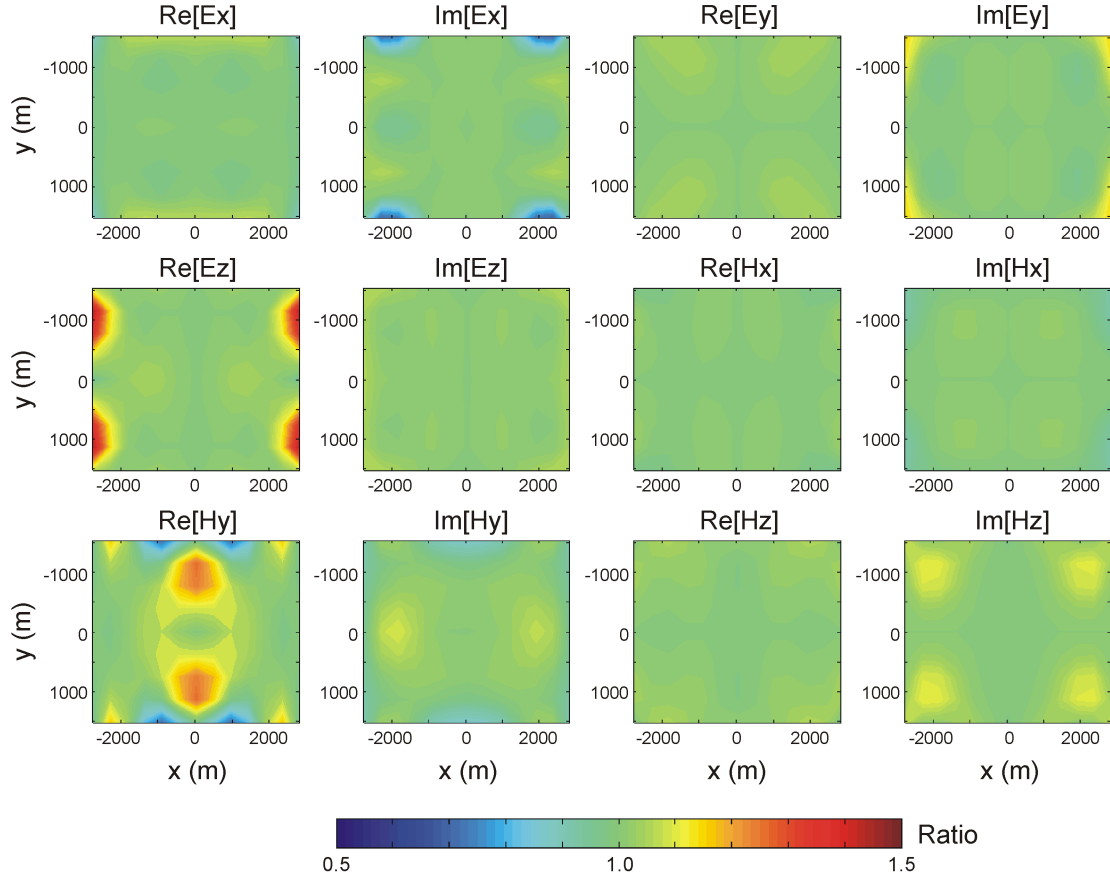


Figure 3.3: Ratio between the sensitivities of the electric and magnetic fields, computed using the Fréchet derivative (defined in equation 3.29), and the numerical integration formulas 3.52a and 3.52b for the adjoint solution.

et al., 2005). However, the Gauss-Newton method is generally avoided in 3D applications as it is computationally very demanding and intensive. In this work are considered methods that only require information of the gradient of the objective function, and this section is devoted to the efficient computation of the gradient.

As aforementioned $\mathcal{L}$ is a sparse matrix. However, as the non-zero elements on each row are known *a priori*, the action of $\mathcal{L}$ over $\mathbf{m}$ is easily computed and the whole matrix is never explicitly stored. Thus the computation of the gradient of the regularization term does not present major difficulties.

A more critical aspect is the calculation of the gradient of the data misfit term as the Jacobian matrix is dense and, therefore, when millions of parameters are involved, its storage can be impractical. Perhaps one of the most elegant approaches to derive the gradient of the data misfit is starting from the discrete form for the solution of the forward modelling problem 2.41. This approach, is generally preferred when the forward modelling problem solution

is achieved using a finite difference or finite element method discretization. Newman & Alumbaugh (1997) derived the expression for the Jacobian matrix when the forward problem is solved using the decomposition of the electric field in primary and secondary components, which is now reviewed. Taking the derivative of 2.41 with respect to the model parameters $\mathbf{m}$:

$$\frac{\partial \mathcal{A}}{\partial \mathbf{m}} \mathbf{e}_s + \mathcal{A} \frac{\partial \mathbf{e}_s}{\partial \mathbf{m}} = \frac{\partial \mathbf{s}}{\partial \mathbf{m}} \quad (3.57)$$

Defining a *projector operator* $\mathcal{P}$, that maps the computed secondary field into the receiver position, the Jacobian matrix reads:

$$\mathcal{J}(\mathbf{m}) = \mathcal{P} \frac{\partial \mathbf{e}_s}{\partial \mathbf{m}} = \mathcal{P} \mathcal{A}^{-1} \left(\frac{\partial \mathbf{s}}{\partial \mathbf{m}} - \frac{\partial \mathcal{A}}{\partial \mathbf{m}} \mathbf{e}_s \right) \quad (3.58)$$

Hence, the gradient of the data misfit term in equation 3.54 is:

$$\nabla_m f_D(\mathbf{m}) = \Re \left\{ \left[\mathcal{P} \mathcal{A}^{-1} \left(\frac{\partial \mathbf{s}}{\partial \mathbf{m}} - \frac{\partial \mathcal{A}}{\partial \mathbf{m}} \mathbf{e}_s \right) \right]^T \Delta \mathbf{d}^* \right\} \quad (3.59)$$

As $\mathcal{A}$ is symmetric, reorganizing the terms of the previous expression yields:

$$\nabla_m f_D(\mathbf{m}) = \Re \left\{ \left(\frac{\partial \mathbf{s}}{\partial \mathbf{m}} - \frac{\partial \mathcal{A}}{\partial \mathbf{m}} \mathbf{e}_s \right)^T \mathcal{A}^{-1} \mathcal{P}^T \Delta \mathbf{d}^* \right\} \quad (3.60)$$

We can now introduce the *backpropagated electromagnetic field*, $\mathbf{v}$, such that:

$$\mathbf{v} = \mathcal{A}^{-1} \mathcal{P}^T \Delta \mathbf{d}^* \quad (3.61)$$

Expressions 3.60 and 3.61 show that the computation of the gradient of data misfit term only requires the equivalent to one forward modelling solution, and is independent of the number of model parameters to be estimated. Equation 3.61 expresses the concept of *back-propagation of the residuals*, a term coined by Tarantola (1984). The back-propagation approach presented above for deriving the gradient of the data misfit term, is equivalent to the well known adjoint-state method (Plessix & Mulder, 2008) based on continuous functionals, however this approach is derived using only linear algebra theory, and has been extensively used in other domains of geophysical imaging, such as full waveform inversion (Chavent & Jacewitz, 1995; Pratt *et al.*, 1998; Virieux & Operto, 2009).

As one can observe, $\mathcal{P}^T \Delta \mathbf{d}^*$ is a sparse vector, with non-zero members corresponding to the edges in the vicinity of receivers. This method was combined with the forward modelling engine proposed in chapter 2. However, such an approach showed to be unreliable, and for this reason, this method was not further considered and an alternative was investigated.

In this section, I demonstrate that the reciprocity principle can be used to achieve an equivalent expression for the computation of the gradient of the data misfit term, requiring,

however, the evaluation of integrals over the support of each model parameter and the previous computation of the primary field at each receiver position. Hence, the computational cost is higher when compared with 3.60. However, the computation of the integrals 3.39 and 3.46 is very fast. Furthermore, when a homogeneous conductivity background model is used, the computational time is meaningless as shown in chapter 2. The only critical aspect is when a layered background model needs to be considered, however, as the background model does not change during the inversion, the computational time is substantially reduced by parallelizing the computation of the primary field over the number of receivers and storing it. This approach, allows to achieve a practical computing time per tomographic iteration. Expressions for the computation of the gradient of the data misfit are derived using results from section 3.6.2 and considering that the forward modelling problem is solved utilizing the decomposition of the electric field in primary and secondary components. It is shown that only the action of the transpose of the Jacobian matrix $\mathcal{J}$, over the vector of residuals $\Delta \mathbf{d}^*$, needs to be stored, that is, the gradient of the data misfit.

The gradient of the functional corresponding to the data misfit is more conveniently represented by:

$$\frac{\partial f_D}{\partial m_k} = \Re \left\{ \sum_{i=1}^{N_D} \Delta \mathbf{d}_i^* \frac{\partial g_i}{\partial m_k} \right\} \quad (3.62)$$

And the arbitrary element of the Jacobian matrix $\frac{\partial g_i}{\partial m_k}$, is given by:

$$\frac{\partial g_i}{\partial m_k} = \frac{1}{s_i} \int_{\mathcal{V}_k} d\mathbf{r}' \mathbf{E}_{n(i)}(\mathbf{r}') \cdot \mathbf{E}_i^\dagger(\mathbf{r}') \quad (3.63)$$

Where $n(i)$ is the number of the source for the i -th observation, $1/s_i$ is the entry in the main diagonal of $\mathcal{D}$ at the i -th row, and $\mathbf{E}_i^\dagger = \mathbf{E}_{J,i}^\dagger$ or $\mathbf{E}_i^\dagger = -\mathbf{E}_{K,i}^\dagger$, depending if g_i is a component of the electric field or magnetic field, respectively. Substituting equation 3.63 in equation 3.62, yields:

$$\begin{aligned} \frac{\partial f_D}{\partial m_k} &= \Re \left\{ \sum_{i=1}^{N_D} \frac{1}{s_i} \Delta \mathbf{d}_i^* \int_{\mathcal{V}_k} d\mathbf{r}' \mathbf{E}_i^\dagger(\mathbf{r}') \cdot \mathbf{E}_{n(i)}(\mathbf{r}') \right\} = \\ &= \Re \left\{ \sum_{i=1}^{N_D} \int_{\mathcal{V}_k} d\mathbf{r}' \left[\frac{1}{s_i} \Delta \mathbf{d}_i^* \mathbf{E}_i^\dagger(\mathbf{r}') \right] \cdot \mathbf{E}_{n(i)}(\mathbf{r}') \right\} = \\ &= \Re \int_{\mathcal{V}_k} d\mathbf{r}' \left[\sum_{i=1}^{N_D} \frac{1}{s_i} \Delta \mathbf{d}_i^* \mathbf{E}_i^\dagger(\mathbf{r}') \right] \cdot \mathbf{E}_{n(i)}(\mathbf{r}') \end{aligned} \quad (3.64)$$

Decomposing the adjoint electric field in primary and secondary components, $\mathbf{E}_i^\dagger = \mathbf{E}_{p,i}^\dagger + \mathbf{E}_{s,i}^\dagger$

yields:

$$\begin{aligned} \frac{\partial f_D}{\partial m_k} &= \Re \int_{\mathcal{V}_k} d\mathbf{r}' \left[\sum_{i=1}^{N_D} \frac{1}{s_i} \Delta \mathbf{d}_i^* \left[\mathbf{E}_{p,i}^\dagger(\mathbf{r}') + \mathbf{E}_{s,i}^\dagger(\mathbf{r}') \right] \right] \cdot \mathbf{E}_{n(i)}(\mathbf{r}') = \\ &\Re \int_{\mathcal{V}_k} d\mathbf{r}' \left[\sum_{i=1}^{N_D} \frac{1}{s_i} \Delta \mathbf{d}_i^* \mathbf{E}_{p,i}^\dagger(\mathbf{r}') + \sum_{i=1}^{N_D} \frac{1}{s_i} \Delta \mathbf{d}_i^* \mathbf{E}_{s,i}^\dagger(\mathbf{r}') \right] \cdot \mathbf{E}_{n(i)}(\mathbf{r}') \end{aligned} \quad (3.65)$$

As the Maxwell operator $\mathcal{M}[\cdot] = -i\omega\mu\sigma[\cdot] + \nabla \times \nabla[\cdot]$ is linear, the superposition principle holds, thus:

$$\mathcal{M} \left[\sum_{i=1}^{N_D} \frac{1}{s_i} \Delta \mathbf{d}_i^* \mathbf{E}_{s,i}^\dagger(\mathbf{r}') \right] = i\omega\mu\Delta\sigma \sum_{i=1}^{N_D} \frac{1}{s_i} \Delta \mathbf{d}_i^* \mathbf{E}_{p,i}^\dagger(\mathbf{r}') \quad (3.66)$$

From 3.66 one concludes that only one extra forward modelling computation is necessary per source and per frequency, for the calculation of the data misfit functional. The solution of 3.66 is solved using the finite element approach presented in chapter 2, and subject to the perfect electric conductor boundary conditions. By inspection of 3.66 one can conclude that a scheme was derived (based on the electromagnetic reciprocity relations) for computing the gradient of the data misfit term of the objective function, that resembles the previously reviewed back-propagation technique. This similarity was expected as the back-propagation method can be interpreted as having virtual sources in the location of the receivers (Pratt *et al.*, 1998), which is the same principle used to derive the reciprocity relations. As aforementioned, this technique is slightly more expensive computationally in comparison to the use of the discrete approach for deriving the gradient, as it requires the evaluation of volume integrals for each model parameter and the computation of the primary field at each receiver position. However, this approach is necessary to avoid the observed numerical instabilities near the source position, when computing the adjoint solution in equation 3.61 using the finite element scheme presented in chapter 2.

An advantage of using a factorization method is the fact that the factors used for the solution of the forward modelling problem, can be re-utilized for the solution of equation 3.66 at each tomographic iteration, and therefore, it is not required an extra factorization for the computation of the gradient.

3.8 Preconditioning of the inverse problem

When using Gauss-Newton or Newton methods, it is used a good approximation of the full Hessian matrix, thus neither preconditioning or scaling of the gradient is necessary. However, as aforementioned, their use can be prohibitive in 3D applications, and the optimization problem is generally solved using gradient based methods, such as steepest descent, nonlinear

conjugate gradients, or quasi-Newton methods such as the L-BFGS method. As pointed out by Newman & Boggs (2004), and Plessix & Mulder (2008) the efficiency of gradient based, and quasi-Newton methods can be further improved using a preconditioner. An efficient preconditioner is expected to satisfy two main properties: decrease the number of iterations necessary for convergence and do it without increasing the computational load significantly (Newman & Boggs, 2004). Preconditioning aims to obtain a new direction for the gradient of the objective function, which is closer to the Newton direction. Another aspect of the preconditioning is that it also scales the gradient thus preventing poor imaging of the geo-electrical structures in the deeper regions of the model, or if one prefers, of the earth (Rodi & Mackie, 2001; Plessix & Mulder, 2008). The development of preconditioners for the electromagnetic inverse problem has been extensively studied. For example, in the scope of 2D MT data inversion, Rodi & Mackie (2001) introduced an approximation of the Hessian based on the Hessian utilized in the previous iteration for the regularization of the inverse problem added to a scaled identity matrix to take into account for the data component of the Hessian. Newman & Boggs (2004) studied the approximation of the Hessian based on the idea of using approximate sensitivities as it was originally introduced by Farquharson & Oldenburg (1996). The approach of Newman & Boggs (2004) consists of using the Born approximation and a simple background model to obtain a semi-analytical approximation of the Hessian at each tomographic iteration. More recently Plessix & Mulder (2008) introduced a physics-based preconditioner that attempts to compensate for the exponential decay of the amplitude of the electromagnetic field with depth. This preconditioner can be understood as a weighting of the model parameters with depth.

For the approximation of the Hessian matrix, or its diagonal, it is necessary to compute the adjoint field at each receiver position, thus it is required as many adjoint solutions as number of receivers. Hence, this approach can be prohibitive when the number of receivers is large. An alternative method was investigated, using the primary adjoint field at each receiver position, for the computation of an approximation of the diagonal of the Hessian matrix. This approach is also based in the ideas first proposed by Farquharson & Oldenburg (1996), however avoiding the computation of the Born approximation as proposed by Newman & Boggs (2004). The main advantage is that the approximate diagonal of the Hessian matrix is obtained with almost no extra computational cost, as the primary adjoint field is computed for the calculation of the gradient, and the diagonal of $\mathcal{L}^T \mathcal{L}$ is also computed rapidly. However, the approximation of the diagonal of the Hessian matrix proved to be unreliable, as in some cases the inversion algorithm diverged. For this reason, this approach was abandoned and the preconditioner introduced by (Plessix & Mulder, 2008) was implemented. The physics-based preconditioner is reviewed in this section for a matter of completeness.

In order to implement the physics-based preconditioner using a smoothing constraint, I introduce a weighted second order operator $\tilde{\mathcal{L}}$, in the regularization term, leading to an

invariance between the value of the functional in the model parameter space and in the weighted model parameter space, keeping the original properties of the updating formula for the model parameters derived by Plessix & Mulder (2008).

