Three-dimensional inversion of transient electromagnetic data using the octree-based finite element method

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PhD thesis
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To my parents and supervisors.
Preface

This thesis is written to fulfill the requirements of the three-year PhD program at the Graduate School of Science and Technology, Aarhus University (Denmark). The work was carried out at the HydroGeophysics Group (HGG), Department of Geoscience, Aarhus University.

The thesis is based on three appended publications. The thesis includes an introductory section that describes the research background and the aim of this project (Chapter 1), an overall description of the methodologies (3D TEM modeling, octree-based finite element method, multi-mesh approach, inversion methods) applied in the papers (Chapter 2), an extended summary of research results affiliated to each paper (Chapter 3-5), and conclusions and an outlook (Chapter 6).

Papers

Xiao, L., G. Fiandaca, B. Zhang, E. Auken, and A.V. Christiansen. 2021, Fast 2.5D and 3D inversion of transient electromagnetic methods using the octree-based finite element methods. (Submitted to Geophysics, under review)


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Summary

The transient electromagnetic method (TEM), an effective and non-invasive geophysical method, has been widely used for mapping the resistivity distribution in the subsurface. With the instrumental advancements that have taken place, TEM data is acquired with increasing quality and quantity. The method is therefore expected to have wider applications, such as serving as a monitoring tool. Besides, an integrated TEM survey combining different systems becomes possible for wider applications. To better interpret the data, a fast and versatile 3D inversion scheme is needed, despite of the challenges on the large complexity in terms of computation and practical set-up in various applications. The thesis aims to give a general solution to these applications, as presented in three appended papers.

Paper I presents two efficient implementations of three-dimensional (3D) and two-and-a-half-dimensional (2.5D) modeling and inversion, which can apply to large-scale TEM explorations. The key novel features are: (1) forward response and Jacobian calculations were implemented using the octree-based finite element method, (2) a mirror approach was used to build a 2.5D inversion scheme for further efficiency, and (3) a flexible link between the forward mesh and inversion model was applied on both 3D and 2.5D schemes based on the voxel formulation. I compared the performance of the new implementations with 3D modeling using tetrahedral meshes, with respect to speed and memory requirements. The 3D octree algorithm requires less than 1/3 of running time than a 3D tetrahedral scheme for equivalent accuracy. The 2.5D octree algorithm further speeded up the process by another factor of two. The inversion used the Levenberg-Marquart approach minimizing the least-squares criterion of the objective function. The devised inversion was successfully applied to a field dataset containing 200 soundings. I performed a 3D inversion on the full survey and a 2.5D inversion on a profile comprising 24-sounding. The 2.5D inversion result showed similar resistivity features as the 3D inversion result at the selected profile. Hence, I concluded that the presented implementations can handle fairly large TEM surveys, where 2D and 3D effects are pronounced, on modern computational platforms.

Paper II presents an inversion scheme for 3D TEM time-lapse data using a generalized minimum support norm with an application to monitor conductivity changes over time. In particular, two challenges for time-lapse TEM applications were addressed: i) the survey repetition with slightly different acquisition layouts; ii) non-optimal data coverage above the time-lapse anomalies. To address these issues, I developed a new TEM time-lapse inversion scheme based on Paper I with the
following features: (1) the multi-mesh approach allows for seamless integration of datasets with different acquisition layouts; (2) 3D sensitivity calculation allows retrieving conductivity changes in-between TEM soundings; (3) simultaneous inversion of two datasets at once, imposing time-lapse constraints defined in terms of a generalized minimum support norm, which ensures sharp time-lapse changes. I assessed the relevance of our implementations through a synthetic example and a field example. In the synthetic model, I studied the capability of the inversion scheme to retrieve compact time-lapse changes and the effect of data density, i.e. spacing of transects in surveys. The synthetic tests were used to interpret time-lapse datasets collected at an Icelandic geothermal site within a monitoring project of H₂S sequestration. Furthermore, I studied the trade-off between data misfit and time-lapse constraints through the tuning settings of the generalized minimum support norm. Based on the results from both the synthetic and real cases, I showed that our implementation of 3D time-lapse inversion has a robust performance for TEM monitoring.

**Paper III** applies the 3D inversion scheme developed from Paper I to an integrated coastal survey using ground-based and waterborne TEM systems, where strong conductivity contrast presents. The method has substantially advanced the data interpretation with the following features: (1) 3D octree-based forward modeling describes the multi-dimensional environment and simulates the field diffusions more accurately. (2) The decoupling of forward and inversion mesh offers the flexibility to model each sounding independently with minimum computation cost regardless of their configuration difference. Still, it keeps the continuity of the earth model in the survey area during inversions. Additionally, I have illustrated that a special refinement is required for meshing models with highly conductive top layers to ensure certain accuracy. In the synthetic coastal model, I first studied the difference of the one-dimensional (1D) and 3D modeling response of the example. Then, the 3D inversion was shown to outperform 1D inversion with a generally lower misfit and a superior model retrieval. Finally, the application on the field case further demonstrated that 3D inversion interprets the data with more consistency, which is verified by the existing borehole data.

The thesis presented a 3D inversion scheme, a 2.5D inversion scheme, and a 3D time-lapse inversion scheme, which have been successfully applied to a hydrogeological field case, a time-lapse dataset collected in a geothermal site, an integrated TEM survey in a coastal area, respectively. I, therefore, concluded that the developed inversion schemes should be considered as a routinely practice in the survey to produce a more reliable earth model from the data.
Résumé

Den transiente elektromagnetiske metode (TEM), er en effektiv og non-invasiv geofysisk metode, der i vid udmåling bliver brugt til at kortlægge resistivitetsfordelingen i undergrunden. På TEM-instrumentsiden sker der løbende udvikling, der øger både datakvalitet og kvantitet. I nærfremtids forventes derfor at TEM metoden også ville kunne bruges til monitoring vha. 'time laps målinger’, samt at man med en integreret TEM kortlægning med en kombination af forskellige TEM systemer, vil kunne opnå en bred anvendelse. For at opnå en bedre og mere præcis inversion, af de indsamlede TEM data, til resistivitets modellen, er der brug for en effektiv og robust 3D TEM inversions kode. For en 3D TEM inversions kode findes der en mængde udfordringer i relation til model opsætning og beregningskompleksiteten til de forskellige TEM applikationer. I denne afhandling er formålet at finde en generel løsning på disse udfordringer, hvilket adresseres t i de tre artikler inkluderet i ph.d.-afhandlingen.