It is assumed the existence of a weighting matrix $\mathcal{W}$ and the relation between the scaled unknowns $\tilde{\mathbf{m}}$, and the model parameters $\mathbf{m}$ (Plessix & Mulder, 2008):

$$\mathbf{m} = \mathcal{W}\tilde{\mathbf{m}} \quad (3.67)$$

Plessix & Mulder (2008) approach requires that:

$$\tilde{f}(\tilde{\mathbf{m}}) = f(\mathbf{m}) \quad (3.68)$$

leading to the identity:

$$\nabla_{\tilde{\mathbf{m}}} \tilde{f}(\tilde{\mathbf{m}}) = \mathcal{W}^T \nabla_{\mathbf{m}} f(\mathbf{m}) \quad (3.69)$$

The weighting matrix $\mathcal{W}$ is assumed to be diagonal, hence $\mathcal{W} = \mathcal{W}^T$, and the expression for the L-BFGS update at the k -th iteration is (Plessix & Mulder, 2008):

$$\tilde{\mathbf{m}}_{k+1} = \tilde{\mathbf{m}}_k - \alpha_k \tilde{\mathcal{H}}_k^{-1}(\tilde{\mathbf{m}}_k) \nabla_{\tilde{\mathbf{m}}} \tilde{f}(\tilde{\mathbf{m}}_k) \quad (3.70)$$

Substituting equations 3.67 and 3.69 in equation 3.70, and considering the symmetry of the weighting matrix, yields:

$$\mathbf{m}_{k+1} = \mathbf{m}_k - \alpha_k \mathcal{W} \tilde{\mathcal{H}}_k^{-1}(\tilde{\mathbf{m}}_k) \mathcal{W} \nabla_{\mathbf{m}} f(\mathbf{m}_k) \quad (3.71)$$

Introducing the weighted second order operator $\tilde{\mathcal{L}} = \mathcal{L}\mathcal{W}$, the objective function in the weighted model parameter space reads:

$$\tilde{f}(\tilde{\mathbf{m}}) = \frac{1}{2} \|\mathcal{D}(\mathbf{G}(\tilde{\mathbf{m}}) - \mathbf{d})\|_2^2 + \frac{1}{2} \lambda \|\tilde{\mathcal{L}}\tilde{\mathbf{m}}\|_2^2 \quad (3.72)$$

Note that the definition $\|\mathbf{a}\|_2^2 = \mathbf{a} \cdot \mathbf{a}^*$, for the L_2 norm of a vector in a space over complex numbers, is being used. It is straightforward to show that the objective function 3.72 satisfies identities 3.68 and 3.69, thus the weighted updating formula (equation 3.71) can be used for the solution of the inverse problem regularized with the smoothing constraint.

Expression 3.71 updates the model parameters directly using the defined preconditioner and the inverse of the Hessian of the weighted objective function, $\tilde{\mathcal{H}}_k^{-1}(\tilde{\mathbf{m}}_k)$. The approximate inverse of the weighted Hessian $\tilde{\mathcal{H}}_k^{-1}(\tilde{\mathbf{m}}_k)$, is obtained by using the weighted model parameters 3.67, and the weighted gradient 3.69 for the computation of $\mathbf{s}_k$ and $\mathbf{y}_k$ in equation 3.23 and the recursive approximation of the inverse of the Hessian, given by equation 3.24. The weighting

matrix $\mathcal{W}$ is defined as (Plessix & Mulder, 2008):

$$\mathcal{W}(x, y, z) = \begin{cases} 1 & \text{if } z \geq z_0 \\ \left[\left(\frac{z_0 - z}{\delta} \right)^{-\gamma} \exp(-\beta \frac{z_0 - z}{\delta}) + \varepsilon \right]^{-1} & \text{if } z < z_0 \end{cases} \quad (3.73)$$

Where γ , β and ε are empirical positive numbers, δ is the skin depth for same frequency as the data being inverted, and z_0 is a reference depth (*e.g.* sea-bottom). It is considered a z-axis pointing upwards, and z-values are negative bellow z_0 . Each model parameter m_k has an associated weight $\mathcal{W}_{kk}$, and (x, y, z) is the coordinate of the centre of $\mathcal{V}_k$, that is the support of the model parameter m_k .

3.9 On the use of a direct solver in the inversion scheme

It is important to note that the main computational effort is related with the solution of the linear system, as it is used the direct solver as described in chapter 2. In the implemented inversion scheme, the linear system is factorized once for the forward modelling solution and the same factors are re-utilized for the computation of the gradient of the data misfit term. A second factorization may be necessary if the Armijo condition is not satisfied, as it is necessary to solve the forward modelling problem for the updated model parameters with the new step length.

The reutilization of the factors, requires the use of a forward modelling grid stretched at the vicinity of each source and each receiver position, thus leading to a rapid increase in the grid dimensions, and, consequently, a rapid increase in the size of the linear system to be solved. This aspect constitutes a drawback in the use of the direct solver as it scales poorly with increasing size of the linear system, thus imposing limitations in the size of the models that can be considered in the inversion scheme. Nonetheless, the direct solver will be used to attain the inversion results as it proved to be more reliable than any of the tested iterative solvers.

As the forward modelling grid is stretched in the vicinity of each source and position, the inversion grid is decoupled from the forward modelling grid to avoid the estimation of redundant model parameters that would be originated. This procedure was explained in more detail in section 3.6.2.1.

3.10 Inversion of a synthetic data example

In this section an example of the inversion of synthetic data is presented, using the principles reviewed and derived in this chapter. For the same synthetic data set, it is compared the performance of both the steepest descent and L-BFGS methods preconditioned with the

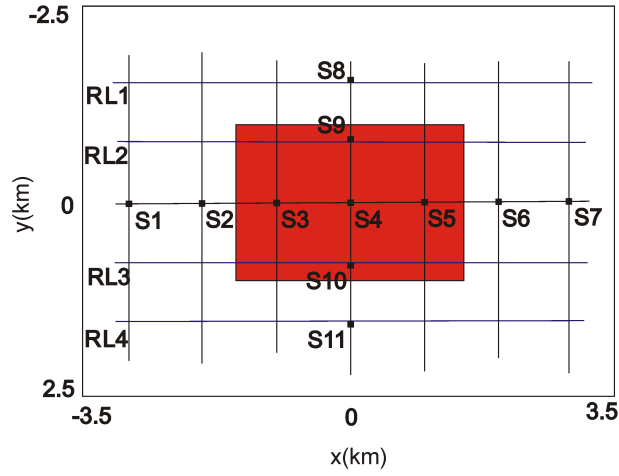


Figure 3.4: Configuration of the source and receivers utilized to generate the synthetic data set, and for the inversion. The labels starting by "S" denote source, and the labels starting by "RL" denote receiver line. The red box represents the boundaries of the resistive anomaly.

method reviewed in section 3.8.

The synthetic model responses for 0.5 and 1 Hz were generated using the conductivity model shown in figure 3.7 a), and the source-receiver configuration illustrated in figure 3.4. The synthetic data set was generated considering eleven sources, denoted by S1-S11 in figure 3.4 and 28 receivers, distributed along four receiver lines RL1-RL4, using the eFEM code developed during this thesis, which is described in chapter 2. The transmitter utilized on each source position is an electric dipole, oriented in the x-direction and operating at 0.5 Hz and 1 Hz. All transmitter positions were located 30 m above the sea-floor and the receivers were placed at the sea-bottom. The synthetic data for 11 sources, recorded on 28 receiver points, includes 924 noise-free measurements. The simulated measurements comprise all the components of the electric field. It is assumed that the noise level at the sea-floor is 10^{-15} Vm^{-1} , thus all the field values in the synthetic data set with an amplitude smaller than the value of the noise level were eliminated from the data set utilized for the inversion. The data set included 714 data samples and 614 data samples for 0.5 Hz and 1Hz, respectively. Each sample was weighted by a fraction of its magnitude, that is, the diagonal members of the weighting matrix $\mathcal{D}$ were defined as:

$$\mathcal{D}_{kk} = \frac{1}{\delta \sqrt{A_k A_k^*}} \quad (3.74)$$

Where δ is an arbitrary positive constant chosen to be 0.05, and A_k is the k -th observation. A_k can be the measurement of a component of the electric or magnetic field. However, in this example, only inversion of electric field observations is considered. By weighting each data residual by a percentage of the magnitude of the respective observation leads

	Processing Groups	Number of Threads	Factorization Memory	Time per Iteration	Number of Iterations	Run Time
One frequency						
Steepest Descent	12	8	2.99 GB	8.4 min	150	21.1 h
L-BFGS	12	8	2.99 GB	8.8 min	58	8.5 h
Two frequencies						
L-BFGS	12	8	2.99 GB	8.1 min	39	5.2 h

Table 3.2: Summary of the allocated computational resources, and number of iterations necessary to decrease the data misfit below the tolerance level, for each one of the inversion examples presented in this section. The number of processing groups corresponds to the number of MPI processes and number of computer nodes; the factorization memory is the average allocated memory per node for the factorization of the linear system.

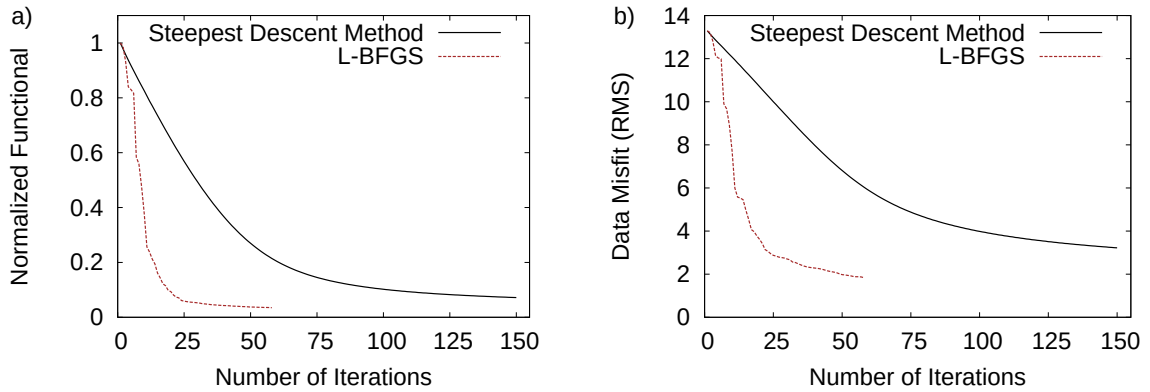


Figure 3.5: Comparison between the decrease of the a) normalized functional and b) data misfit, using the preconditioned steepest descent method and the preconditioned L-BFGS algorithm. In this example, inversion was carried out for 0.5 Hz only.

to a uniformization of the residuals and sensitivities with respect to the model parameters (Zhdanov, 2002).

The dimension of the forward modelling grid is $139 \times 95 \times 32$ representing a computational domain of $7 \times 5 \times 3 \text{ km}^3$, corresponding to approximately 1.25×10^6 unknowns in the forward modelling solution. The inversion grid has dimensions $118 \times 80 \times 18$ corresponding to 157131 model parameters. Table 3.2 summarizes the allocated computational resources, execution times, and number of iterations necessary to decrease the data misfit below the tolerance level, for the inversion examples presented in this section.

I compared the performance of the steepest descent and L-BFGS methods, inverting only the synthetic data set for 0.5 Hz. For the approximate L-BFGS Hessian are only stored 5 vector pairs. Some preliminary tests with the inversion algorithm showed that a good solution could be obtained using the preconditioning parameters $\gamma = 2.1$, $\varepsilon = 1.0$ and $\beta = 6.0$ (See section 3.8 for a description of the preconditioner). Generally, were obtained good results

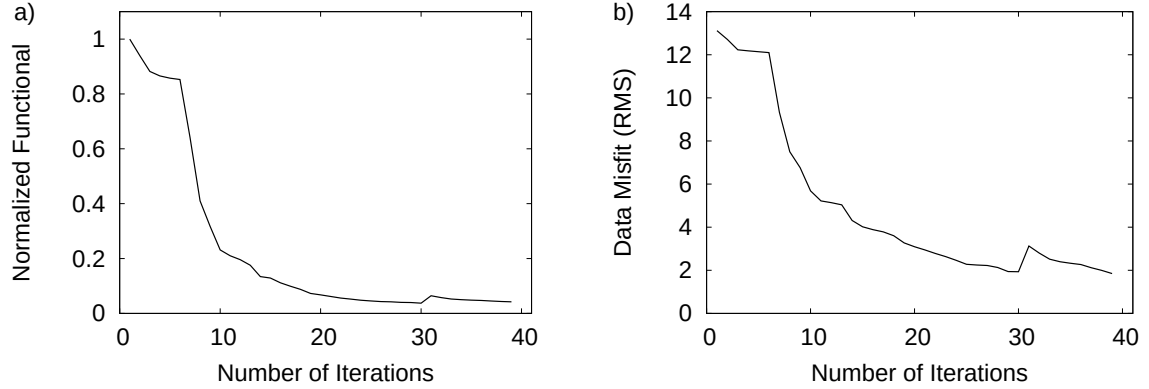


Figure 3.6: Decrease of the a) normalized functional and b) data misfit with the number of iterations, using the preconditioned L-BFGS method, and inverting for 0.5 Hz and 1 Hz.

utilizing these parameters, as well as for β ranging between 2 and 6. However, I cannot be absolutely sure that these parameters always work, thus experimentation is needed for each case. For a more complete discussion on the setting of the parameters controlling the preconditioner see Plessix & Mulder (2008).

The regularization parameter λ , was set to 100 and decreased during the inversion using the cooling algorithm 3 (see section 3.4). The stopping criterion used for this example, was a value of root mean square of the residuals equal or less than 1.85, where the root mean square (RMS) is defined as:

$$\text{rms} = \sqrt{\frac{1}{N_D} \Delta \mathbf{d}^T \Delta \mathbf{d}^*} \quad (3.75)$$

Note that $\Delta \mathbf{d}$ contains weighted residuals, as defined in equation 3.74. Figure 3.5 shows the decrease of the a) normalized functional and b) data misfit for the case when the steepest descent and the L-BFGS algorithms are used. The normalized functional, is computed dividing the parametric functional 3.3, by its magnitude, at the first iteration. As expected the L-BFGS algorithm decreased the data misfit below the tolerance level with fewer iterations than the steepest descent algorithm. In fact, 150 iterations were not sufficient to achieve the desired misfit, when using the steepest descent method. The L-BFGS algorithm converged to a data misfit of 1.83 in 58 iterations. Thus the higher complexity of the L-BFGS algorithm, is compensated by its superior performance in comparison to the steepest descent algorithm. Figure 3.7 b) shows a slice of the recovered conductivity model at $y = 0$ km (left column) and at $x = 0.5$ km (right column), using the L-BFGS algorithm. It can be observed a very good agreement for both the spatial positioning of the conductivity anomaly and the magnitude of the values of the recovered model parameters.

In order to increase the quality of inverted models, inversions are generally carried out for

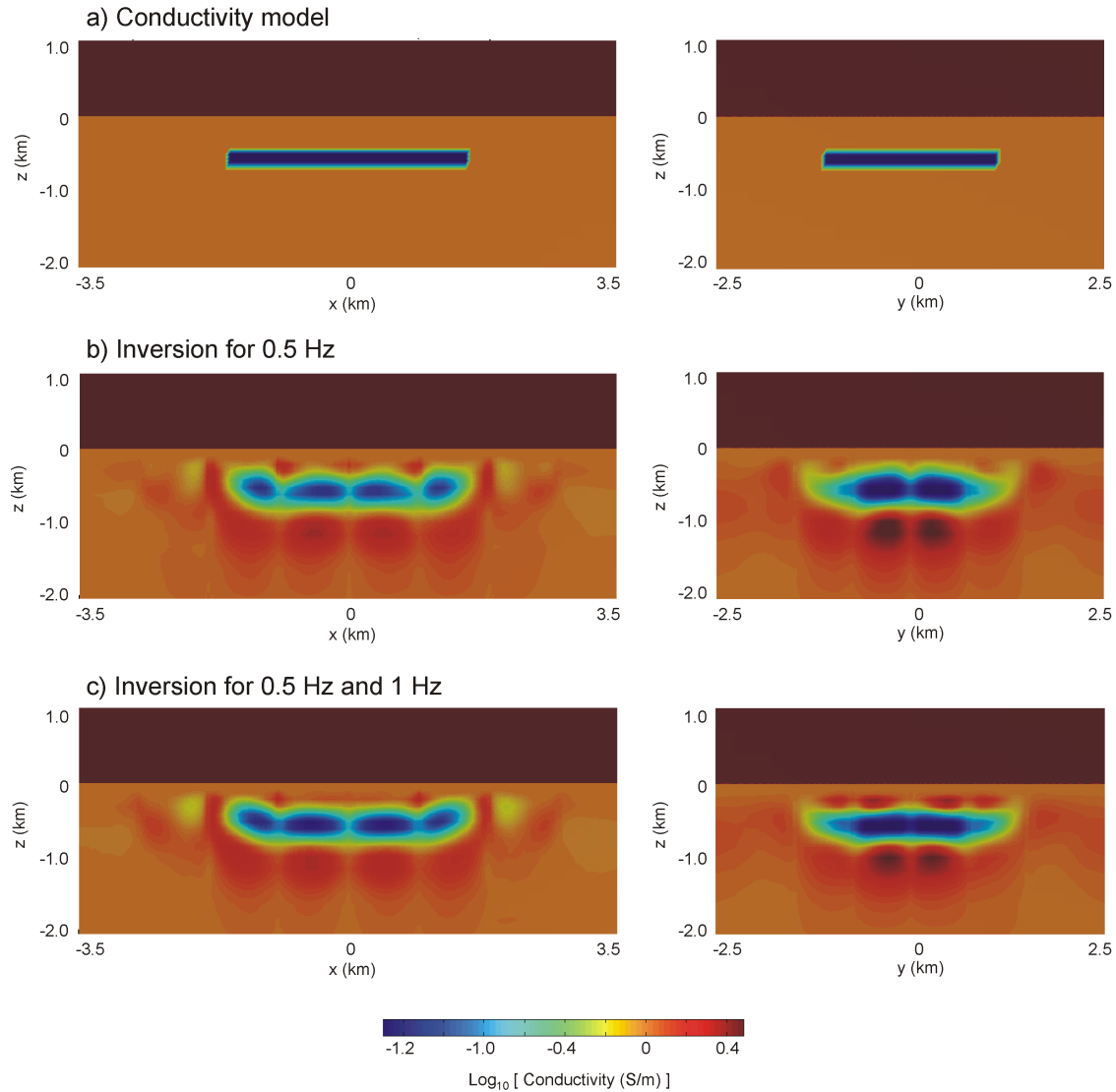


Figure 3.7: Slice of the conductivity model at $y = 0$ km (left column) and $x = 0.5$ km (right column); a) model used to generate synthetic data for both frequencies, b) reconstructed conductivity inverting for 0.5 Hz, c) reconstructed conductivity inverting for 0.5 Hz and 1 Hz.

data sets containing several frequencies, as different frequencies (or wavelengths) have different sensitivities to the same geological, or if one prefers, geo-electrical structures depending on their depth and dimension. An important aspect is the fact that models with shorter length scales lead to objective functions with higher number of local minima than smooth models (Sirgue & Pratt, 2004). Thus, data dominated by higher frequency (or higher wavelengths) content, generate objective functions which have a higher number of local minima. The so called *multiscale* method mitigates this problem, and consists in inverting sequentially for each frequency, starting at the lowest frequency and ending at the highest. For each fre-

quency, the inversion algorithm iterates a predefined number of iterations, or until the data misfit is below a predefined threshold. This approach is widely used by the geophysical community (Song *et al.*, 1995; Ravaut *et al.*, 2004; Jaiswal *et al.*, 2009) and was also implemented in the developed inversion algorithm.

For this reason I include an example of an inversion for which a synthetic data set was generated using 2 frequencies: 0.5 and 1 Hz. Again, it is utilized the source-receiver configuration illustrated in figure 3.4, and the same modelling and inversion grids as in the example for just one frequency. It is important to note that the modelling grid satisfied the Nyquist criterion (Press *et al.*, 2002) for both 0.5 Hz and 1 Hz. Table 3.2 lists the allocated computational resources utilized to carry out the inversion for two frequencies. In this example only the L-BFGS algorithm was used, as it proved to be more efficient and reliable than the preconditioned steepest descent method, considering the results of the inversion for just one frequency. The stopping criterion was a maximum value of 1.85 for the root mean square of the weighted data misfit. The initial regularization parameter was again set to 100 and decreased using algorithm 3. The multi-frequency inversion scheme runs the inversion algorithm, for a predefined number of tomographic iterations, starting inverting for 0.5 Hz. The inversion for the last frequency (1 Hz) runs until one of the stopping criteria is satisfied, that is, the maximum number of iterations is reached or the desired level of data misfit is attained. I selected 30 iterations for 0.5 Hz and the algorithm stopped after 9 iterations for 1 Hz, as the data misfit level reached the defined RMS threshold tolerance of 1.85.

Figure 3.6 shows the decrease of the a) normalized parametric functional and of the b) data misfit for the inversion using two-frequencies. In figure 3.6 it can be observed a slight increase in the value of the data misfit (and consequently in the value of the parametric functional, as it depends on the data misfit), at iteration 30, corresponding to the transition to the inversion for the 1 Hz data set. Figure 3.7 c) shows a slice of the reconstructed conductivity model at $y = 0$ km (left column) and at $x = 0.5$ km (right column), using two frequencies in the inversion scheme. As it can be observed, the shape of the anomaly is better defined and the magnitude of the conductivity is closer to the true values of the conductivity, than when inverting for a single frequency (Figure 3.7 b). Figures 3.8 and 3.9, compare the electromagnetic field responses of the conductivity model shown in figure 3.7 c), and the synthetic data, for a selected set of source gathers and, for both frequencies. It is shown a very good agreement between the response of the recovered model of conductivity and the synthetic data for both frequencies.

3.11 Conclusions

In this chapter, a strategy was presented for three-dimensional inversion of marine CSEM data in the frequency domain, after reviewing the most important aspects of non-linear

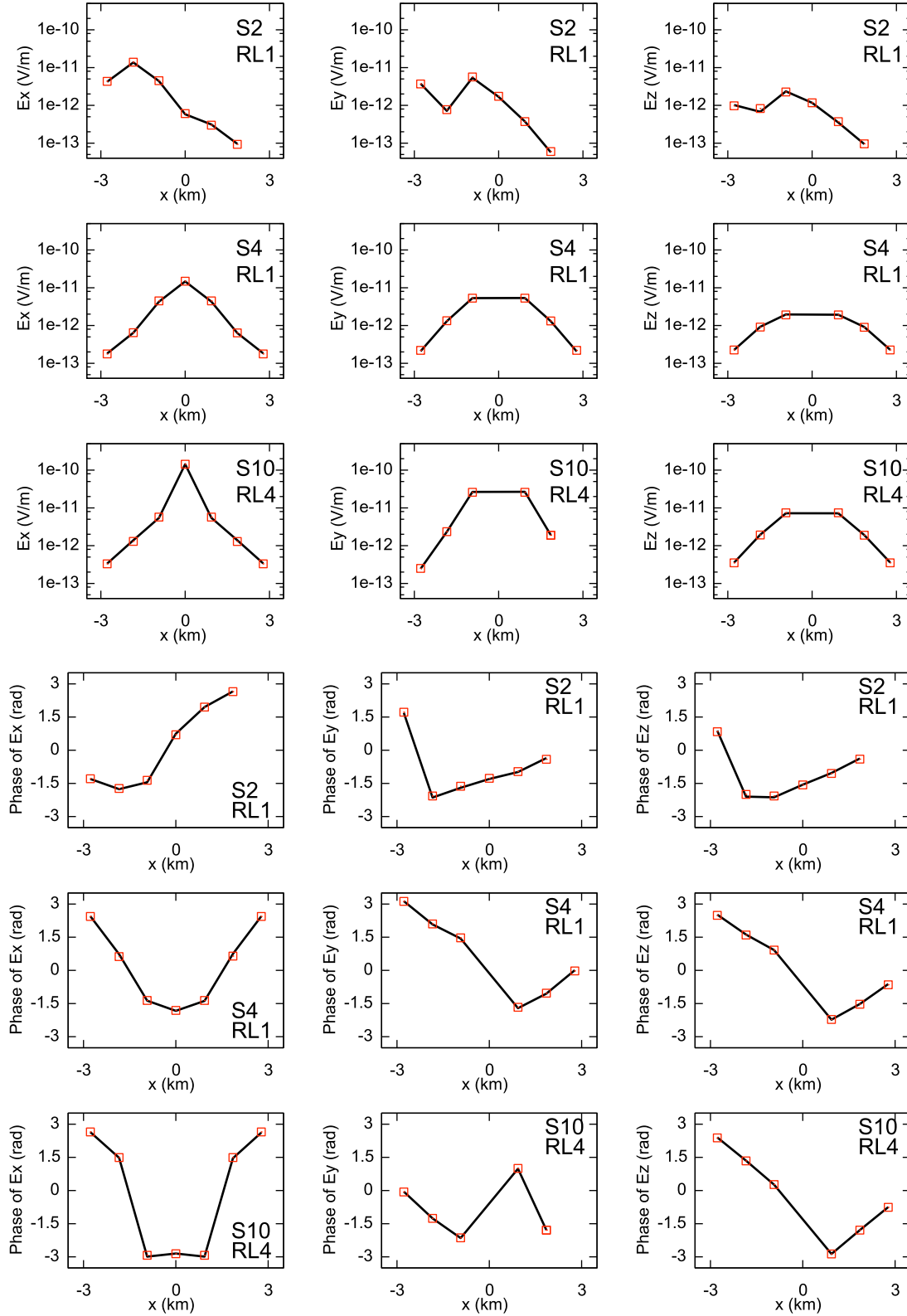


Figure 3.8: Data fitting for the 0.5 Hz data set. Black lines represent the responses of the reconstructed conductivity model, and red squares represent synthetic data

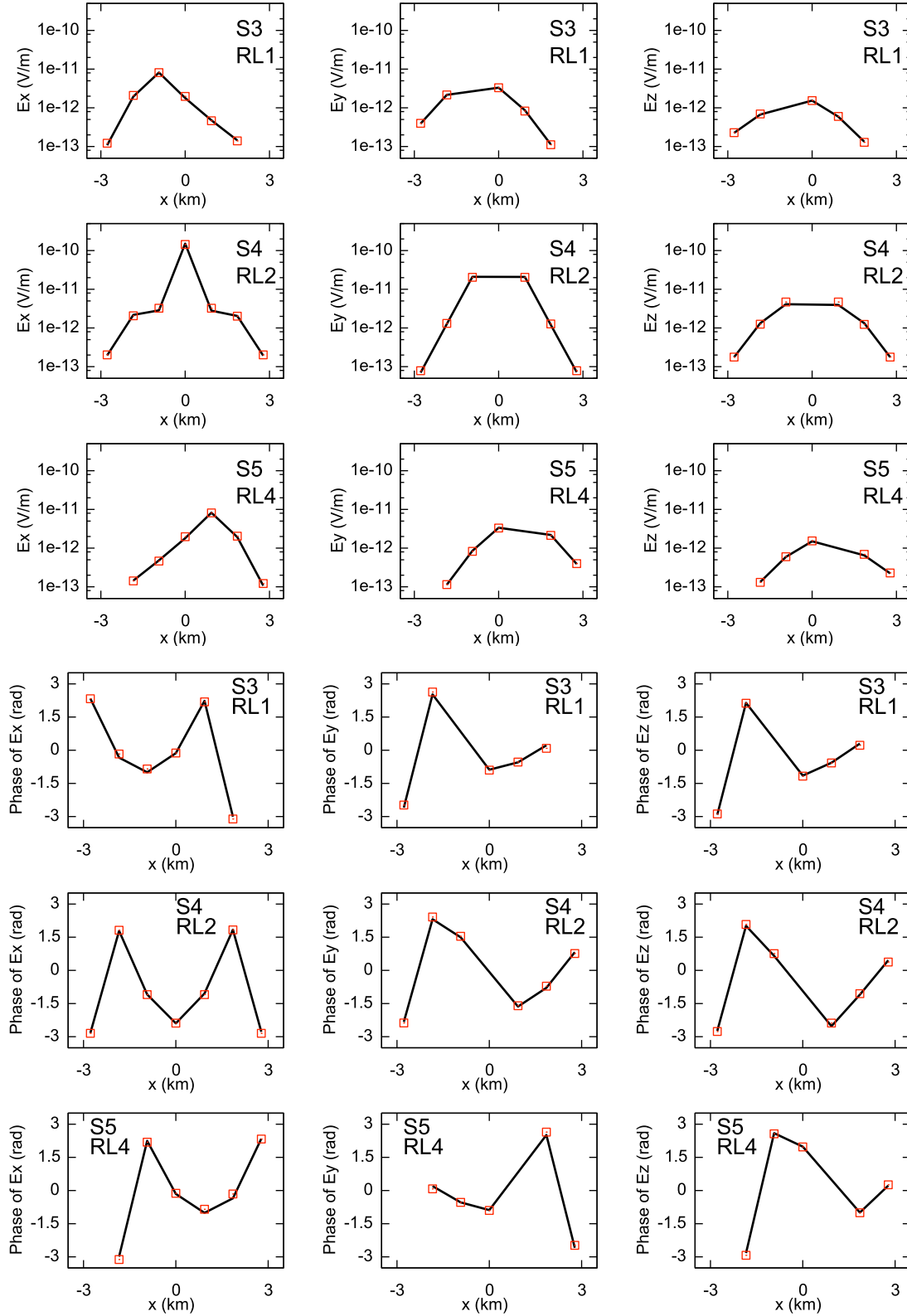


Figure 3.9: Data fitting for the 1 Hz data set. Black lines represent the responses of the reconstructed conductivity model, and red squares represent synthetic data.

inversion in the context of geophysical electromagnetic problems.

The non-linear inverse problem is generally solved by recasting the original problem as a non-linear optimization problem. This strategy was also used in the scope of this thesis. The parametric functional has a measure of the data misfit and regularization term, and the L_2 norm was chosen.

The inclusion of a regularization term is critical to mitigate the non-uniqueness and ill-posed properties of the non-linear inverse problem, and weights the contributions of the data misfit and of other constraints to the model parameters. In the scope of this thesis it was considered penalizing for the norm of the second derivative of the model parameters, that is, imposing a smoothing constraint to the estimated model parameters. The use of an additive parametric functional, that is, the parametric functional is the sum of the contributions of a measure of the data misfit and of a measure of an imposed constraint to the model, requires the estimation of the regularization parameter during the inversion.

It is required an adaptive weight for the regularization term, because if the regularization parameter is too high, the inversion algorithm will produce an over-smoothed model, if it is too small, it will lead to a model with large variations in conductivity.

In the context of non-linear inverse problems, the regularization parameter is generally estimated by choosing an initially relatively large value, and is decreased for each tomographic iteration using a pre-defined mathematical law. This approach is generally known as the *cooling method*. The cooling method is a heuristic approach based in the fact that, in the limit when the regularization parameter and the data misfit tend to zero, the estimated model should be very close to the true distribution of the model parameters or, if one prefers, of the true conductivity. In this work I decided to implement a cooling method that uses the decrease in the data misfit between successive tomographic iterations as a criterion to decrease the regularization parameter. This approach for the cooling method is based in the idea that if the regularization parameter is fixed, then the inversion scheme is over smoothing. Thus, if the data misfit does not decrease by a certain amount, the regularization parameter is probably overweighting the smoothing constraint and it should be decreased, or in the next iterations a decrease in the data misfit may not be achieved. This method has proved to be a valid approach as demonstrated by the synthetic example presented in section 3.10. To my knowledge this approach is original, and was not implemented in previous inversion algorithms. As aforementioned the use of a multiplicative cost function allows to determine automatically the regularization parameter λ , however its benefits and drawbacks were not explored during this work. Its implementation should be considered in future research.

Three-dimensional inverse problems generally involve a large number of parameters to be estimated, thus methods that only use information of the gradient of the parametric functional are generally preferred. As shown, the gradient of the regularization term is easily computed. Furthermore, the use of a finite-difference approximation for the Laplacian oper-

ator leads to a sparse matrix which essentially only requires the storage of the pattern of the non-zero terms.

More critical is the derivation of the gradient of the data misfit term. The theory for the efficient computation of the gradient of the data misfit term is well established and generally the solutions derived from the adjoint-state method are implemented. One of the main problems I encountered when implementing a code for 3D CSEM forward modelling was the representation of the source. This problem was overcome with the use of the well known decomposition of the electric field in primary and secondary components. When solving the linear system for the back-propagated field, or if one prefers for the adjoint solution, the same problem was found, as the adjoint solution essentially requires a solution of a linear system with the data residuals on the right-hand side. The solution of the adjoint linear system in the frequency domain, can be interpreted as the equivalent to a forward modelling solution with virtual point sources weighted by the corresponding data residual at the position of the receivers. Thus, the same numerical instability and inaccuracy is found in the adjoint solution when solving the adjoint linear system.

This problem led me to use the electromagnetic field reciprocity properties to derive an expression for the gradient of the data misfit term. By starting from the well known expressions for the computation of the electromagnetic field sensitivities, I derived an expression for the explicit computation of the gradient, which requires the computation of the primary electromagnetic field at each receiver position. Apart from the computation of the primary field, the proposed approach only requires the solution of a linear system for each source and frequency, and the integration of electric and adjoint electric fields over the support of each model parameter. This approach can be interpreted as computing the back-propagated secondary field for the computation of the gradient. Even though computationally more costly than using the gradient for the data misfit term derived from the discrete form of the linear system of equations, the presented method proved to be stable. In addition, it is important to note that, by using this approach, it is only required one extra solution for the adjoint problem, per source and per frequency. If the original adjoint solutions were implemented as they are described in the literature it would be necessary to compute as many forward modelling solutions as number of receivers per source and frequency. However, the implemented approach cannot be used to compute the terms of the Hessian matrix.

For the computation of the gradient of the data misfit term it is used a numerical integration scheme based in the Gauss-Legendre method, which is widely used in *isoparametric* finite element schemes. The implementation of the numerical integration scheme was tested for the computation of the sensitivities for both magnetic and electric fields. The adjoint solution for the sensitivities was compared with the direct computation of the Fréchet derivative. A qualitative analysis of the results using both methods showed a very good agreement between solutions. Generally small errors were observed for both real and imaginary parts of the sen-

sitivities. Furthermore, the sign (positive or negative) was always correct. It is important to note that the larger errors, are very localized, are most likely caused by the inaccuracy of the computation of the Fréchet derivative, since the formula used was only approximated. Furthermore, there is propagation of errors from the computation of the electromagnetic field for the computation of the Fréchet derivative.

Each term of the gradient of the data misfit, is the sum of the sensitivities of the electromagnetic field weighted by the respective residual, over the receiver positions, for the same model parameter. As the integration operation is commutative for the sum, the numerical integration is only performed once.