Artikel I præsenterer to effektive implementeringer af 3D og 2.5D TEM modellering og inversion, som kan anvendes ved stor skala TEM kortlægninger. De væsentligste nye implementeringer er: (1) beregning af forward responser og modelafledte til Jacobian matricen ved brug af et octree-baserede finitte-element grid; (2) Opbygning af en 2.5D inversionsmetode for øget effektivitet ved hjælp af en spejling betragtning, og (3) et fleksibelt link mellem 'forward' griddet og inversionsmodellen, både i 3D- og 2.5D tilfællet, ved hjælp af en voxel-formulering. Vi sammenligner inversionsresultater med vores nye implementeringer med 3D-modelleringskode der anvender et tetrahedriske grid, med hensyn til beregnings hastighed og hukommelsesforbrug. Sammenligningen af vores 3D octree-algoritmen viser en reduktion på beregningstid på minimum 1/3 i forhold til et 3D-tetrahedrisk formulering for en tilsvarende nøjagtighed. 2.5D octree-algoritmen reducerer beregningstiden yderligere en faktor to. Vores inversionen algoritme anvender en Levenberg-Marquart tilgangen, men en 'least squares’ minimering af objektive funktionen. Vi har men med succes anvendt vores 2.5 og 3D inversions algoritme på et TEM kortlægning med 200 sonderinger. 3D-inversionen omfatter hele TEM datasæt mens 2,5D-inversionen blev udført på en enkelt sektion med 24 sonderinger. Langs 2.5D sektionen giver 3D og 2.5D-inversionenerne sammenlignelige resultater. Konklusionen er, at de præsenterede implementeringer er i stand til at håndtere relative store TEM kortlægninger med udtalte 2D- og 3D-effekter i undergrunden på en hurtig og effektiv måde.
**Artikel II** præsenterer en inversionskode for 3D TEM time-lapse data, der anvender en ’generalized minimum support’ norm, og med applikation muligheder for monitoring af konduktivitetsændringer over tid. Der er fokus på to udfordringer for time-lapse TEM-inversion: i) gentagende TEM-kortlægningerne med små geografiske ændringer i målepositionerne; ii) dårlig datadækning over selve time-lapse-anomalien. For at adressere disse forhold videreudviklede vi inversionskoden fra artikel I til en TEM time-lapse-inversionskode med de følgende funktioner: (1) ’multi-mesh’ tilgangen, hvilket giver problemfri integration af time-laps datasæt med ændringer i målepositionerne; (2) beregning af 3D sensitiviteten, hvilket gør det muligt at opfange ændringer i mellem TEM- målepositionerne; (3) Samlet inversion af to datasæt, hvilket muliggør at man kan anvende ’generalized minimum support’ bånd i modelrummet, som gør at man kan opnår relative skarpe modelændringer. Vi evaluerer vores implementeringer via et syntetisk eksempel og et feltexempl. I det syntetisk eksempel studerer vi inversionskodens evne til at håndtere time-lapse-ændringer, samt effekten af datadækningen. Erfaringerne med opsætning af inversionen for det syntetisk eksempel anvendes for time-lapse inversion af et feltdatasæt. Feltdatasættet stammer fra et geotermisk moniteringsprojekt på Islandsk. Endvidere undersøges afvejningen mellem datatilpasning og time-lapse bånd. Baseret på resultaterne fra det syntetiske eksempel og feltexempl påviser vi, at vores 3D time-lapse inversion er robust og kan anvendes til inversion af TEM-moniteringsdata.

**Artikel III** anvender 3D inversionsmetoden udviklet i Artikel 1 på en kystnær TEM kortlægning, som indeholder både on-shore og off-shore TEM data og derved med store konduktivitetskontraster primært pga. tilstedeværelse af saltvand. I forhold til 1D-inversion resulteret 3D-inversion i forbedrede resultaterne da: (1) 3D octree-baseret forward modellering, kan beskrive det multidimensionelle miljø og simulerer de diffusionen EM-felten mere nøjagtigt; (2) afkoblingen af forward and inversion griddene giver fleksibilitet til at modellere de enkelte sonderinger uafhængig og hurtigt, og samtidig bevarer kontinuiteten i model griddet. Vi viser, at det kræver et ekstra fin model grid i tilfældet men et relativt konduktiv toplag for at opnå en tilfredsstillende beregning præcision. For et syntetisk kystnært eksempel, studerede vi først forskellen mellem 1D og 3D-inversionsresuldataer. Her resulterede 3D inversionen i en bedre gengivelse af den sande model ift. 1D-inversion. Feltdata eksemplet vise at 3D inversion, specialit i overgangszone fra kyst til vand, resultater i et mere realistiske og troværdige resultater ift. En 1D-tolkning, hvilket er verificeret af borehulsdata.

Afhandlingen præsenterer en 3D inversionsmetode og en 2,5D inversionsmetode, der med succes er blevet anvendt på et TEM-feltexempl i en et hydrologisk sammenhæng, et time-lapse
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datasæt for TEM-monitorering i et geotermisk område på Island, samt i en integreret TEM kortlægning i et kystnært område. Vi konkluderer derfor, at man bør overvej at anvende de udviklede TEM-inversion koder rutinemessing til inversion af TEM-data for at opnå en bedre beskrivelse af undergrunden ud fra de indsamlede TEM-data.
1. Introduction

Environmental challenges such as climate change and anthropogenic contamination caused by human activities have shown knock-on effects on the ecosystems on this planet and will continue to do so. Assessment tools for mapping the subsurface resistivity distribution and monitoring variations are needed to deliver valuable policy-making and environment management services. Although transient electromagnetic method (TEM) was initially developed to effectively characterize the distribution of mineral deposits within an economical budget before mining production, the non-intrusive and cost-effective geophysical exploration method, has been continuously developed to solve environmental problems for more than two decades. The method provides imperative information for drilling and largely improves the odds of success. The technique also offers valuable knowledge for multi-disciplinary interpretation to achieve earth models with reduced ambiguity. Compared to other resistivity geophysical methods, such as electrical resistivity tomography (ERT), the method is much more productive and can achieve similar depths of investigation.

In response to a need from various applications, TEM instrumentation has been evolving to offer high-quality data, robust performance and rapid acquisition. This has included different platforms (airborne, ground-based and waterborne systems) that have been developed to cater to different needs according to the geological setting. Innovative dual-moment technology (Sørensen and Auken, 2004), with fast turn-off and small current in the low moment for near surface resolution, and long turn-off and strong current in the high moment for deep detection allows for high near surface resolution concurrently with large depths of investigation (DOI) (Christiansen and Auken, 2012). Simultaneously, increased suppression of very low and high-frequency noise sources enhances the signal-to-noise ratio and delivers more informational data for exploration (Larsen et al., 2021, Wu et al., 2019, Gisselø et al., 2020). In addition, real-time review and remote operation provide the flexibility to reconfigure the system parameters during the survey and minimize the survey expense. Furthermore, fast-moving measurement technology (Eadie et al., 2018, Auken et al., 2019) further brings cost-efficiency benefits and drives us into a geophysical big-data age.

The increase of data quality and quantity allows us to explore the near-surface with better resolution than ever. One-dimensional (1D) inversion algorithms (Auken and Christiansen, 2004, Viezzoli et al., 2009, Brodie and Fisher, 2008) are still the common practice after TEM data collection and routine processing. However, although this is sufficient to give a quick overview, the approach is less satisfactory when three-dimensional (3D) anomalies exist within data coverage. With advanced
modern computation architectures, 3D TEM modeling is no longer a computational luxury as in the last century, and multi-dimensional interpretation is more likely to become routine in the near future. So far, 3D TEM modeling has been realized using different numerical methods: integral equation (IE), finite difference (FD), finite volume (FV) and finite element (FE) (Cox et al., 2012, Commer et al., 2015, Haber and Schwarzbach, 2014, Um et al., 2010). Among these methods, FV and FE have more flexibility at model meshing, such as structured meshes, unstructured meshes, or non-uniform structured meshes (Jahandari and Farquharson, 2014, Zhang et al., 2021). Non-uniform meshes only locally refine the domains of interest, such as places representing geological features and with fast field variations, which largely decrease the unknown parameters and thus accelerate the calculation. This is vital, since the modeling is conducted twice for each inversion iteration, one forward and one adjoint problem. On top of this, the direct solvers (Schenk and Gärtner, 2004, Amestoy et al., 2006) recycle factorization information during the time-stepping which speeds up the modeling development process. In addition, the constant improvement of solvers further optimizes the solving of linear system equations.

3D TEM inversion is computationally demanding. More than thousands of soundings are collected for a moderate-size survey, which means a massive Jacobian matrix is to be solved due to the number of datasets and cells needed to cover the survey area. Many solutions have been proposed to mitigate the challenge over the years. The footprint concept (Cox et al., 2010) was introduced to show that only the elements close to the system with strong impacts are considered for Jacobian calculation, which significantly downsizes the matrix. Domain decomposition strategies (Yang et al., 2013) alleviate the problem by decoupling the modeling mesh and inversion mesh: a local modeling mesh for each sounding and one inversion mesh for the entire area. The triple mesh approach (Zhang et al., 2021) suggests that a coarser tetrahedral mesh can be used for Jacobian calculation than forward modeling. Despite all the efforts, fulfilling a full-scale or large-scale 3D TEM inversion remains a challenging problem and needs further investigation.

TEM surveys provide an opportunity to serve as a monitoring tool of temporal resistivity variations, which has a big market in agricultural production, seawater intrusion, gas sequestration, etc. To the best of my knowledge, most time-lapse inversion algorithms reported in the literature are devised for the application of ERT, magnetotelluric (MT), and controlled-source electromagnetic (CSEM) methods (Bretaudeau et al., 2021, Carbajal et al., 2012, Fiandaca et al., 2015), and not for TEM data. However, to conduct a time-lapse inversion of TEM data, some special features need attention: i) a moving measurement has difficulty in repeating the soundings at the same locations, or
with same system configurations if the time period is too long; ii) TEM surveys at a different time have different data density due to varying field conditions, processing parameters, or human errors; iii) to obtain a more focused image of the changes, an emphasis on model variation is required, compared to a standard L2-norm inversion.

Multiple systems or different configurations can be utilized if nontrivial geologic variation appears. For example, when the survey covers both onshore and offshore areas (Bücker et al., 2021, Christiansen et al., 2021), airborne or a combination of physically different systems is required to collect data in both areas. Besides, in some projects, measurement in the region where the anomaly is located requires different configurations to achieve the same DOI as other areas, even though the same instruments are used. For instance, in mineral exploration, when the ore bodies lie below a conductive layer, the transmitter’s magnetic moment should be increased substantially to penetrate the top layer and reach the deep target. Another challenge for such cases is that conventional 1D inversions are incapable of fitting data and delivering an agreeable model when 3D effects present, especially when strong conductivity contrasts occur. Therefore, a proper 3D inversion is needed to solve the problems in practice, where multiple technologies are combined in areas consisting of different geological settings and 3D effects manifest.