As the gradient of the misfit term of the parametric functional is obtained by integration of the electromagnetic and adjoint electromagnetic fields, it is provided a natural framework to decouple an inversion grid from a forward modelling grid. This aspect is advantageous, as the forward modelling grid is finer near the position of sources and receivers, thus it is avoided the estimation of redundant model parameters. The implemented approach uses an inversion grid conformal with the forward modelling grid. A more general scheme can be considered, where the use of non-conformal grids can be used, requiring however an efficient interpolation scheme to map the electromagnetic field and the conductivity from the forward modelling grid to the inversion grid. This is a topic to be considered in future research.

The gradient derived using adjoint methods is unscaled and if used without scaling, it will update the regions of the model in the vicinity of the positions of sources and receivers. It is important to note that when Gauss-Newton methods are used, this difficulty does not exist as the inverse of the approximate Hessian matrix scales the gradient. During this work I experienced that, using the action of the approximate inverse of the Hessian, obtained using the L-BFGS formula, leads to very poor scaling. Hence, preconditioning is necessary. It was investigated the approximation of the diagonal of the Hessian matrix using the primary adjoint field. However, this approach revealed to be unreliable and in fact it was not verified any improvement. Alternatively the physics-based preconditioner was implemented. This preconditioner takes into consideration the decrease of the amplitude of the electric field with depth, and can be interpreted as weighting the model parameters with depth. A particular aspect of using a direct solver (as presented in chapter 2) is the fact that the same factors can be used to compute both the forward modelling solution and the gradient of the parametric functional. An extra factorization is needed if the Armijo conditions are not satisfied. The performance of the preconditioned steepest descent and L-BFGS methods, was compared when inverting for one frequency, in section 3.10. Tests showed that, by storing a small number of vector pairs with the approximate solution and gradient of the previous iterations, it was possible to accelerate dramatically the convergence rate in comparison to the steepest descent method. In fact, the steepest descent method did not converged for the desired level of data misfit in 150 iterations. This result was naturally expected, however it

is presented here because it shows that the physics-based preconditioner is a good scaling method for the gradient, and can possibly be implemented in other optimization algorithms as the non-linear conjugate gradient methods, constituting an alternative to other previously implemented preconditioners based in other approximations of the Hessian. Furthermore, it shows that the additional complexity of the L-BFGS method is compensated by its superior performance in comparison to the steepest descent method, even when the gradient is scaled by an approximation of the diagonal of the Hessian (the scaled gradient is closer to the Newton direction).

An example inverting sequentially for two frequencies was also presented. The inversion for several frequencies is needed in order to adequately reconstruct conductivity, as different frequencies are sensitive to different length scales and differently sensitive to geo-electrical structures at different depths, thus improving the resolution of the model. Thus, as expected, inverting for two frequencies led to a better reconstructed conductivity model, and the algorithm converged in fewer iterations to the desired level of data misfit, showing the importance of using several frequencies in inversion schemes.

In conclusion, tests with a synthetic data example showed that a scheme for inverting 3D CSEM data was successfully implemented. The presented approach can constitute an alternative to existing schemes. The use of a direct solver has attractive characteristics in the sense that the same factors can be used to obtain the solution of the forward modelling problem and compute the gradient of the data misfit functional. However, as expected, it imposes limitations on the size of the models that can be considered.

In addition, the approach for 3D CSEM inversion presented here is general and can be implemented with alternative forward modelling engines.

Constrained Inversion of Resistivity

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4.1 Introduction to constrained and joint inversion

As previously stated, inverse problems aim to reconstruct the distribution of one or several physical properties of a domain, from a limited number of measurements affected by noise and carried out at the boundary or in a small portion of the probed domain. Hence the solution of the inverse problem is inherently non-unique and unstable, leading to ambiguities as different models can explain the same observations (Parker, 1994; Tarantola, 2005). The regularization of the inverse problem alleviates these problems, however, regularization introduces a *bias* (Aster *et al.*, 2005) in the estimated models as it relies on including constraints in the parametric functional, which do not have in general correlation with geological structures.

Joint inversion algorithms, essentially aim to mitigate the underlying non-uniqueness of the solution of inverse problems, by including disparate physical data sets in the inversion scheme. It is assumed that there are available two or more complementary data sets obtained through the realization of different experiments $\mathbf{d}_i$, thus the inverse problem for each complementary data set can be stated as:

$$\mathbf{G}_i(\mathbf{m}_{p(i)}) = \mathbf{d}_i, \quad i = 1, \dots, N_{exp} \quad (4.1)$$

Where N_{exp} denotes the number of different experimental realizations, and $p(i)$ relates the experimental realization with the respective model domain. It is important to note, that the disparate data sets do not have to be necessarily connected with different model domains *i.e.*

data sets recorded in different experimental realizations, can be sensitive to the same physical parameter.

In addition, there is not an unique approach when implementing joint inversion algorithms. For example, Stefano *et al.* (2011) categorized joint inversion algorithms in the following way:

1. Single domain joint inversion inverts complementary data sets for the same model domain. For example, Commer & Newman (2009) and Abubakar *et al.* (2011a) jointly inverted marine CSEM and MT for electrical resistivity.
2. Cooperative joint inversion integrates complementary data sets, that are related with different model domains in a single workflow. This approach consists in inverting each complementary data set separately and using the inverted models to constrain subsequent inversions for one or several model domains. The constraint can be imposed using a mathematical or empirical law which establishes a relation between the different model domains. For example (Saunders *et al.*, 2005), constrained inversion of DC data imposing a structural constraint derived from seismic travel-time inversion, and Hu *et al.* (2009a) jointly inverted electromagnetic and seismic data by using one model domain to constrain the other at each successive iteration by imposing a structural term in the parametric functional. That is, the estimated conductivity at a given iteration k , is used to constrain the inversion for velocity at the next iteration, and the new estimated velocity model at iteration $k+1$ is used to constrain the inversion for conductivity in the next iteration. The process is repeated until one of the stopping criteria is satisfied.
3. Simultaneous joint inversion tries to invert all complementary data sets simultaneously, and can also include a constraint linking the different model domains. Gallardo & Meju (2003, 2004) jointly inverted DC and seismic data, Stefano *et al.* (2011) presented a joint inversion algorithm for seismic, magnetotelluric and gravity data, aimed at improving subsalt imaging, Santos *et al.* (2006) jointly inverted gravity and magnetotelluric data, and Gao *et al.* (2010) presented an algorithm for the estimation of porosity and fluid saturation, from joint inversion of seismic and electromagnetic measurements.

The mathematical solution of the single domain joint inversion is generally formulated as minimizing the parametric functional:

$$f(\mathbf{m}) = \sum_i^{N_{exp}} \|\mathcal{D}_i(\mathbf{G}_i(\mathbf{m}) - \mathbf{d}_i)\|_2^2 + \lambda \mathcal{R}(\mathbf{m}) \quad (4.2)$$

Where the same conventions for the mathematical symbols are used, and $\mathcal{D}_i$ is the data weighting matrix for the i -th experimental realization. For the cooperative joint inversion

the constrained parametric functional for the k -th model domain can be defined as:

$$f(\mathbf{m}_1, \dots, \mathbf{m}_{N_p}) = \|\mathcal{D}_k(\mathbf{G}_k(\mathbf{m}_{p(k)}) - \mathbf{d}_k)\|_2^2 + \lambda \mathcal{R}(\mathbf{m}_{p(k)}) + \beta \mathcal{C}(\mathbf{m}_1, \dots, \mathbf{m}_{N_p})$$

Where N_p is the number of different model domains, $\mathcal{C}(\mathbf{m}_1, \dots, \mathbf{m}_{N_p})$ is the link between the model domains and β weights the contribution of the constraining term to the parametric functional. Finally, the solution for the simultaneous joint inversion problem can be obtained through the minimization of (Haber & Oldenburg, 1997):

$$f(\mathbf{m}_1, \dots, \mathbf{m}_{N_p}) = \sum_i^{N_{exp}} \|\mathcal{D}_i(\mathbf{G}_i(\mathbf{m}_{p(i)}) - \mathbf{d}_i)\|_2^2 + \sum_i^{N_p} \lambda_i \mathcal{R}_i(\mathbf{m}_i) + \beta \mathcal{C}(\mathbf{m}_1, \dots, \mathbf{m}_{N_p}) \quad (4.3)$$

Where λ_i and $\mathcal{R}_i$ are the regularization parameters and regularization terms corresponding to each model domain.

It is important to note that the solution of the joint inversion problem can also be formulated in terms of the minimization of a multiplicative cost function (Hu *et al.*, 2009a; Abubakar *et al.*, 2011a), however, in the scope of this thesis, only the additive cost functions were considered and for this reason, this topic is not further developed here.

The constraining term $\mathcal{C}(\mathbf{m}_1, \dots, \mathbf{m}_{N_p})$, can be constructed using structural (Haber & Oldenburg, 1997; Gallardo & Meju, 2004, 2003; Hu *et al.*, 2009a), petrophysical (Heincke *et al.*, 2010; Liang *et al.*, 2011), or empirical (Roy *et al.*, 2005) relations between the model domains. In this thesis a structural link is used, and its construction is discussed in the next section.

4.2 3D constrained inversion of marine CSEM with acoustic velocity

Cooperative joint inversion is essentially a constrained inversion algorithm or a combination of constrained inversion algorithms, and can be interpreted as an additional regularization of the inverse problem (Kaipio *et al.*, 1999). One of the main motivations to use a constrained inversion algorithm is to improve the quality of estimated models and reduce inherent ambiguities. A classical example with geophysical implications is the well known fact that acoustic velocity has much higher spatial resolution than electrical conductivity (Harris & MacGregor, 2006). This fact has been considered in previous constrained inversion schemes for resistivity. For example, Saunders *et al.* (2005) constrained inversion of DC data utilizing a structural factor derived from a velocity model obtained by travel-time tomography. This approach

proved to be effective as the conductivity model inverted with a structural constraint had better spatial resolution than the conductivity models inverted from DC data alone.

This is also the methodology used in this thesis. It is assumed that a velocity model is available for the constraining of electromagnetic inversion with a structural term. In a practical situation, one must have available CSEM and seismic data sets acquired with the aim of imaging the same geological structures. The velocity model can be obtained using modern seismic waveform inversion methods (Warner *et al.*, 2006; Ben-Hadj-Ali *et al.*, 2008), which are known to lead to velocity models with a better spatial resolution than the ones obtained from seismic travel-time inversion. The approach presented in this chapter, aims to investigate the benefit of integrating acoustic velocity in 3D CSEM inversion, without jointly invert CSEM and seismic data, taking in consideration that such an approach does not increase the complexity of the inversion algorithm dramatically, nor the computational capabilities requirements. Future work will be oriented to extend the presented methodology to jointly invert seismic and CSEM in a single workflow, and apply both algorithms in the inversion of real data sets.

The link term lies at the heart of cooperative joint inversion. This work aims to develop a scheme to improve the quality and spatial resolution of resistivity, or conductivity, images obtained from the inversion of CSEM data. For this reason only the use of structural links is discussed here.

There are available several approaches to derive a structural link. For example, (Haber & Oldenburg, 1997) defines the Laplacian of each model domain as a measure of structure for that model domain, and a measure of similarity of structures is imposed to a parametric functional, and minimized together with the data misfit terms. Saunders *et al.* (2005) introduced a structure operator based on the local Hessian of the *a priori* known velocity field, and it is imposed as a regularization of the conductivity model in the parametric functional. A third approach is to use the cross product of the gradients of the physical parameters to be estimated, defined as (Gallardo & Meju, 2004, 2003):

$$\mathbf{t}(\mathbf{r}) = \nabla m(\mathbf{r}) \times \nabla v(\mathbf{r}) \quad (4.4)$$

Where $m(\mathbf{r})$ represents the logarithm with respect to the base 10, of the conductivity, and $v(\mathbf{r})$ represents the acoustic velocity. The condition $\mathbf{t}(\mathbf{r}) = \mathbf{0}$, imposes that all spatial changes in electrical conductivity and acoustic velocity point in the same or opposite directions regardless of their amplitude. This constitutes a substantial advantage over the structural links proposed by Haber & Oldenburg (1997) and Saunders *et al.* (2005), as they require a scaling in the constraint term. Furthermore, the cross product of gradients is identically zero if $\nabla m(\mathbf{r}) = \mathbf{0}$ or $\nabla v(\mathbf{r}) = \mathbf{0}$. Thus, it allows for the existence of strong discontinuities in one of the model domains even if the same discontinuity does not exist in the other (Gallardo & Meju, 2003).

I now define the augmented parametric functional in the weighted parameter space (as described in section 3.8), with the added constraint term derived from an *a priori* known velocity model:

$$\tilde{f}(\tilde{\mathbf{m}}) = \frac{1}{2} \|\mathcal{D}(\mathbf{G}(\tilde{\mathbf{m}}) - \mathbf{d})\|_2^2 + \frac{1}{2} \lambda \mathcal{R}(\tilde{\mathbf{m}}) + \frac{1}{2} \beta \sum_{n=1}^{N_m} \|(\nabla [\mathcal{W} \tilde{\mathbf{m}}]_n \times \nabla v_n)\|_2^2 \quad (4.5)$$

Where $\tilde{m}_n$ is the weighted logarithm (base 10) of the conductivity, and v_n is the acoustic velocity at the n -th inversion cell, N_m is the number of inversion cells.

As stated in section 3.8 the preconditioning matrix $\mathcal{W}$ is symmetric, thus it is relatively straightforward to show that the parametric functional 4.5 satisfies identities 3.68 and 3.69. These properties are necessary for the use of the updating expression 3.71 and $\nabla_m f$, which is given by:

$$\nabla_m f = \nabla_m f_D + \lambda \nabla_m f_R + \beta \nabla_m f_C \quad (4.6)$$

Where, $\nabla_m f_D$, $\nabla_m f_R$ and $\nabla_m f_C$ are the gradients of the data misfit, of the regularization term and of the acoustic velocity constraining terms, respectively. The computation of the gradients of the data misfit and of the regularization terms were discussed in chapter 3. For the computation of the gradient of the structural term, it is more convenient to make the analysis for the k -th component of the gradient in the model parameter space:

$$\frac{\partial f_C}{\partial m_k} = \sum_{n=1}^{N_m} (\nabla m_n \times \nabla v_n) \cdot \frac{\partial}{\partial m_k} (\nabla m_n \times \nabla v_n) \quad (4.7)$$

Before deriving an explicit expression for the computation of ∇m_n and ∇v_n it is also convenient to use a parameterization for the n -th inversion cell. That is, each inversion cell can be identified by the triplet (i, j, k) , such that $n = n(i, j, k)$. By using a finite difference formula, each component of ∇m_n is approximated by:

$$\frac{\partial m_n}{\partial x} \approx \frac{m_{i+1,j,k} - m_{i,j,k}}{x_{i+1,j,k} - x_{i,j,k}} \quad (4.8a)$$

$$\frac{\partial m_n}{\partial y} \approx \frac{m_{i,j+1,k} - m_{i,j,k}}{y_{i,j+1,k} - y_{i,j,k}} \quad (4.8b)$$

$$\frac{\partial m_n}{\partial z} \approx \frac{m_{i,j,k+1} - m_{i,j,k}}{z_{i,j,k+1} - z_{i,j,k}} \quad (4.8c)$$

Where $(x_{i,j,k}, y_{i,j,k}, z_{i,j,k})$ are the coordinates of the centre of the n -th inversion cell. A similar expression can be obtained for ∇v_n . I consider $\nabla m_n = \mathbf{0}$ and $\nabla v_n = \mathbf{0}$ for all cells on the boundary.

Using Gibbs's notation, the gradients $\nabla \mathbf{m}$ and $\nabla \mathbf{v}$ are more conveniently represented by a

matrix to vector multiplication, that is:

$$\nabla \mathbf{m} = (\mathcal{D}_x \mathbf{m}, \mathcal{D}_y \mathbf{m}, \mathcal{D}_z \mathbf{m}) \quad (4.9a)$$

$$\nabla \mathbf{v} = (\mathcal{D}_x \mathbf{v}, \mathcal{D}_y \mathbf{v}, \mathcal{D}_z \mathbf{v}) \quad (4.9b)$$

where $\mathbf{m}$ and $\mathbf{v}$ are vectors containing the logarithm (base 10) of the conductivity, and the acoustic velocity for each inversion cell. Each row of $\nabla \mathbf{m}$ and $\nabla \mathbf{v}$ contains the gradient of m and v for each inversion cell, respectively. Sparse matrices $\mathcal{D}_x$, $\mathcal{D}_y$, $\mathcal{D}_z$, allow for a compact representation of the finite difference approximation for each component of the gradient in the Cartesian space. For example:

$$\mathcal{D}_x = \begin{pmatrix} -\frac{1}{Lx_1} & \frac{1}{Lx_1} & \cdots & & \\ & -\frac{1}{Lx_2} & \frac{1}{Lx_2} & \cdots & \\ & & \vdots & & \\ & & & -\frac{1}{Lx_n} & \frac{1}{Lx_n} & \cdots \\ & & & \vdots & & \end{pmatrix} \quad (4.10)$$

Where $1/Lx_i = 1/(x_{i+1,j,k} - x_{i,j,k})$. Similar expressions are relatively straightforward to derive for the remaining components.

The expressions above derived, allow for a straightforward computation of the cross product of the spatial gradients. It is now derived an explicit expression, for the computation of the derivative of the cross-product of gradients with respect to the k -th model parameter. From 4.7:

$$\begin{aligned} \frac{\partial}{\partial m_k} (\nabla m_n \times \nabla v_n) &= \\ \frac{\partial}{\partial m_k} \left(\hat{\mathbf{i}} \frac{\partial m_n}{\partial x} \times \nabla v_n \right) + \frac{\partial}{\partial m_k} \left(\hat{\mathbf{j}} \frac{\partial m_n}{\partial y} \times \nabla v_n \right) + \frac{\partial}{\partial m_k} \left(\hat{\mathbf{k}} \frac{\partial m_n}{\partial z} \times \nabla v_n \right) &= \\ \hat{\mathbf{i}} \frac{\partial}{\partial m_k} [\mathcal{D}_x \mathbf{m}]_n \times \nabla v_n + \hat{\mathbf{j}} \frac{\partial}{\partial m_k} [\mathcal{D}_y \mathbf{m}]_n \times \nabla v_n + \hat{\mathbf{k}} \frac{\partial}{\partial m_k} [\mathcal{D}_z \mathbf{m}]_n \times \nabla v_n &= \\ \hat{\mathbf{i}} [\mathcal{D}_x \delta_{\bullet,k}]_n \times \nabla v_n + \hat{\mathbf{j}} [\mathcal{D}_y \delta_{\bullet,k}]_n \times \nabla v_n + \hat{\mathbf{k}} [\mathcal{D}_z \delta_{\bullet,k}]_n \times \nabla v_n & \end{aligned} \quad (4.11)$$

Where $\delta_{\bullet,k}$ is the k -th column of the identity matrix using Kronecker's delta notation, and $(\hat{\mathbf{i}}, \hat{\mathbf{j}}, \hat{\mathbf{k}})$ are the versors of a three-dimensional Cartesian coordinate system. Finally, the k -th component of the gradient of the structural constraining term, is given by:

$$\frac{\partial f_C}{\partial m_k} = \sum_{n=1}^{N_m} (\nabla m_n \times \nabla v_n) \cdot \left(([\mathcal{D}_x \delta_{\bullet,k}]_n, [\mathcal{D}_y \delta_{\bullet,k}]_n, [\mathcal{D}_z \delta_{\bullet,k}]_n) \times \nabla v_n \right) \quad (4.12)$$

As matrices $\mathcal{D}_x$, $\mathcal{D}_y$ and $\mathcal{D}_z$ are sparse, and only contain a maximum of two non-zero elements

per column, the computational operations for the computation of $\frac{\partial f_C}{\partial m_k}$ can be accomplished rapidly and efficiently. The expressions presented in this section cover the principal schemes for the implementation of constrained or joint inversion algorithms utilizing a structural constraint based on the cross product of the spatial gradients of different physical parameters or, if one prefers, model domains. It is important to note that the approach presented in this chapter is completely general and can be implemented for any kind of complementary geophysical domain, as for example gravity.

As in chapter 3, it is utilized a smoothing stabilizer in the developed constrained inversion algorithm. All the necessary expressions for the computation of the gradient of the data misfit and of the regularization term are derived in chapter 3. Expression 4.12 was implemented for the computation of the gradient of the augmented objective function 4.5.

4.3 Static versus adaptive weighting parameter

The minimization of 4.5 requires the estimation of an appropriate weighting parameter β , for the structural constraint term.

As in the case of the regularization term, a parameter too high will lead to the structural term dominating the inversion, whereas a parameter too low will lead to a solution which is close to the one without imposing the structural constraint.

Hence the estimation of β resembles the estimation of the regularization parameter λ . Naturally, one can choose empirically an initial value for β that is sufficiently high and decrease it when the progress in the improvement of the data misfit term does not meet some pre-defined criterion. However, this route can lead to some confusion, as it would be difficult to set a rule that could decide which weighting parameter should be decreased, that is, λ , β , or both, at each tomographic iteration. Thus, there is a strong subjective component associated to this approach. In addition, a rapid decrease of β can lead to a solution of the inverse problem that is not constrained by the structural term. Hence, a cooling method is probably not the best approach for estimating the weighting parameter of the structural term.

Two different approaches were investigated, in order to determine how the structural constraining term should be weighted in the inversion scheme. One consists of setting a value for β and keeping it constant through the inversion, as in Saunders *et al.* (2005). Following this approach requires setting an appropriate value for β , which is not straightforward in most part of the cases, as a value too large can lead to an insufficient decrease in the data misfit. This route essentially requires some testing in order to determine an appropriate weighting parameter, that is, a parameter that leads to a constrained inverted model consistent with the structural term and with geological significance. I will call this the *static* approach.

The second approach, consists in setting a value for β , which weights the constraint term in relation to the decrease of the contribution of the data misfit and of the regularization

terms to the objective function. This approach is also empirical, however, it is intuitive as the weight is automatically interpreted as a fraction of the remaining contributions to the objective function. In addition, as in principle both the data misfit and the regularization terms decrease through the inversion, it is also guaranteed that the contribution of the structural constraining term also decreases, keeping its relative contribution to the parametric functional. I will call this the *adaptive* approach. The weighting parameter β_k at the k -th iteration is given by:

$$\beta_k = \beta_0 [f_D + \lambda f_R] \quad (4.13)$$

Where β_0 is a constant that represents the fraction of the contributions of the data misfit and of the regularization terms. The determination of β_0 also requires experimentation.

4.4 Constrained inversion of a synthetic data example

In this section, I present an example that shows the effectiveness of the implemented constraining methodology in improving the spatial resolution of conductivity (or resistivity) images. As aforementioned it is assumed that the velocity model is known *a priori*, and determined from separate inversion of seismic data.

In practical inversion of a seismic data set, the structure of the inverted velocity model does not match the structure of the true distribution of velocity in the subsurface, due to the resolution limits of seismic data, which is controlled by several factors such as, the use of a band limited source and existence of noise in the recorded data. For inversions that model the full waveform, the spatial resolution depends essentially on the component with highest wavenumber in the recorded data (Hicks & Pratt, 2001; Sirgue *et al.*, 2010). In addition, geophysical inversion has a natural limitation, as it aims to reconstruct a continuous distribution from a sparsely collected data set (Aster *et al.*, 2005).

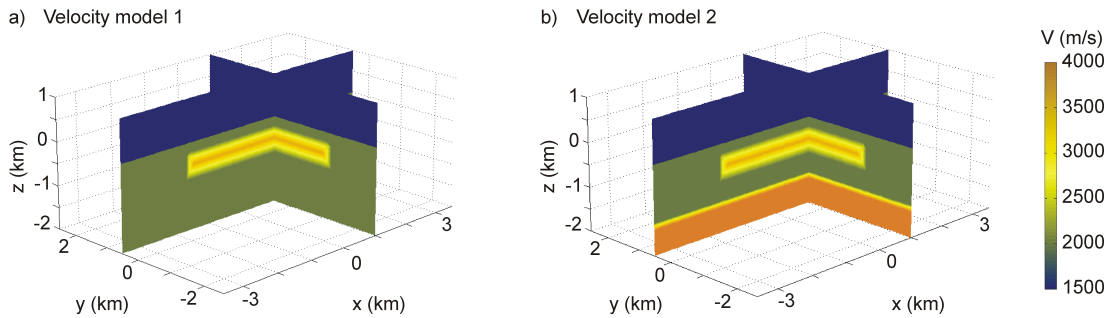


Figure 4.1: Velocity models utilized for the computation of the cross-gradient constraining term.

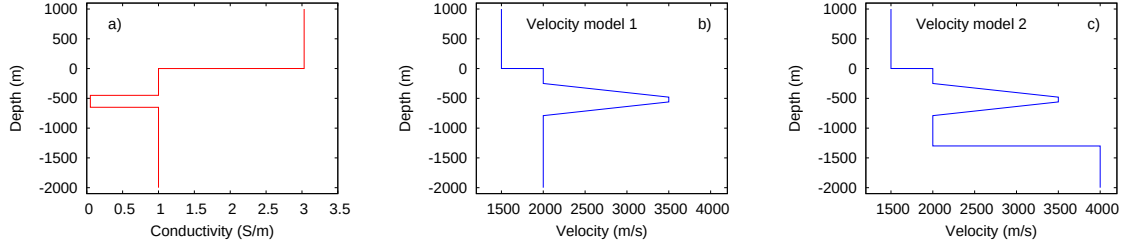


Figure 4.2: Vertical profiles of the a) conductivity model, b) velocity model 1, c) velocity model 2, at the centre of the model ($x = 0$ m and $y = 0$ m).

Consequently, the structure of the inverted model cannot exactly match the structure of the conductivity model. To replicate this in the synthetic inversion tests, the velocity model was smoothed over several hundred meters, which corresponds to the expected resolution of seismic tomography at the depths considered in this example.

In this section are presented constrained inversions of a noise-free CSEM synthetic data set using two different velocity models (figure 4.1). Both velocity model 1 and velocity model 2, have a velocity anomaly in the region of the conductivity anomaly in the synthetic conductivity model (figure 4.3 a). Velocity model 2, however, also has a higher velocity anomaly in the lower part of the model, and which is not correlated with any resistivity structure in the synthetic resistivity model. Figures 4.2 a)-c), show vertical profiles of the conductivity model, and velocity model 1 and 2, respectively. One can observe that the block velocity anomaly occupies a region larger than the conductivity anomaly. The purpose of inverting CSEM data with structural constraints from velocity model 2 was to investigate the effect of changes in velocity that do not correlate with changes in resistivity.

The CSEM data is generated using the conductivity model shown in figure 4.3 a), and the same source-receiver configuration as in the example presented in section 3.10, and shown in figure 3.4. The synthetic data set was generated using eleven x-oriented sources (denoted by S1-S11) for frequencies 0.5 Hz and 1 Hz, and 28 receivers, distributed along four receiver lines: RL1-RL4. All transmitters were positioned 30 m above the sea-floor. Figure 4.3 shows slices of the conductivity model utilized to generate the synthetic data, at $y = 0$ km and $x = 0.6$ km. The data set includes 924 noise-free measurements, comprising the three components of the electric field. I considered a case for which the sea-floor noise level is 10^{-15} Vm^{-1} , thus all synthetic measurements with an amplitude smaller than the noise level estimate were disregarded in the inversion tests. All data residuals were weighted accordingly with the expression for the weight of the k -th data residual:

$$\mathcal{D}_{kk} = \frac{1}{\delta \sqrt{A_k A_k^*}} \quad (4.14)$$

Where $\mathcal{D}_{kk}$ is a generic term in the main diagonal of $\mathcal{D}$ (equation 4.5), δ is an empirical constant, chosen to be 0.05 for all inversion tests presented in this section. The asterisk in superscript stands for complex conjugation, and A_k is the value of the k -th sample of the data set.

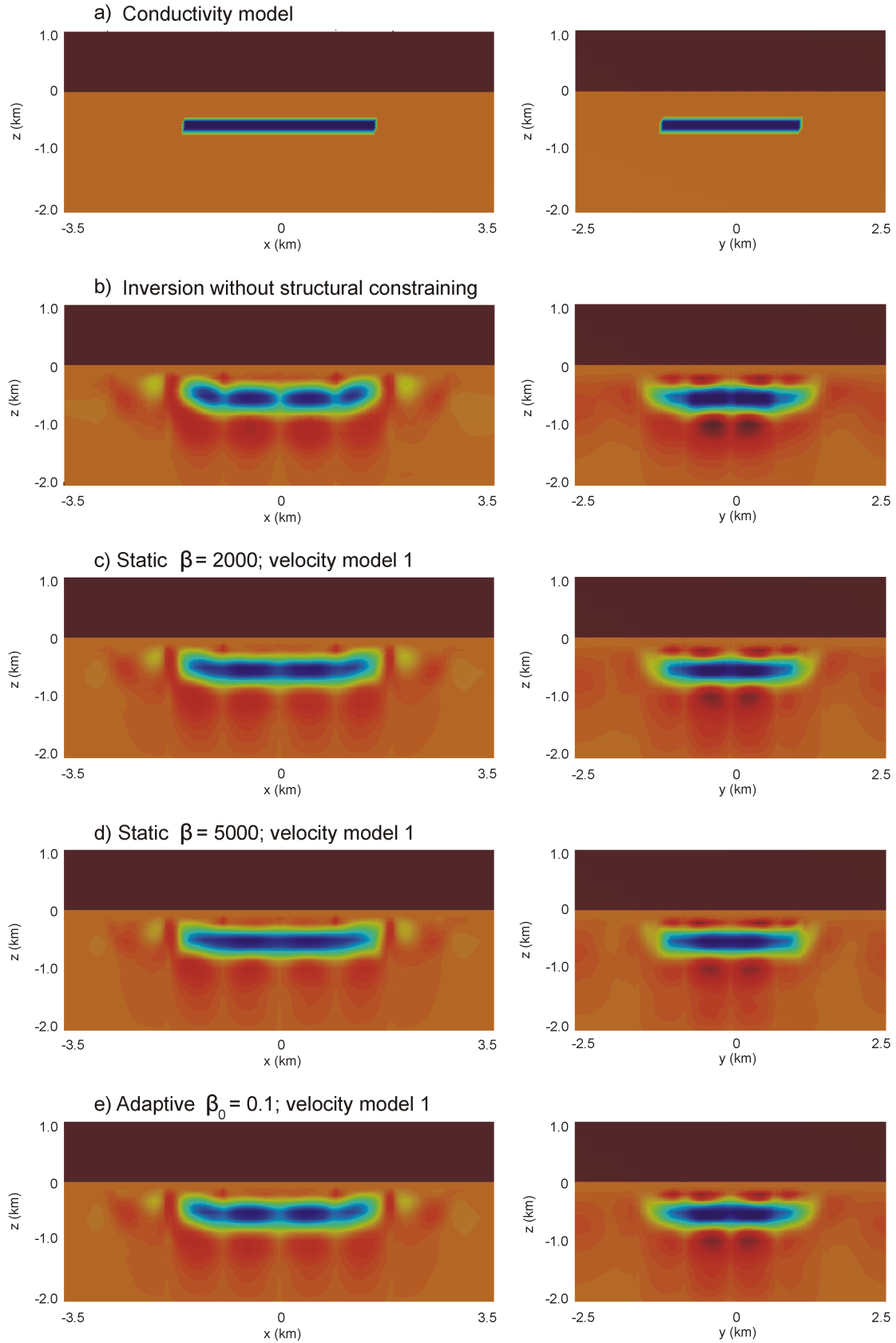
As in the example presented in section 3.10, the computational domain is a volume with $7 \times 5 \times 3 \text{ km}^3$, corresponding to approximately 1.25×10^6 unknowns in the forward modelling solution. The forward modelling grid has dimensions $139 \times 95 \times 32$ and the inversion grid has dimensions $118 \times 80 \times 18$, corresponding to 157131 inversion cells. For all the inversion examples shown in this section it is used the L-BFGS method, preconditioned with the physics-based approximation of the inverse of the diagonal of the Hessian matrix, and the parameters of the preconditioner are $\gamma = 2.1$, $\varepsilon = 1.0$ and $\beta = 6.0$

The inversions are carried out sequentially for each frequency. It is chosen a maximum of 30 tomographic iterations for 0.5 Hz and the inversion proceeds for 1 Hz until one of the chosen stopping criteria is satisfied, that is, the root mean square of the data misfit is smaller than 1.85, or the accumulated number of iterations exceeds 130.

As aforementioned one of the most problematic issues with the implementation of the constraining inversion algorithm, is how to set the weighting parameter for the structural constraining term, β . In this example, the two approaches described in section 4.3, are investigated. The so called static method, where the parameter is kept constant during the inversion, and the adaptive method, where the parameter changes through the inversion accordingly to equation 4.13. One must note that both methods require experimentation in order to determine the best structural weighting, however, the use of the adaptive approach is more *intuitive*, in the sense that it represents a fraction of the summed contributions of the data misfit and regularization terms, to the parametric functional.

In the examples presented in figures 4.3 c)-f), the cross-product term is computed with the velocity model 1. Figure 4.3 c)-d) shows slices of the reconstructed conductivity model at $y = 0 \text{ km}$ and $x = 0.6 \text{ km}$, using fixed weighting parameters $\beta = 2000$ and $\beta = 5000$, respectively. By inspection of figures 4.3 c)-d) it is possible to identify an improvement of the spatial resolution due to the structural constraining term, and the best reconstructed model is the one for $\beta = 5000$ (figure 4.3 d). For values of β higher than 6000, the solution had not converged by iteration 130. For values of β below 1000 was observed a residual effect of the structural constraining term. Thus, one can conclude that there is a limited interval in which exists one or a set of optimal values for the structural weighting β . In practice, one cannot determine *a priori* what is the best value for the weighting parameter, and its estimation relies essentially upon experimentation.

The results of the inversions carried out with the adaptive weighting parameter, are rendered in figures 4.3 e)-f), for $\beta_0 = 0.1$ and $\beta_0 = 0.3$, respectively. The cross-gradient constraining term is computed using velocity model 1.