1.1 Aim of the project

The project proposes a general solution for classic 3D inversion, 3D time-lapse inversion, and 3D multi-system inversion. This work is built on an existing voxel Gauss-Newton (GN) inversion scheme. In terms of code implementations, I have implemented the algorithms of hexahedral modeling, the hexahedral and octree Jacobian calculation, and the integration with the software AarhusInv (https://hgg.au.dk/software/aarhusinv/), as well as contributed to develop octree modeling.

Specifically, the modeling in classic 3D inversion is developed using the octree-based finite element method, which effectively reduces the number of unknowns by local refinement in the domain of interest. The multi-mesh approach, with locally refined octree meshes for modeling at each sounding and a regular mesh for the inversion model update, provides a link between forward and inversion. In addition, to further accelerate the inversion, a mirror approach is proposed to realize the 2.5D inversion, based on the classic 3D inversion and an approximation. In the time-lapse inversion, I proposed a minimum support norm to obtain a focused temporal variation image established on the developed classic 3D inversion. Furthermore, I demonstrated the versatility of the devised schemes in applying a multi-system measurement at a coastal area, where strong 3D effects exist.
Although the work presented is applied only to ground-based and waterborne TEM examples, the implementation can readily be used for a wider range of applications such as measurement with airborne and marine platforms.

The rest of the thesis is structured as follows: firstly, I introduce the methodology including TEM modeling, the mirror approach, the multi-mesh approach, classic inversion and time-lapse inversion. Then, I will show the results of three subtopics: i) Fast 2.5D and 3D inversion of transient electromagnetic surveys using the octree-based finite element method; ii) Three-dimensional time-lapse inversion of transient electromagnetic data, with an application at an Icelandic geothermal site; iii) 3D inversion of an integrated ground-based and waterborne TEM survey. Finally, I conclude the thesis and discuss the outlook of TEM numerical computing. In the Appendix, I attached the hexahedral finite element method formulations, and three papers that I submitted to journals.
2. Methodology

2.1 3D TEM Modeling

I derive the time-domain forward problem from Maxwell’s equations:

$$\nabla \times \mathbf{e}(\mathbf{r}, t) = -\mu \frac{\partial \mathbf{h}(\mathbf{r}, t)}{\partial t}$$

(2.1)

and

$$\nabla \times \mathbf{h}(\mathbf{r}, t) - \frac{\partial \mathbf{D}(\mathbf{r}, t)}{\partial t} = \mathbf{j}(\mathbf{r}, t) + \mathbf{j}_s(t).$$

(2.2)

where the electric field $\mathbf{e}(\mathbf{r}, t)$, magnetic field intensity $\mathbf{h}(\mathbf{r}, t)$, the dielectric displacement $\mathbf{D}(\mathbf{r}, t)$ and the current density $\mathbf{j}(\mathbf{r}, t)$ are functions of space, $\mathbf{r}(\mathbf{r} \in \Omega)$, and time, $t \in (0, T)$; $\mu$ is the magnetic permeability of free space and $\mathbf{j}_s$ denotes the current source.

With the quasi-static approximation (displacement currents $\frac{\partial \mathbf{D}}{\partial t} = 0$), the use of Ohm’s law for current density ($\mathbf{j} = \sigma \mathbf{E}$, where $\sigma$ represents the electric conductivity), and the assumption that the medium is isotropic and non-magnetizable and that electrical properties are independent on time (so induced polarization is neglected), the electrical field $\mathbf{e}(\mathbf{r}, t)$ obeys a diffusion equation:

$$\nabla \times \nabla \times \mathbf{e}(\mathbf{r}, t) + \mu \sigma(\mathbf{r}) \frac{\partial \mathbf{e}(\mathbf{r}, t)}{\partial t} = -\frac{\partial \mathbf{j}_s(t)}{\partial t}$$

(2.3)

For this boundary-value problem, the initial conditions are given as:

$$\mathbf{e}(\mathbf{r}, 0) = \mathbf{e}_0(\mathbf{r})$$

(2.4)

When the modeling domain is big enough and boundary effects are negligible, I can apply the homogeneous Dirichlet boundary condition:

$$\mathbf{e}(\mathbf{r}_{\Omega}, t) = 0$$

(2.5)

Using the Galerkin method, I obtain the weak form of Eq.(2.3):

$$\iint_{\Omega} \iint_{\mathcal{V}} \frac{1}{\mu} (\nabla \times \mathbf{N}) \cdot (\nabla \times \mathbf{e}) + \sigma \mathbf{N} \cdot \frac{\partial \mathbf{e}}{\partial t} + \mathbf{N} \cdot \frac{\partial \mathbf{j}_s}{\partial t} d\mathcal{V} = 0$$

(2.6)
where $N$ is the vector interpolation functions (i.e. basis functions or shape functions) at the edges.