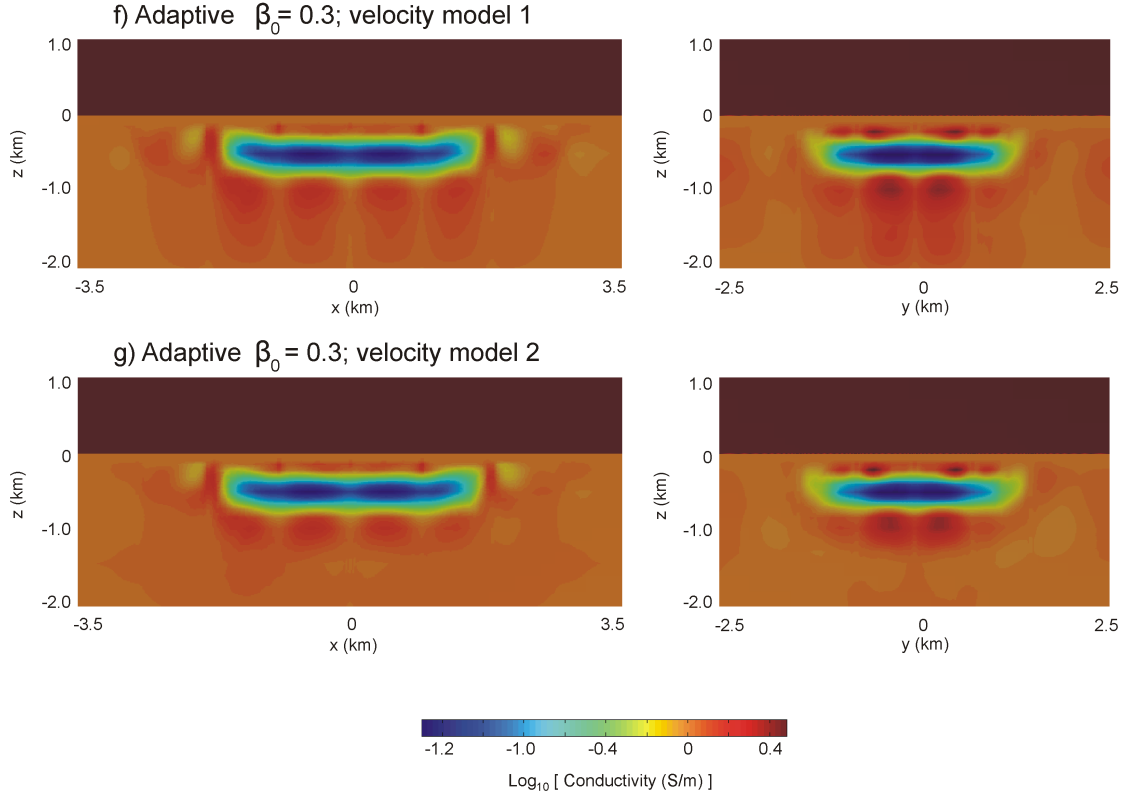


Figure 4.3: Slices of the a) synthetic conductivity model, reconstructed conductivity model b) without structural constraints, c) fixed $\beta = 2000$ and velocity model 1, d) fixed $\beta = 5000$ and velocity model 1, e) adaptive with $\beta_0 = 0.1$ and velocity model 1, f) adaptive with $\beta_0 = 0.3$ and velocity model 1, g) adaptive with $\beta_0 = 0.3$ and velocity model 2, at $y = 0$ km (left row) and $x = 0.6$ km (right row).

For the case $\beta_0 = 0.1$ one can observe that there is almost no improvement in the spatial resolution, in comparison to the inverted conductivity model utilizing the non-constrained inversion scheme (figure 4.3 b). The best recovered model can be observed for $\beta_0 = 0.3$. As in the case of a fixed weighting parameter approach, experimentation is necessary in order to determine which parameter can lead to the most meaningful inverted model of conductivity. However, this approach is more intuitive as it can be interpreted as a relative weighting. Generally, convergence was obtained within an acceptable number of iterations for values of β_0 between 0.1-0.45. Naturally, the structural constraining is proportional to β_0 . Nonetheless one must note that these weights were determined on a heuristic basis, and for a limited number of cases. Experimentation is therefore necessary on a case-by-case basis. Figure 4.4 a)-d) compares the constrained conductivity models for $\beta = 5000$ and $\beta_0 = 0.3$, with the original synthetic model and the unconstrained inverted model.

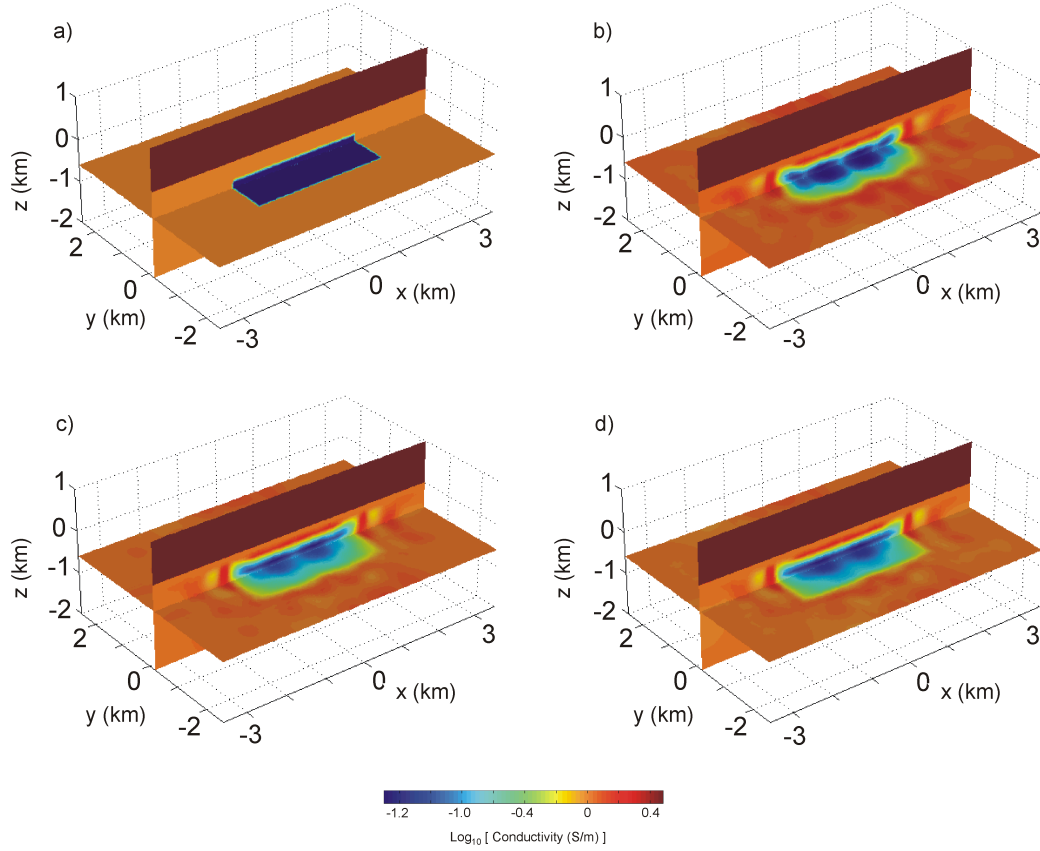


Figure 4.4: Slices of the a) original resistivity model, b) inverted resistivity model without structural constraining, c) inverted model using adaptive structural weighting ($\beta_0 = 0.3$), d) inverted model using static structural weighting ($\beta = 5000$), at $y = -200$ m and $z = -600$ m. All inversions were carried out with 2 frequencies (0.5 Hz and 1 Hz).

Figure 4.3 g) shows slices of the inverted conductivity model constrained with velocity model 2 (figure 4.1 b), at $y = 0$ km and $x = 0.6$ km. Comparing figures 4.3 f) and 4.3 g) one can observe that the inverted conductivity model constrained with velocity model 2 presents less conductivity artifacts in the lower region of the model, than the inverted conductivity model constrained with velocity model 1. This observation, is explained by the fact that in the first case (figure 4.3 f), the gradient of the velocity is non-zero in the vicinity of the transition to the layer in the lower part of the model. Thus, a structural constraint is being imposed in this region of the model eliminating conductivity artifacts and, imposing the update of the conductivity model in the right positions in space, at each tomographic iteration. Consequently, the number of tomographic iterations increases as the structural term of the objective function is also larger, in comparison to the example using velocity model 1 (figure 4.5 b).

Structural Weighting	Processing Groups	Number of threads	Factorization Memory	Time per Iteration	Number of Iterations	Run Time
Static						
$\beta = 2000$ (vm1)	12	8	2.99 GB	9.4 min	49	7.7 h
$\beta = 5000$ (vm1)	12	8	2.99 GB	9.2 min	65	9.9 h
Adaptive						
$\beta = 0.1$ (vm1)	12	8	2.99 GB	9.5 min	44	6.9 h
$\beta = 0.3$ (vm1)	12	8	2.99 GB	9.4 min	53	8.3 h
$\beta = 0.3$ (vm2)	12	8	2.99 GB	9.9 min	96	15.8 h

Table 4.1: Summary of the allocated computational resources, execution time, and number of iterations necessary to decrease the data misfit below the tolerance level, for each one of the inversion examples presented in this section. The number of processing groups corresponds to the number of MPI processes and number of computer nodes; the factorization memory is the average allocated memory per node for the factorization of the linear system; vm1 stands for velocity model 1; vm2 stands for velocity model 2.

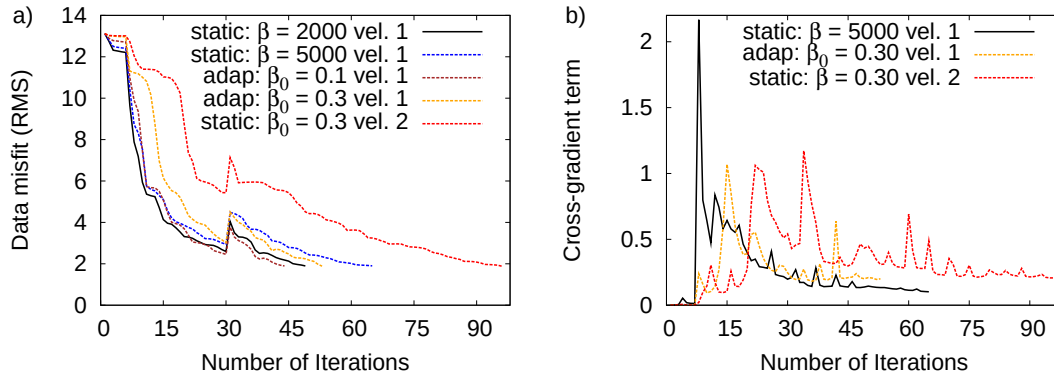


Figure 4.5: Plot of the a) data misfit and of the b) cross-product of the gradient, for different structural weighting parameters and velocity models, as a function of the iteration number.

As aforementioned, this example demonstrates that no artificial structures are added to inverted models, if velocity structures are uncorrelated with conductivity anomalies. Another important aspect, is the fact that source and receiver effects are strongly attenuated, when using the constraining inversion scheme presented here, as shown in figure 4.4. The same conclusions are valid if the structural weighting parameter is kept constant during the inversion. Both the static approach and the adaptive approach for the structural weighting parameter yielded conductivity models that are constrained spatially. However, the cross-product term is more effectively minimized when the structural weighting parameter is constant, *i.e.*, the static method is chosen (figure 4.5 b). This result is further confirmed comparing figure 4.3

d) and 4.3 f), and figure 4.4 c), 4.4 d) and 4.4 a). This is explained by the fact that for $\beta = 5000$ the value of the cross-gradient term is more effectively minimized, as shown in figure 4.5 b). Thus a constant value for the structural weighting parameter leads to better constrained conductivity models. Figure 4.5 a) shows the decrease of the data misfit with the number of iterations, for the examples presented in this section. The visible jump of the value of root mean square (see equation 3.75) at iteration 30 (figure 4.5), occurs when the inversion moves from the data set corresponding to 0.5 Hz to the data set corresponding to 1 Hz.

Table 4.1 summarizes the allocated computational resources, execution time, and number of iterations necessary to decrease the data misfit below the tolerance level, for the inversion examples presented in this chapter.

4.5 Conclusions

An approach was presented for three-dimensional inversion of marine CSEM data constrained with acoustic wave velocity. This is based on two main assumptions: changes of electrical conductivity and acoustic velocity have the same direction and occur at the same spatial positions, and the acoustic velocity model is known *a priori*. Therefore it is assumed that seismic data is inverted separately, using a waveform inversion algorithm, for example. From the several methodologies available to determine the structural constraint, the cross-product method was the one adopted as it does not require any scaling for the complementary model parameters *i.e* the acoustic velocity. Furthermore, it does not add artificial structures in the inverted model, in the regions of the model where there is no spatial correlation between conductivity and velocity anomalies. The constraining term of the parametric functional is weighted to allow the use of the physics-based preconditioner introduced by Plessix & Mulder (2008).

It is a fact that seismic data has a higher spatial resolution and is more sensitive to the fine-scale of geological structures than electromagnetic data. Therefore, it is reasonable to determine the velocity model separately and use it to compute the structural term. However, one must note that inverted conductivity models, and constrained with the presented approach, can only be improved within the limits of seismic resolution. For this reason, the algorithm was tested with smoothed velocity models to take into account this factor.

A particular aspect of extending the parametric functional by including the link term, is the fact that a suitable trade off, or if one prefers, weighting parameter must be determined. One may consider to use a cooling approach, similarly to Tikhonov's regularization for non-linear inverse problems. Nonetheless, such an approach may lead to a fast decrease of the structural weighting parameter, and therefore, the inverted model will not be constrained.

In addition, this route does not lead to a clear methodology on how to decrease both the Tikhonov's regularization parameter and the structural weighting parameter at each tomographic iteration, hence two options (both empirical) were investigated. The first consists in choosing a parameter and keeping it constant during the inversion (Saunders *et al.*, 2005). I called this route, the static approach. The second approach consists of weighting the structural constraining term with a fraction of the accumulated contributions of the data misfit and the regularization functionals to the parametric functional. I called this route, adaptive approach. The inversion of a synthetic data set demonstrated that both approaches yielded inverted models which are spatially better resolved, provided that appropriate weighting parameters were chosen. However the static method yielded constrained models with better resolution. This statement is supported by a qualitative comparison of the conductivity models inverted, and quantitatively as the static approach is more effective in decreasing the value of the cross-gradient term with the increasing number of iterations. The adaptive approach has the advantage of offering an intuitive interpretation of the structural weighting parameter, in the sense that it represents a ratio between the contribution of the structural term and the summed contributions of the data misfit and regularization terms.

In summary, it has been demonstrated that a scheme for the integration of an *a priori* known velocity model in the inversion of CSEM data, using the cross product of gradients, leads to a conductivity model which is better resolved spatially, reduces the source and receiver printing, and can help to reduce artifacts in inverted conductivity models. However, the method was only tested with synthetic models. Future research, will aim to test the algorithm with more realistic cases, apply the methodology to field data, and extend it to a full joint inversion algorithm.

Final Conclusions

This thesis presents developed and implemented methods for three-dimensional forward modelling, inversion and constrained inversion of CSEM data in the frequency domain. These methods have been implemented in a computer code using Fortran 90. Three-dimensional CSEM modelling and inversion is computationally intensive and demanding. To alleviate this problem codes were parallelized using openMP and MPI to take advantage of a hybrid model of parallelism *i.e.*, both shared and distributed memory paradigms are used.

Chapter 2 presents a numerical scheme for three-dimensional modelling of marine CSEM data, by decomposing the electric field in primary and secondary components, and discretizing the equation for the secondary field utilizing edge finite elements. The edge finite element method is a discretization consistent with the discontinuity of the normal component of the electric field at interfaces across different materials, and enforces the divergence-free condition locally. In this work, cartesian grids were considered as this allows to facilitate the task of building a grid and implement a grid generator in the code. The primary field is calculated using a homogeneous or two half-space resistivity model. The latter was shown to be particularly important in improving the accuracy of the solution when the air layer is represented in the resistivity model. Comparisons between the solutions obtained using the scheme developed in this thesis and 1D and 3D integral equation solutions, demonstrated a good agreement between solutions. The proposed approach is more demanding computationally in comparison to the integral equation solution, nonetheless, geological resistivity models can be represented with significantly less effort. The method was also shown to be reliable in the range of frequencies typically used in CSEM surveys.

Preconditioners for the solution of the linear system of equations derived from the edge finite element discretization were investigated. All the tested options yielded slow convergence rates, making their practical use unfeasible, hence an implementation of a multifrontal solver was used. The examples presented in this thesis, showed that the approach used for the numerical solution is robust for large grid spacing ratios, and can cope with the large null space of the linear system, that results from the discretization of the vector Helmholtz equation in the air. It was shown that it is possible to achieve a solution for relatively large models for one source in an acceptable run time. Nonetheless, it requires the use of large computational capabilities to cope with the computationally intensive multifrontal solver. As

the factorization is computationally intensive, the reutilization of the factors and successive forward and back-substitutions are used to achieve a multiple source solution. However, this requires the grid to be refined at each source position (and each receiver position for the computation of the adjoint field), thus limiting the size of the models that can be considered. In this work, two levels of parallelism were applied for the calculation of the primary field: A shared memory parallelism model for its calculation at each source point, and a distributed memory parallelism model for its calculation at different source positions. When using a two half-space model and, by extension, a layered background medium, this aspect is particularly important as it is required the calculation of Hankel transforms, which is very time consuming for a large number of grid points. The same model of parallelism is applied for the computation of the adjoint field. A full-field formulation has a clear advantage in this aspect, and therefore its effective implementation should be investigated in future research.

The examples presented in chapter 2 showed the usefulness of the approach for survey simulation and data inversion for limited sized models, and it constitutes an alternative to existing forward modelling methods, requiring however the use of a parallel computing system. In order to improve the effectiveness of the presented approach for 3D CSEM forward modelling, future research should be oriented essentially on three topics: development of a preconditioner, improving the representation of the source term and optimizing the discretization of the computational domain. The first aspect is particularly important in order to improve the scalability of the code. Representing directly the source term, avoids the need to compute the primary field, thus leading to a substantial reduction of computing time in the case when an air layer is represented in the resistivity model. Finally, optimizing the discretization of the computational domain, is crucial to improve the effectiveness of the code in terms of computing storage, allowing to consider resistivity models with larger dimensions. Options include the use of elements with higher-order basis functions in the vicinity of the source, implementation of *Octrees* (Bespalov, 2009) or tetrahedra, alleviating the problem of generating an excessive number of redundant elements in the vicinity of the sources (or receivers) due to finer grid spacing. The use of tetrahedra is particularly attractive, as the discretization of complex shapes, such as bathymetry, do not need to be approximated with a staircase, as in the case of hexahedra.

In chapter 3 is presented a scheme for three-dimensional CSEM inversion in the frequency domain based upon the forward modelling scheme presented in chapter 2.

The marine CSEM inverse problem is non-linear as the electromagnetic field responses depend non-linearly upon the model parameters (*i.e.* resistivity/conductivity). For this reason the inverse problem is recast into an optimization problem. The inverse problem is known to be ill-posed and a well known remedy for this problem is the use of a regularization term. In this work a smoothing stabilizer was implemented. When using the additive cost function, as in the case of this thesis, it is required the estimation of the regularization parameter,

which balances the contribution of the data misfit and the regularization term to the parametric functional. For the case of non-linear problems this parameter is estimated at each tomographic iteration using a cooling approach. An alternative approach for the cooling method was introduced, based upon the decrease of the data residual between successive iterations. An example of a successful inversion of a synthetic data set showed that the adopted cooling method is as valid as the more common cooling approach, that utilizes an artificial mathematical law to determine the regularization parameter.

Three-dimensional inversion requires the estimation of a large number of parameters, thus only methods that require the use of information from the gradient of the objective function were implemented. The gradient of the parametric functional for the regularized inverse problem, comprises two terms: the gradient of the regularization term and the gradient of the data misfit term. The first is trivial to compute as it only requires linear algebra operations. The latter is generally computed using adjoint methods.

Early tests implementing the calculation of the gradient of the misfit term as described in Newman & Alumbaugh (1997), led to unfeasible solutions using the edge finite element forward modelling code, described in chapter 2. For this reason, a method was introduced to compute the gradient of the misfit term, which uses the adjoint primary and secondary field electric fields. The presented approach is effective as it constitutes an automatic method for the computation of the action of the Jacobian matrix over the vector of the data residuals, thus avoiding the explicit storage of the Jacobian matrix, which can be very large in 3D applications. It is also important to note that, the presented approach only requires one extra linear system solution, as in the case of the more widely used approaches based on the discrete form of the forward modelling problem and linear algebra concepts (Newman & Alumbaugh, 1997; Pratt *et al.*, 1998). The importance of such an approach lies also in the fact that it shows a link between the so called *back-propagation of the residuals* using electromagnetic reciprocity and the more commonly approach using notions of linear algebra. Furthermore, the introduced approach for the calculation of the gradient of the misfit term is general, and can be implemented with other forward modelling engines.

This approach is computationally more costly in comparison to the use of the discretized linear system, as it requires the computation of the adjoint primary field, and the integration of the dot product of the electric and adjoint electric field over the volume occupied by the inversion cell (also referred to as the support of the model parameter). However, it is important to note that the computing time for the integration of the electric and adjoint electric fields is negligible and, furthermore, the second factor is only time consuming in the case of considering a layered background model. However, one must observe that the background medium is constant during the inversion, thus the primary field only needs to be computed once and, by parallelizing the computation of the adjoint field over receivers and edges, the computational overhead for this case, is reduced.

An advantage of using electromagnetic reciprocity principles is the fact that the inversion and forward modelling grids are easily decoupled, thus avoiding the estimation of the conductivity at redundant inversion cells generated by a refined forward modelling grid in the vicinity of sources and receivers. In this work, were considered only, inversion grids conformal with the forward modelling grid. However, the methodology is general and therefore non-conforming grids can also be considered. The Gauss-Legendre method was used for the numerical integration scheme, and comparisons between the sensitivities computed using the Fréchet derivative, and the inversion of synthetic data example, showed that an eight point integration rule is sufficient to accurately determine the sensitivities, and therefore the gradient of the data misfit term.

Only methods that use information of the gradient were considered in this project. However, the use of the negative direction of the gradient of the cost function generally is not reliable, and the search direction is improved by preconditioning the gradient. Preconditioners based on the use of the background conductivity model for the approximation of the diagonal of the Hessian were investigated. However, results were disappointing, as no improvement was observed. Instead an existing physics-based preconditioner (Plessix & Mulder, 2008) was implemented, and a weighted second order operator was introduced to obtain a consistent formulation for the weighted parametric functional. As shown for a synthetic example (section 3.10), the presented approach is capable of inverting synthetic data for a configuration with multiple sources and receivers, and for multiple frequencies.

In chapter 4 is presented an approach for a 3D CSEM constrained inversion. The algorithm relies upon the use of the cross-product of the gradients of conductivity and velocity. It is assumed that the velocity distribution is determined *a priori* using a seismic inversion algorithm, and an augmented functional in the weighted model parameter space was defined, in order to obtain a consistent formulation for using the physics-based preconditioner, in the constrained inversion algorithm.

It is important to note that, in a practical application, the structures of velocity and conductivity do not match exactly. For this reason, it was used a synthetic velocity model that was smoothed, in comparison to the conductivity model that was used to generate the CSEM data. Two methods were investigated in order to determine a suitable weighting of the structural constraining term. Both the static and adaptive approaches led to constrained inverted models, however, the static approach was more effective. Synthetic model examples showed that this approach is suitable for improving the spatial resolution, reduce source and receiver printing, and reduce artifacts of inverted conductivity models.

The inversion algorithms developed can be applied to many and diverse electromagnetic imaging problems. For example hydrocarbons exploration, mineral exploration, monitoring of CO₂ storage and oceanic crustal studies. The computational performance of the inversion algorithms (constrained and unconstrained) is driven essentially by the performance of the

multifrontal solver. The computational overhead of the multifrontal solver, combined with grid stretching in the vicinity of sources and receivers, requires extremely large computational resources. Hence, the performance of the inversion algorithms will improve substantially by implementing an effective iterative solver and representing directly the source term. Nonetheless, it is important to note that, both inversion algorithms (unconstrained and constrained) are completely general and independent of the forward modelling engine, and therefore can be adapted to alternative forward modelling engines. In particular, the constraining inversion algorithm constitutes a fundamental module for the implementation of a full joint inversion scheme for CSEM and seismic data, and for future applications.

Marine CSEM field data suggest the presence of strong anisotropy in the resistivity of rocks. Tompkins (2005) demonstrated that interpreting CSEM data based on the assumption of isotropic conductivity can lead to inaccurate models from the inversion. Hence, future research should aim to extend the current inversion algorithms to include anisotropic conductivity.

In summary, a solver for the 3D CSEM forward modelling problem was developed. Arbitrary resistivity distributions can be represented within the limitations of cartesian grids. State-of-the-art algorithms for inversion and constrained inversion of CSEM data were also developed and implemented. These algorithms are independent of the forward modelling engine and therefore can be implemented with alternative codes. With further improvement of the forward modelling engine, large-scale applications of the presented inversion algorithms will follow. In addition, a structured framework was set for future research on 3D CSEM forward modelling and inversion, integration of these methodologies in practical workflows, and extension to a joint inversion of CSEM and seismic data. The latter is of particular importance for imaging structurally complex domains, such as thrust belts (Colombo & Stefano, 1996), sub-salt (Stefano *et al.*, 2011) and sub-basalt imaging (MacGregor & Sinha, 2000), where conventional seismic data leads to poor imaging, and for improved estimation of reservoir parameters (Gao *et al.*, 2010).

Mathematical Symbols

$\mathbf{E}$	Electric field
$\mathbf{D}$	Electric displacement field
$\mathbf{E}_p$	Primary electric field
$\mathbf{E}_s$	Secondary electric field
$\mathbf{J}$	Current density
$\mathbf{J}_c$	Conduction currents
$\mathbf{K}$	Magnetic source
$\mathbf{B}$	Magnetic induction field
$\mathbf{H}$	Magnetic field
$\mathbf{H}_p$	Primary magnetic field
$\mathbf{H}_s$	Secondary magnetic field
ρ_c	Charge density
σ	Electrical conductivity
ρ	Electrical resistivity
σ_p	Background conductivity
$\Delta\sigma = \sigma - \sigma_p$	Conductivity anomaly
μ	Magnetic permeability
ε	Electric permittivity
ω	Angular frequency
i	Imaginary unit
$\partial\Omega$	Boundary of the computational domain
$\mathbf{n}$	Normal vector to a surface
N_e	Total number of elements
Ω^e	Polyhedral domain of a finite element
Ω	Computational domain
$\mathcal{R}_k$	Weighted residual
$\mathcal{K}^e$	Element stiffness matrix
$\mathcal{N}^e$	Element mass matrix
$\mathbf{N}_i$	Basis function for the i -th edge.

(ξ, η, ζ)	Local coordinate system of an element
(ξ_i, η_i, ζ_i)	Local coordinates of the center for the i -th edge on an element
$\tilde{\mathcal{J}}(\xi, \eta, \zeta)$	Jacobian matrix in the local coordinate system
l_x^e, l_y^e, l_z^e	Lengths of an element in the x, y and z directions respectively
$\mathbf{x}^e = (x^e, y^e, z^e)$	General physical coordinates in the element e
$\mathbf{x}_i = (x_c^e, y_c^e, z_c^e)$	Coordinates of the centre of the element e
$\mathbf{r} = (x, y, z)$	Coordinates in the three-dimensional space
$\mathbf{P}$	Electric dipole moment
$\mathbf{G}(\mathbf{m})$	Forward modelling operator, or mathematical model
$\mathbf{m}$	Vector with the model parameter for each inversion cell
$\mathbf{d}$	Vector of observed data
$\Delta \mathbf{d}$	Vector of data residuals
$f(\mathbf{m})$	parametric functional, objective function, or cost function
λ	Regularization (or trade off) parameter
$\mathcal{D} = \text{diag}\{\frac{1}{s_1}, \frac{1}{s_2}, \dots\}$	Data weighting matrix. Generally, the inverse of data standard deviation, data amplitude, or the identity matrix
N_D	Number of observations
N_m	Number of model parameters
N_{exp}	Number of physical realizations
N_p	Number of model domains
$\mathcal{I}$	Identity matrix
$\mathcal{W}$	Weighting matrix for the model parameters
$\mathcal{H}$	Hessian of a function
$\mathcal{J}$	Jacobian matrix
$\mathbf{p}_k$	Search direction at iteration k
$\mathcal{P}$	Projection operator, maps the field computed in a grid into a receiver position.
$\mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}')$	Dyadic Green's function for the electric field due to a current source $\mathbf{J}$, in $\mathbf{r}'$
$\mathcal{G}^{EK}(\mathbf{r}, \mathbf{r}')$	Dyadic Green's function for the electric field due to a magnetic source $\mathbf{K}$, in $\mathbf{r}'$
$\mathcal{G}^{HJ}(\mathbf{r}, \mathbf{r}')$	Dyadic Green's function for the magnetic field due to a current source $\mathbf{K}$, in $\mathbf{r}'$
$\mathcal{M}[\cdot]$	Maxwell operator
$\ \cdot\ _2$	L_2 norm
$\delta_{i,k}$	Kronecker's delta
$\Re$	Real part of a complex number
W_i	Integration weight
$Sup(f)$	Support of function f

Table A.1: Mathematical Symbols.

Tables

$N_x \times N_y \times N_z$	DOF	N_{mpi}	$\mathbf{T}_f/s$	$\mathbf{T}_b/s$	$\mathbf{M}_{node}/\text{GB}$
$75 \times 75 \times 37$	613200	1	267	6.8	2.2
		4	131	3.6	1.91
		8	69	4	1.05
		12	68	2.9	1.04
		18	69	5.5	0.77
		24	83	6.5	0.54
		32	$\diamond$	$\diamond$	$\diamond$
$95 \times 95 \times 37$	985720	1	533	12	3.35
		4	232	9	2.89
		8	168	5.7	1.95
		12	145	6.15	1.7
		18	126	7.6	1.25
		24	152	6.9	0.82
		32	$\diamond$	$\diamond$	$\diamond$
$135 \times 135 \times 37$	1994760	1	1599	618	7.05
		4	660	31	6.13
		8	436	16	4.33
		12	433	12	3.44
		18	268	8.63	2.58
		24	346	12	1.8
		32	328	8.8	1.43
$153 \times 108 \times 69$	3385935	1	-	-	-
		4	-	-	-
		8	2144	75	11.2
		12	1936	59	8.73
		18	1621	27	6.61
		24	1517	24	4.71
		32	1215	20	3.33
$153 \times 134 \times 69$	4203609	1	-	-	-
		4	-	-	-
		8	4248	228	15
		12	2400	108	12.2
		18	2321	51	8.95
		24	2344	37	6.26
		32	2165	26	4.44

Table B.1: Scalability study for the parallel solution. $N_x \times N_y \times N_z$ grid dimension, DOF: degrees of freedom, N_{mpi} : number of mpi processes, $\mathbf{T}_f$: time for factorization, $\mathbf{T}_b$: time for back-substitution, $\mathbf{M}_{node}$: average allocated memory per node. (-) Not enough memory; ($\diamond$) Test disregarded.

Primary Field

Homogeneous conductivity domain

The solution for the electric field in the frequency domain originated by an electric dipole in a homogeneous medium can be determined from the Schelkunoff's potentials, which satisfy the Helmholtz equation (Ward & Hohmann, 1988):

$$\nabla^2 \mathbf{A} + i\omega\mu\sigma \mathbf{A} = -i\omega\mu\delta(\mathbf{x} - \mathbf{x}_0)\mathbf{P} \quad (\text{C.1})$$

where $\mathbf{x}_0$ is the coordinate of the centre of an infinitesimal dipole, $\mathbf{x}$ is a generic position in the three-dimensional space and $\mathbf{P}$ is the dipole moment. Equation C.1 has fundamental solution:

$$\mathbf{A} = \frac{e^{-ik\|\mathbf{x}-\mathbf{x}_0\|}}{4\pi\|\mathbf{x}-\mathbf{x}_0\|}\mathbf{P} \quad (\text{C.2})$$

where $k^2 = i\omega\mu\sigma$. The relation between the electric field $\mathbf{E}$, field and the vector potential $\mathbf{A}$, is:

$$\mathbf{E} = \mathbf{A} + \frac{\nabla\nabla \cdot \mathbf{A}}{i\omega\mu\sigma} \quad (\text{C.3})$$

Two half-spaces

The general solution for the electric field in the frequency domain, originated by an infinitesimal electric dipole centered at $(0, 0, z_s)$ in a cylindrical coordinate system (r, θ, z) , for the configuration shown in figure C.1, where z_s is the height in relation to some conveniently defined datum, is given by:

$$E_r = E_r^{TM} + E_r^{TE} \quad (\text{C.4})$$

E_r^{TM} and E_r^{TE} are the transverse magnetic and transverse electric components of the radial component of the electric field, respectively, and:

$$E_r^{TM} = \frac{\|\mathbf{P}\| \cos(\theta)}{4\pi\sigma_0} \int_0^\infty \beta_0 \left[kJ_0(kr) - \frac{J_1(kr)}{r} \right] \left(-e^{-\beta_0|z-z_s|} + R_{air}^{TM} e^{\beta_0(z+z_s)} \right) \quad (\text{C.5a})$$

$$E_r^{TE} = \frac{\|\mathbf{P}\| \cos(\theta)}{4\pi\sigma_0} \int_0^\infty \frac{i\omega\mu\sigma_0 J_1(kr)}{r\beta_0} \left(e^{-\beta_0|z-z_s|} + R_{air}^{TE} e^{\beta_0(z+z_s)} \right) \quad (\text{C.5b})$$

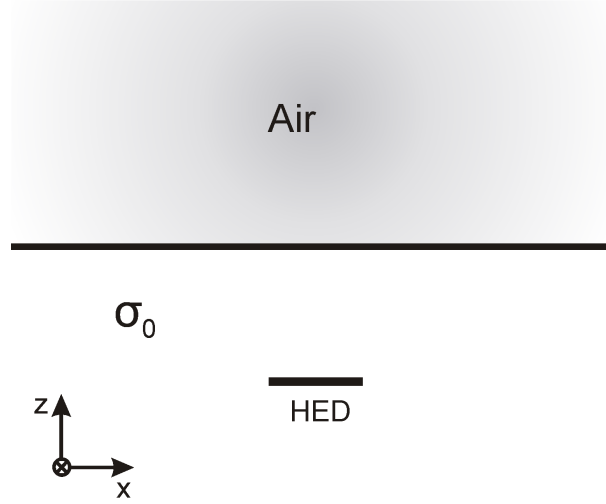


Figure C.1: Configuration with two half-spaces for the calculation of the primary field. The centre of the horizontal electric dipole (HED) is located at $(0, 0, z_s)$.