The derivative of the electric field to time, $\frac{\partial e}{\partial t}$, is discretized using the second-order backward Euler method (Butcher and Goodwin, 2008):

$$\frac{de(t)}{dt} = \frac{1}{2\Delta t}[3e(t) - 4e(t - \Delta t) + e(t - 2\Delta t)]$$

(2.7)

The equation is spatially discretized using the vector FE method (Jin, 2015), and field $e$ at any position can be calculated by a weighted sum of the tangential electric fields $e_i$ along the edges of the located cell:

$$e = \sum_{i=1}^{12} N_i e_i$$

(2.8)

Combining the equations of all the elements at all time gates, a sparse linear system of equations is therefore yielded as

$$Ke(r, t) = b$$

(2.9)

where the right-hand side $b$ is a source term, and $K$ is a symmetric stiffness matrix:

$$K = \begin{pmatrix}
A^1 & B^2 & A^2 \\
B^3 & C^3 & A^3 \\
\vdots & \vdots & \vdots \\
C^{n_t-2} & B^{n_t-2} & A^{n_t-2} \\
C^{n_t-1} & B^{n_t-1} & A^{n_t-1} \\
C^{n_t} & B^{n_t} & A^{n_t}
\end{pmatrix}$$

(2.10)

where $n_t$ denotes the number of time steps, and $A, B, C$ at $k$th element are

$$A^k = 3Q^k + 2\Delta t S^k$$

(2.11)

$$B^k = -4Q^k$$

(2.12)

$$C^k = Q^k$$

(2.13)

$$Q^k = \iiint \sigma^k N^k \cdot N^k dV^k$$

(2.14)
\[
S^k = \iiint 1/\mu (\nabla \times \mathbf{N}^k) \cdot (\nabla \times \mathbf{N}^k) \, dV^k
\]  
(2.15)

I keep the step size for a number of steps, and increase the size by an integer number of step rate on the condition that the response difference between two steps is smaller than a certain standard, i.e., tolerance value. Since the problem is designed for local meshes (Yang et al., 2013), the matrix associated with each time gate is relatively small. In this case, direct solvers are favorable as the matrix factorization can be shared when the time step size is constant (Oldenburg et al., 2013).

The time derivative of the vertical magnetic induction, i.e. the simulated impulse response \( \mathbf{d}_{\text{imp}} \), will be obtained from the electrical field \( \mathbf{e} \) through Faraday’s law, followed by multiplication of the interpolation matrix \( \mathbf{L} \):

\[
\mathbf{d}_{\text{imp}} = \mathbf{Le} = \mathbf{L}_t \mathbf{L}_s \mathbf{e}
\]  
(2.16)

\( \mathbf{L}_t \) denotes the linear interpolation matrix in the time-domain according to the actual time gates, and \( \mathbf{L}_s \) represents the interpolation matrix in the space-domain at the location of receivers.

### 2.1.1 The finite element method

The FE method is a numerical solution to differential equations (i.e. boundary-value problems), which can be divided into scalar (node-based) FE and vector (edge) FE. I formulate the vector FE using brick/hexahedral elements for all the applications, which assigns a constant tangential electrical field to each edge of the element. Because of their linear variation in the direction normal to the vector, these elements exhibit the same convergence rate as the first-order nodal elements. In the meanwhile, normal continuity could be guaranteed by taking the cross product of normal vector \( \mathbf{N}^e_i \) with \( \mathbf{N}^f_i \), which efficiently represents surface currents.

Fields at any position of an element can be calculated through the sum of the multiplication of shape function \( \mathbf{N} \), an interpolation function, and tangential electric fields along the edges of the located cell through Eq.(2.8). The definition of shape function \( \mathbf{N} \) is essential to build two fundamental elemental matrices Eq.(2.14) and Eq.(2.15), and thereby the stiffness matrix \( \mathbf{K} \) for solving Eq.(2.9) and obtaining electric fields.

The construction of \( \mathbf{N} \) follows the descriptions from Jin (2015). Specifically, if the cells are rectangular bricks, the basis function \( \mathbf{N} \) is easily calculated through the edge lengths and cell center. If the element is a non-structured, the basis function \( \mathbf{N} \) is constructed to keep a tangential component
only along the certain edge and none along other edges. The detailed expression of the basis function and the curl of the function, and the integral calculation of hexahedral elements under finite element system is listed in the Appendix 4.

However, unlike the vector basis functions for the rectangular and tetrahedral elements, hexahedral cells are not divergence-free. The divergence depends on deformation degree, thus one should avoid using the hexahedra that deviate greatly in shape from a rectangular brick (Jin, 2015).

2.1.2 Octree-based finite element method

Mesh generation

Octree mesh generation is a spatial partition topology that recursively subdivides a cell into eight blocks (see Fig. 2.1) until a stopping criterion is met (Frey and George, 2007); for example, in our case, the criterion is the volume of the cell. Firstly, I divide the model uniformly in all directions and set the level of these ancestor cells as zero. Based on this basic skeleton, I set several nested regions from the model margin to the center where the transmitter is located. Elements in each region are refined to different levels, with the refinement increasing from the outer regions to the inner ones. The level, or subdivision times, of each cell is stored as a tree structure. One stand-out feature of mesh gradation management is that the level difference between adjacent cells may not exceed 1. Moreover, hanging nodes appear when two adjacent cells do not share the same level (Legrain et al., 2011). Two types of hanging nodes can be noted as shown in the Fig. 2.1: hanging nodes on the edges and hanging nodes on the faces (Grayver, 2015), which require special treatment when I compose the system matrix.

Hanging nodes

I need to handle the added parameters from the edges associated to hanging nodes, to ensure the compatibility of the finite element approximation and the continuity of the finite element fields even on the interface. The solution is inspired by the work of Bielak et al. (2005), who selected the added parameters and treated them using a properly weighted constraint during the stiffness matrix assembly process in Eq.(2.10).
Based on the classic FE solution $\mathbf{e}$ as Eq. (2.8), the field definition in the octree-based FE is extended as

$$
\mathbf{e} = \sum_{i_1=1}^{12-n_h} N_{i_1} e_{i_1} + \sum_{i_2=1}^{n_h} N_{i_2} \left( \sum_{j=1}^{n_{ed}} d_j^{i_2} \cdot \phi_j^{i_2} \right)
$$

(2.17)

where $n_h$ represents the number of edges with hanging nodes, $d_j^{i_2}$ are fields on the edges of lower-level master cell that are associated with the added parameters, $\phi_j^{i_2}$ denotes the enrichment function applied on the added parameters, and $n_{ed}$ is the number of related edges. Given the property of the edge element and all the elements being regular, I define the enrichment function as

$$
\phi_j^{i_2} = \begin{cases} 
1 & \text{on the edge, } n_{ed} = 1 \\
(1/2, 1/2) & \text{on the face, } n_{ed} = 2
\end{cases}
$$

(2.18)

Note that when the hanging node is on the face, two parallel edges on the face share the contribution equally, as the field varies linearly in the normal direction to the vector. In general, the main idea of my approach is to redefine the shape function of edges at the hanging nodes by linear combinations of the previous shape functions, similarly to Grayver (2015).