For the azimuthal component we have:

$$E_\theta = E_\theta^{TM} + E_\theta^{TE} \quad (\text{C.6})$$

where E_θ^{TM} and E_θ^{TE} are the transverse magnetic and transverse electric components of the azimuthal component of the electric field, respectively, and:

$$E_\theta^{TM} = \frac{\|\mathbf{P}\| \sin(\theta)}{4\pi\sigma_0} \int_0^\infty \frac{\beta_0 J_1(kr)}{r} \left(e^{-\beta_0|z-z_s|} - R_{air}^{TM} e^{\beta_0(z+z_s)} \right) \quad (\text{C.7a})$$

$$E_\theta^{TE} = -\frac{\|\mathbf{P}\| \sin(\theta)}{4\pi\sigma_0} \int_0^\infty i\omega\mu\sigma_0 \frac{kJ_0(kr) - J_1(kr)/r}{\beta_0} \left(e^{-\beta_0|z-z_s|} + R_{air}^{TE} e^{\beta_0(z+z_s)} \right) \quad (\text{C.7b})$$

and,

$$E_z = \frac{\|\mathbf{P}\| \cos(\theta)}{4\pi\sigma_0} \int_0^\infty k^2 J_1(kr) \left(\mp e^{-\beta_0|z-z_s|} + R_{air}^{TM} e^{\beta_0(z+z_s)} \right) \quad (\text{C.8})$$

for the vertical component of the electric field. The upper and lower signs correspond to the cases $z_s > z$, and $z_s < z$, respectively. The reflection coefficients, R_{air}^{TM} and R_{air}^{TE} , are

determined from (Andreis & MacGregor, 2008):

$$R_{air}^{TM} = \frac{\beta_0 \sigma_{air} - \sigma_0 \beta_{air}}{\beta_0 \sigma_{air} + \sigma_0 \beta_{air}} e^{-2H_0 \beta_0} \quad (C.9a)$$

$$R_{air}^{TE} = \frac{\beta_0 - \beta_{air}}{\beta_0 + \beta_{air}} e^{-2H_0 \beta_0} \quad (C.9b)$$

where $\beta_0 = \sqrt{k^2 - i\omega\mu\sigma_0}$ and H_0 is the distance between the interface that separates the two half-spaces, and the origin of the z-axis. These particular solutions, were obtained by simplifying the expressions for the general case of a horizontal electric dipole in a horizontally layered resistivity model in the frequency domain, and can be found in the work of Chave & Cox (1982), and Andreis & MacGregor (2008).

Equations C.5, C.7 and C.8 are only valid in the lower half-space. In practice, when applying this background model for the calculation of the primary field, the upper-half space overlaps the representation of the air-layer in the finite element mesh, and the lower half-space overlaps the representation in the model, of the sea-water resistivity and of the geo-electrical structures in the crust. When $\sigma_{air} = 0$ S/m, the reflection coefficients simplify to $R_{air}^{TM} = -e^{-2H_0 \beta_0}$ and $R_{air}^{TE} = \frac{\beta_0 - k}{\beta_0 + k} e^{-2H_0 \beta_0}$.

Green's functions and reciprocity in electromagnetics

D.0.1 Introduction to Green's functions

Given a differential operator $\mathcal{L}_{\mathbf{r}}$ and $\mathbf{r} = (x, y, z)$, let's consider the following equation:

$$\mathcal{L}_{\mathbf{r}}u(\mathbf{r}) = f(\mathbf{r}) \quad (\text{D.1})$$

The Green's function $G(\mathbf{r}, \mathbf{r}')$ for D.1 satisfies (Morse & Feshbach, 1953):

$$\mathcal{L}_{\mathbf{r}}G(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \quad (\text{D.2})$$

Where $\delta(\mathbf{r} - \mathbf{r}')$ is the Dirac delta function with origin at $\mathbf{r}' = (x', y', z')$. The Dirac delta function satisfies:

$$\int_{\mathbb{R}^3} \delta(\mathbf{r} - \mathbf{r}')f(\mathbf{r}') d\mathbf{r}' = f(\mathbf{r}) \quad (\text{D.3})$$

From the definition of the Green's function D.2, the Dirac delta function D.3 and D.1:

$$\begin{aligned} \mathcal{L}_{\mathbf{r}}u(\mathbf{r}) = f(\mathbf{r}) &= \int_{\mathbb{R}^3} \delta(\mathbf{r} - \mathbf{r}')f(\mathbf{r}') d\mathbf{r}' = \\ \int_{\mathbb{R}^3} \mathcal{L}_{\mathbf{r}}G(\mathbf{r}, \mathbf{r}')f(\mathbf{r}') d\mathbf{r}' &= \mathcal{L}_{\mathbf{r}} \int_{\mathbb{R}^3} G(\mathbf{r}, \mathbf{r}')f(\mathbf{r}') d\mathbf{r}' \end{aligned} \quad (\text{D.4})$$

Therefore, the solution of D.1 is:

$$u(\mathbf{r}) = \int_{\mathbb{R}^3} G(\mathbf{r}, \mathbf{r}')f(\mathbf{r}') d\mathbf{r}' \quad (\text{D.5})$$

This identity is general for any linear differential operator, being important for the derivation of some important electromagnetic properties, such as the reciprocity relations.

D.0.2 Dyadic Green's functions

In the case of electromagnetic problems, the definition for Green's function has to take into account oriented sources and three components for the electric or the magnetic field.

Thus the Green's function for the electric/magnetic fields have components and are referred to as dyadic Green's functions.

Dyadic Green's functions satisfy the following identity:

$$\nabla \times \nabla \times \mathcal{G}(\mathbf{r}, \mathbf{r}') - i\omega\mu\sigma\mathcal{G}(\mathbf{r}, \mathbf{r}') = i\omega\mu\mathcal{I}\delta(\mathbf{r} - \mathbf{r}') \quad (\text{D.6})$$

Where $\mathcal{I}$ represents the identity and $\sigma = \sigma(\mathbf{r})$. If we now consider the partial differential equation for the electric field :

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) - i\omega\mu\sigma\mathbf{E}(\mathbf{r}) = i\omega\mu\mathbf{J}(\mathbf{r}) \quad (\text{D.7})$$

and identity D.5, the solution for the electric generated by a current density $\mathbf{J}$ at $\mathbf{r}_R$ is (Bladel, 2007):

$$\mathbf{E}(\mathbf{r}) = \int_{\mathcal{V}} \mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}(\mathbf{r}') d\mathbf{r}' \quad (\text{D.8})$$

and $\mathcal{V}$ is the support of the current density, and the superscript EJ is used to designate that it is the dyadic Green's function for the electric field due to a current density source. From the Faraday's law the following identity must hold:

$$\nabla \times \mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}') = i\omega\mu\mathcal{G}^{HJ}(\mathbf{r}, \mathbf{r}') \quad (\text{D.9})$$

Where $\mathcal{G}^{HJ}(\mathbf{r}, \mathbf{r}')$ is the dyadic Green's for the magnetic field due to a current density source. Similar identities can be obtained for dyadic Green's functions for the electric and magnetic fields due to a magnetic source.

To better understand the meaning of the dyadic Green's functions lets rewrite equation D.8 in terms of components utilizing Einstein's sum convention:

$$E_i(\mathbf{r}) = \int_{\mathcal{V}} \mathcal{G}_{ij}^{EJ}(\mathbf{r}, \mathbf{r}') J_j(\mathbf{r}') d\mathbf{r}' \quad (\text{D.10})$$

Thus, $\mathcal{G}_{ij}^{EJ}$ represents the contribution of a source oriented in the j -th direction at $\mathbf{r}'$, to the i -th component of the electric field at $\mathbf{r}$. Similar interpretations can be made for dyadic Green's functions for the magnetic field and when magnetic sources, such as a magnetic dipole, are considered.

D.0.3 Reciprocity in electromagnetics

The reciprocity relations establish the relation between the sources and the electromagnetic field when the position of the sources and the position in space where the electromagnetic field is measured, or calculated, are interchanged, in a medium whose physical properties are time-invariant, and under some constraints (*e.g.* symmetry of the magnetic permeability ten-

sor in anisotropic media, absence of current sources at the boundary). Complete derivations of the reciprocity principle in electromagnetic can be found in the literature (Jackson, 1998; Chew, 1999), thus only the final result is reviewed in this thesis.

Lets define the inner product:

$$\langle \mathbf{u}, \mathbf{v} \rangle = \int_{\Omega} \mathbf{u}(\mathbf{r}) \cdot \mathbf{v}(\mathbf{r}) d\mathbf{r} \quad (\text{D.11})$$

Lets consider the electromagnetic field pair $[\mathbf{E}_1, \mathbf{H}_1]$ originated by sources $[\mathbf{J}_1, \mathbf{K}_1]$, and the electromagnetic field pair $[\mathbf{E}_2, \mathbf{H}_2]$ related with sources $[\mathbf{J}_2, \mathbf{K}_2]$. The following relation between the electromagnetic and the source pairs holds (Chew, 1999):

$$\langle \mathbf{E}_2, \mathbf{J}_1 \rangle - \langle \mathbf{H}_2, \mathbf{K}_1 \rangle = \langle \mathbf{E}_1, \mathbf{J}_2 \rangle - \langle \mathbf{H}_1, \mathbf{K}_2 \rangle \quad (\text{D.12})$$

Equation D.12 is known as the reciprocity theorem in electromagnetism, and it will be used in this text to derive suitable expressions for the sensitivities calculation.

D.0.4 Reciprocity and dyadic Green's functions

In this section is reviewed the extension of the reciprocity principle to electric and magnetic dyadic Green's functions using the reciprocity theorem D.12.

Lets consider two electric dipoles generating current densities $\mathbf{J}_1$ and $\mathbf{J}_2$, and located at $\mathbf{r}_{R_1}$ and $\mathbf{r}_{R_2}$, respectively, and lets consider that there are no magnetic sources present. Hence the following relation holds:

$$\langle \mathbf{E}_2, \mathbf{J}_1 \rangle = \langle \mathbf{E}_1, \mathbf{J}_2 \rangle \quad (\text{D.13})$$

Thus the response of the respective electric fields are:

$$\mathbf{E}_1(\mathbf{r}) = \int_{\mathcal{V}} \mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_1(\mathbf{r}') d\mathbf{r}' \quad (\text{D.14a})$$

$$\mathbf{E}_2(\mathbf{r}) = \int_{\mathcal{V}} \mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_2(\mathbf{r}') d\mathbf{r}' \quad (\text{D.14b})$$

From the inner product definition D.11 and from D.13:

$$\int_{\mathcal{V}} \mathbf{E}_2(\mathbf{r}) \cdot \mathbf{J}_1(\mathbf{r}) d\mathbf{r} = \int_{\mathcal{V}} \mathbf{E}_1(\mathbf{r}) \cdot \mathbf{J}_2(\mathbf{r}) d\mathbf{r} \quad (\text{D.15})$$

The support of the current densities $\mathbf{J}_1$ and $\mathbf{J}_2$ is assumed to be the same, as we want to study the relations between the fields and the sources by exchanging the sources positions in the space. As a consequence of the definition of support, the current densities are zero outside the support, hence the domain of integration for the inner product is assumed to be the support of the current densities $\mathcal{V}$.

Substituting equations D.14a and D.14b into D.15 yields:

$$\begin{aligned} \int_{\mathcal{V}} \int_{\mathcal{V}} [\mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_2(\mathbf{r}')] \cdot \mathbf{J}_1(\mathbf{r}) \, d\mathbf{r}' d\mathbf{r} &= \int_{\mathcal{V}} \int_{\mathcal{V}} [\mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_1(\mathbf{r}')] \cdot \mathbf{J}_2(\mathbf{r}) \, d\mathbf{r}' d\mathbf{r} \iff \\ \int_{\mathcal{V}} \int_{\mathcal{V}} [(\mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}'))^T \cdot \mathbf{J}_1(\mathbf{r})] \cdot \mathbf{J}_2(\mathbf{r}') \, d\mathbf{r}' d\mathbf{r} &= \int_{\mathcal{V}} \int_{\mathcal{V}} [\mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_1(\mathbf{r}')] \cdot \mathbf{J}_2(\mathbf{r}) \, d\mathbf{r}' d\mathbf{r} \end{aligned} \quad (\text{D.16})$$

As both integrals are evaluated in the same domains the integration variables can be exchanged in the arguments of the functions (Altman & Suchy, 1991), hence:

$$\int_{\mathcal{V}} \int_{\mathcal{V}} [(\mathcal{G}^{EJ}(\mathbf{r}', \mathbf{r}))^T \cdot \mathbf{J}_1(\mathbf{r}')] \cdot \mathbf{J}_2(\mathbf{r}) \, d\mathbf{r}' d\mathbf{r} = \int_{\mathcal{V}} \int_{\mathcal{V}} [\mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_1(\mathbf{r}')] \cdot \mathbf{J}_2(\mathbf{r}) \, d\mathbf{r}' d\mathbf{r} \quad (\text{D.17})$$

Reorganizing the terms in D.17 yields:

$$\int_{\mathcal{V}} \int_{\mathcal{V}} \mathbf{J}_2(\mathbf{r}) \cdot [(\mathcal{G}^{EJ}(\mathbf{r}', \mathbf{r}))^T - \mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}')] \cdot \mathbf{J}_1(\mathbf{r}') \, d\mathbf{r}' d\mathbf{r} = 0 \quad (\text{D.18})$$

Thus the following reciprocity relation holds for the dyadic Green's function for the electric field:

$$[\mathcal{G}^{EJ}(\mathbf{r}', \mathbf{r})]^T = \mathcal{G}^{EJ}(\mathbf{r}, \mathbf{r}') \quad (\text{D.19})$$

Lets now consider an electric dipole source $\mathbf{J}_1$ at $\mathbf{r}_{R_1}$, and a magnetic dipole source $\mathbf{K}_2$ at $\mathbf{r}_{R_2}$. Thus from D.12 the following identity holds:

$$\langle \mathbf{E}_2, \mathbf{J}_1 \rangle = -\langle \mathbf{H}_1, \mathbf{K}_2 \rangle \quad (\text{D.20})$$

The responses for the electric and magnetic fields are:

$$\mathbf{H}_1(\mathbf{r}) = \int_{\mathcal{V}} \mathcal{G}^{HJ}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_1(\mathbf{r}') \, d\mathbf{r}' \quad (\text{D.21a})$$

$$\mathbf{E}_2(\mathbf{r}) = \int_{\mathcal{V}} \mathcal{G}^{EK}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{K}_2(\mathbf{r}') \, d\mathbf{r}' \quad (\text{D.21b})$$

From D.11 and D.20:

$$\int_{\mathcal{V}} \mathbf{E}_2(\mathbf{r}) \cdot \mathbf{J}_1(\mathbf{r}) \, d\mathbf{r} = - \int_{\mathcal{V}} \mathbf{H}_1(\mathbf{r}) \cdot \mathbf{K}_2(\mathbf{r}) \, d\mathbf{r} \quad (\text{D.22})$$

As in the previous case the support for the electric dipole source and the magnetic dipole source are assumed to be the same, as the reciprocity relation D.20 establishes the relation between the fields and the sources by exchanging the position of the sources in the same

physical space. Substituting the field responses D.21 in D.22 yields:

$$\begin{aligned} \int_{\mathcal{V}} \int_{\mathcal{V}} [\mathcal{G}^{EK}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{K}_2(\mathbf{r}')] \cdot \mathbf{J}_1(\mathbf{r}) \, d\mathbf{r}' d\mathbf{r} &= - \int_{\mathcal{V}} \int_{\mathcal{V}} [\mathcal{G}^{HJ}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_1(\mathbf{r}')] \cdot \mathbf{K}_2(\mathbf{r}) \, d\mathbf{r}' d\mathbf{r} \iff \\ \int_{\mathcal{V}} \int_{\mathcal{V}} [(\mathcal{G}^{EK}(\mathbf{r}, \mathbf{r}'))^T \cdot \mathbf{J}_1(\mathbf{r})] \cdot \mathbf{K}_2(\mathbf{r}') \, d\mathbf{r}' d\mathbf{r} &= - \int_{\mathcal{V}} \int_{\mathcal{V}} [\mathcal{G}^{HJ}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_1(\mathbf{r}')] \cdot \mathbf{K}_2(\mathbf{r}) \, d\mathbf{r}' d\mathbf{r} \end{aligned} \quad (\text{D.23})$$

Exchanging the mute integration variable in the left term of the equation yields:

$$\int_{\mathcal{V}} \int_{\mathcal{V}} [\mathcal{G}^{EK}(\mathbf{r}', \mathbf{r}) \cdot \mathbf{J}_1(\mathbf{r}')] \cdot \mathbf{K}_2(\mathbf{r}) \, d\mathbf{r}' d\mathbf{r} = - \int_{\mathcal{V}} \int_{\mathcal{V}} [\mathcal{G}^{HJ}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_1(\mathbf{r}')] \cdot \mathbf{K}_2(\mathbf{r}) \, d\mathbf{r}' d\mathbf{r} \quad (\text{D.24})$$

Reorganizing the terms of D.24:

$$\int_{\mathcal{V}} \int_{\mathcal{V}} \mathbf{K}_2(\mathbf{r}) \cdot [(\mathcal{G}^{EK}(\mathbf{r}', \mathbf{r}))^T + \mathcal{G}^{HJ}(\mathbf{r}, \mathbf{r}')] \cdot \mathbf{J}_1(\mathbf{r}') \, d\mathbf{r}' d\mathbf{r} = 0 \quad (\text{D.25})$$

Hence the following conditions between the dyadic Green's functions $\mathcal{G}^{EK}(\mathbf{r}, \mathbf{r}')$ and $\mathcal{G}^{HJ}(\mathbf{r}, \mathbf{r}')$ hold:

$$[\mathcal{G}^{EK}(\mathbf{r}', \mathbf{r})]^T = -\mathcal{G}^{HJ}(\mathbf{r}, \mathbf{r}') \quad (\text{D.26})$$

Following the same procedure it is possible to derive reciprocity identities using other combinations of sources, for the respective dyadic Green's functions. Nonetheless, the identities derived here are the ones necessary to derive expressions for the gradient of the functional to be minimized in the inversion scheme, thus those relations are not derived here.

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