Therefore, the fields at the edges associated with hanging nodes can be expressed by the edges from master cells, and the dimension size of the stiffness matrix is always smaller than the number of physical edges.

2.1.3 Mirroring approach

During a TEM survey, it is common that the transmitter, either in offset configuration or in a central loop configuration, is geometrically symmetric. Here I take the tTEM system (Auken et al.,
as an example to illustrate the principle of the mirror approach, which is the base of the 2.5D implementation. I assume that the resistivity model has variations in the x and z directions and is symmetric in the y-direction. The x-direction is defined by a line passing through the center of the transmitter and the receiver. In this condition, the magnetic fields on the xy plane are symmetric, with values mirrored from the left side to the right side of the xz plane, and has no y component along the xz-plane, because of the system and 2D model symmetry. No y component of the magnetic field in the xz plane means that the electric field has zero x and z components on the plane, because of Faraday's law. These are exactly the Dirichlet boundary condition I set in the 3D modeling on the outer faces of the forward mesh.

![Diagram](image)

**Figure 2.2 Mirror approach illustration, where the red rectangle symbolizes the transmitter of rTEM system (the size of the transmitter is 4m x 2m) and the red dot symbolizes a dipole receiver.**

a) Magnetic field on the bisector plane; b) Octree forward mesh in the 2.5D

Consequently, if I remove a flank of the original 3D model according to the bisector of the system (see Fig. 2.2) as well as the transmitter, and I apply the Dirichlet boundary condition on all mesh outer faces including the mirroring xz plane, I will obtain a forward modeling equivalent to the full problem in which the resistivity is defined in the entire mesh, left and right of the xz plane.
mirroring plane. Defining the model in the half mesh and using a resistivity model in the half mesh that does not change along the y direction, I obtain a pseudo 2.5D solution to the problem, using a 3D implementation with proper source definition and boundary conditions.

An analogous point of view is the one that looks at the stiffness matrix of the problem. If I take Eq. (2.9) with a size of 4*4 matrix (4 unknowns) as an example, the original 3D system matrix would be:

\[
\begin{align*}
K_{11}e_1 + K_{12}e_2 + K_{13}e_3 + K_{14}e_4 &= b_1 \\
K_{21}e_1 + K_{22}e_2 + K_{23}e_3 + K_{24}e_4 &= b_2 \\
K_{31}e_1 + K_{32}e_2 + K_{33}e_3 + K_{34}e_4 &= b_3 \\
K_{41}e_1 + K_{42}e_2 + K_{43}e_3 + K_{44}e_4 &= b_4
\end{align*}
\] (2.19)

With the symmetric conditions of fields and the information of cells from the mirror approach, namely:

\[
\begin{align*}
e_1 &= e_2 \\
e_3 &= e_4 \\
K_{i1} &= K_{i2}, (i \in 1,4) \\
K_{i3} &= K_{i4}, (i \in 1,4)
\end{align*}
\] (2.20)

and Eq. (2.19) in the half mesh will be

\[
\begin{align*}
K_{11}e_1 + K_{13}e_3 &= b_1/2 \\
K_{21}e_1 + K_{23}e_3 &= b_2/2
\end{align*}
\] (2.21)

In this manner, half of the cells can be saved from computation without the accuracy being affected. To achieve this, I simply need to use only half of the transmitter as the source input, since the entire system still follows the same physical law on half of the 3D forward mesh. Consequently, this is de-facto mathematical optimization, where the 2.5D problem is characterized as a 3D source on a mirrored model using a 3D octree mesh.

2.1.4 Arbitrary source shape

In real explorations, especially airborne TEM (AEM), the transmitter loop is always polygon, which is a good approximation of a circle as well as an ease of controlling loop hanging in the air. For example, for a heptagon transmitter loop shown as Fig. 2.3, one should consider both intersecting and collinear situation. Unlike the tetrahedral mesh, it is impractical to ensure the physical edges along the orientation of transmitter edges under the octree-based hexahedra meshing. The traditional practice is that, I approximate the transmitter shape as much as possible with a given magnetic
moment. However, this may be hard to recover the information in the early times, since the generation of fields varies in three dimensions.

Figure 2.3 A heptagon source loop (red) on an octree meshed plane.

I developed an interpolating scheme for a transmitter loop of arbitrary shape to better simulate the actual field distribution. It is assumed that the loop is laid on a plane. Firstly, I determine if two given line segments intersect or are parallel with each other. Then, I get the intersection point, and obtain the segment length in the belonging cell. Next, I utilize the orientation of every triplet of points in the plane to determine the relation of two segments is intersected or colinear.

The source term is in the right hand side of Eq.(2.9). under the finite element system can be written as:

\[ b_s = \iiint_{V_e} N_e \cdot \frac{\partial J_{imp}(r, t)}{\partial t} dV \]  

(2.22)

The contribution of each loop segment \( i \) is

\[ b_{si} = \int_{l_i} N_i^e \cdot \frac{\partial J_{imp}(r, t)}{\partial t} dl \]  

(2.23)

2.1.5 Topography

In the finite element method, the matrix calculation of a single element (i.e. Eq.(2.14) and Eq.(2.15)) has the analytical solution from Jin (2015) when the model is meshed with brick cells, which result in a faster calculation speed, compared with the hexahedral elements. However, it
presents less elegance when simulating earth surface, if topography varies. Therefore, I consider using the octree-based hexahedral meshes: the hexahedral meshes can align better with real geological situation, while lower the unknown numbers through octree topology.

\[ x = \sum_{i=1}^{12} N_i e_i \]  \hspace{1cm} (2.24)

The fields on the opposite face (with node 7-3-4-8, see Fig. 2.4) have no contribution to field e:

\[ N_2 = N_4 = N_{11} = N_{12} = 0 \]  \hspace{1cm} (2.25)

It can also be demonstrated through mathematical proof that

\[ N_5 = N_6 = N_7 = N_8 = 0 \]  \hspace{1cm} (2.26)

Therefore, only edges on the face of hanging node contribute to the field value x. Eq.(2.24) can be simplified to

\[ x = N_1 e_1 + N_3 e_3 + N_9 e_9 + N_{10} e_{10} \]  \hspace{1cm} (2.27)

Assume the unit vector of the hanging edge \( \hat{u}(u_x, u_y, u_z) \), the enrichment function in Eq.(2.17) becomes
\[
\phi_j = \begin{cases} 
1 & \text{on the edge, } n_{ed} = 1 \\
(\mathbf{u} \cdot \mathbf{N}_1, \mathbf{u} \cdot \mathbf{N}_3, \mathbf{u} \cdot \mathbf{N}_9, \mathbf{u} \cdot \mathbf{N}_{10}) & \text{on the face, } n_{ed} = 4
\end{cases}
\]  

(2.28)

### 2.1.6 Applying waveform and filters

![Illustration of obtaining system response from the impulse response](image)

*Figure 2.5 Illustration of obtaining system response from the impulse response*

A TEM response excited by an impulse is the ideal reaction of fields from the ground following the immediate current turn-off, a Heaviside function, whereby the time derivative is a delta function. In the practice of TEM measurement, current with waveform, such as a trapezoidal pulse, is used in the transmitter since current takes time to ramp up and down due to the Tx coil inductance. In addition, several filters are present due to system design and hardware limitations: i) low-pass filter, ii) receiver coil filter, iii) front-gate filter (Fig 2.5). A low-pass filter on receiver board is designed for the sake of anti-aliasing. The stray capacitance and self-inductance of Rx coil limit its receiving bandwidth. Gating using a window will involve integrating over the given width, which also has a low-pass filtering effect on data.

Therefore, the simulation of actual response is indispensable before inverting the measured data. In numerical modeling, the impulse response \( \mathbf{d}_{imp} \) is a discrete signal. A cubic spline interpolation is therefore applied to the impulse response and model the system response \( \mathbf{d}_{sys} \) by convolving a transfer function (Zhang *et al.*, 2021):

\[
\mathbf{d}_{sys} = \left[ (\mathbf{d}_{imp} \ast \mathbf{h}_2 \ast \mathbf{w}_t) \mathbf{h}_3 \right] \ast \mathbf{h}_1
\]  

(2.29)

where \( \mathbf{w}_t \) denotes the time derivative of the waveform, which can be approximated as the slope of a piece-wise linear function \( I \) with \( n \) segments:
\begin{equation}
\omega_t^i = \frac{l_{i+1} - l_i}{t_{i+1} - t_i}, i = 1, ..., n - 1. \tag{2.30}
\end{equation}

the receiver low-pass filter and coil filter are applied numerically with the convolution of the first-order Butterworth filter \( h_1 \) and the second-order critically damped filter \( h_2 \), or two first order filters (Auken et al., 2019):

\begin{align*}
    h_1 &= \omega \cdot e^{-\omega t} \tag{2.31} \\
    h_2 &= \omega^2 \cdot t \cdot e^{-\omega t} \tag{2.32}
\end{align*}

Front-gate filter is simulated as a logistics function:

\begin{equation}
    h_3(t) = \frac{1}{1 + e^{-k(t-t_0)}} \tag{2.33}
\end{equation}

Here \( t_0 \) relates to the turned-off moment of front-gate. The coefficient \( k \) determines the growth rate of the function curve.

### 2.2 Multi-mesh approach

The definition of model parameters and forward meshes is obtained by adapting the approach of Christensen et al. (2017) and Madsen et al. (2020) with domain decomposition. Domain decomposition breaks the full-survey forward problem into small tasks at the soundings, minimizing the computing expenses without sacrificing modeling accuracy. Specifically, I used two sets of separate octree meshes for forward modeling and Jacobian calculation at each transmitter, where I compute the forward response from Eq. (2.16) and the Jacobian from Eq. (2.42) using the adjoint modeling method.

#### 2.2.1 Mesh Interpolation

I designed one voxel mesh for the full-scale model update in the inversion, where the model parameters are defined in two different ways for 3D and 2.5D inversions (see Fig. 2.6). In 3D, the parameters are determined on the nodes of a 3D regular structured mesh, with uniform node spacing in \( x \) and \( y \) direction and log-increasing node spacing in \( z \) direction. In 2.5D, the parameters are specified on the nodes of 2D sections, which follow the acquisition lines, with uniform node spacing along lines and log-increasing vertical spacing. The inversion model parameters are linked to the center of the forward mesh elements through interpolation with an inverse distance function:
where the vector \( \mathbf{m} \) represents the values of model parameters in the forward mesh elements, and \( \mathbf{M} \) holds the values at the voxel nodes. \( \mathbf{F} \) is an interpolation matrix with weights, which merely rely on the relative distances between the forward mesh elements with the model nodes used for interpolation.

Since the interpolation function is a linear operation, and applying the chain rule for derivatives, so that

\[
\frac{\partial \mathbf{d}}{\partial \mathbf{M}_i} = \sum_j \frac{\partial \mathbf{d}}{\partial \mathbf{m}_j} \frac{\partial \mathbf{m}_j}{\partial \mathbf{M}_i} = \sum_j \frac{\partial \mathbf{d}}{\partial \mathbf{m}_j} F_{j,i}
\]

I, therefore, write the Jacobian on the model mesh mapping from Jacobian mesh as:

\[
\mathbf{J}_M = \mathbf{J}_m \cdot \mathbf{F}^T
\]

where the \( \mathbf{J}_M \) is the Jacobian of the inversion model space, the voxel mesh, and \( \mathbf{J}_m \) is the Jacobian computed in the forward mesh through Eq.(2.42).

This multi-mesh approach, with model parameters defined on the regular meshes and forward/Jacobian computations, carried out on octree meshes, one for each transmitter, allows for minimizing computation time and resource requirements while maintaining an inversion model space.
well suited for inversion. In this fashion, enforcing vertical and horizontal constraints for the inversion becomes easily applicable and incorporating other prior knowledge, when present.

2.2.2 Application on time-lapse inversion

The advantage of this method is three-fold for time-lapse TEM inversions. Firstly, the computational expense is multiplied in time-lapse inversion, since the size of data space and model space is proportional to the number of time-lapse steps. Fortunately, the complexity is minimized to local soundings through the domain decomposition so that parallelization can perform while the forward accuracy is maintained. Secondly, it eases the process of enforcing spatial constraints for the inversion or incorporating prior knowledge, thanks to the regularity of the inversion mesh. Last, it overcomes the challenge of data repetition with matching layouts, providing the flexibility that surveys at different time-lapse steps can be carried out at different locations within the research area.

2.2.3 Application on multi-system inversion

For an integrated survey, a combination of multiple systems are used according to the geological settings. For instance, a coastal survey can involve ground-based and waterborne systems, which increase the complexity of the inversion. Compared to the strategy of breaking into several regions and inverting the datasets regionally, the benefits of applying the approach to a dual-system inversion are several: i) the survey area is decomposed into independent tasks in the modeling process, which allows us to design meshes with different density accordingly if different configurations are adopted, so that the computational complexity is minimized while sufficient modeling accuracy maintains; ii) one inversion mesh representing the whole survey area makes it easier to incorporate the 2D or 3D structures between different geological settings, this is especially important for coastal models, as the multi-dimensional effects present at the shoreline – the boundary of land and seawater, beside which ground-based and waterborne systems are used separately.

2.3 Inversion

2.3.1 Jacobian calculation

The Jacobian is the matrix of sensitivities with size $N_d$ (the number of data) by $N_e$ (the number of elements), and each element in the matrix reflects the contribution to the response of conductivity at this point (Christensen, 2014). I calculate the Jacobian in an explicit backward stepping scheme (Börner, 2010) through adjoint forward modeling. This methodology is applied to both the
3D and 2.5D inversion, since I calculate the Jacobian in the octree mesh firstly and then interpolate to the inversion model mesh, as illustrated in Fig. 2.6.

Let us define the Jacobian matrix for each step, $n$, as:

$$J^n = \frac{\partial d^n_{sys}}{\partial \mathbf{m}}$$  \hspace{1cm} (2.37)

The derivative of Eq.(2.9) with respect to model parameters $\mathbf{m}$ will be:

$$\frac{\partial \mathbf{e}}{\partial \mathbf{m}} = \mathbf{K}^{-1} \mathbf{G}$$  \hspace{1cm} (2.38)

where

$$\mathbf{G} = - \frac{\partial \mathbf{K}}{\partial \mathbf{m}} \mathbf{e}$$  \hspace{1cm} (2.39)

Combing the interpolation matrix $\mathbf{L}$ in Eq.(2.16), the Jacobian matrix is derived to:

$$\mathbf{J}^T = \mathbf{G}^T \mathbf{K}^{-T} \mathbf{L}^T$$  \hspace{1cm} (2.40)

If I define a vector $\mathbf{V} = \mathbf{K}^{-T} \mathbf{L}^T$, then I have the adjoint modeling equation:

$$\mathbf{K}^T \mathbf{V} = \mathbf{L}^T$$  \hspace{1cm} (2.41)

Solving the Eq.(2.41) through the backward propagation from the last time step, I have the temporary vector $\mathbf{V}$. I thus obtain the Jacobian through the relation:

$$\mathbf{J}^T = \mathbf{G}^T \mathbf{V}.$$  \hspace{1cm} (2.42)

### 2.3.2 GN method

For inversion, I adopted the framework from AarhusInv (Auken et al., 2015), which provides means for minimizing a general multi-component objective function

$$\Phi(\mathbf{m}) = \frac{\Phi_{obs}(\mathbf{m}) + \Phi_{prior}(\mathbf{m}) + \Phi_{reg}(\mathbf{m})}{N_{obs} + N_{prior} + N_{reg}}$$  \hspace{1cm} (2.43)

where each component of the objective function describes the norm misfit of the solution with respect to the observed data, prior information, and regularizing constraints, respectively ($N_{obs}$, $N_{prior}$ and $N_{reg}$ being the number of data, the number of prior constraints and the number of roughness constraints).
In our algorithm, the objective function is minimized iteratively following the Levenberg-Marquardt adaptive minimization scheme (Menke, 2018, Hanke, 1997), which combines the gradient descent method with the GN method to get the optimal convergence rate. Hence, the \( n + 1 \)th iterative model update vector \( m \) becomes:

\[
m_{n+1} = m_n + \left[ J^T(n) C^{-1}(n) J(n) + \lambda(n) I \right]^{-1} \cdot \left[ J^T(n) C^{-1}(n) \delta d^*(n) \right]
\]  

(2.44)

Here, the damping parameter \( \lambda(n) \) is regenerated at each step, which determines the contribution amount of the gradient descent and the GN method on the current iteration by scaling the identity matrix \( I \); \( J^*(n) \) denotes the Jacobian matrix of partial derivatives; \( \delta d^*(n) \) is the data vector update and \( C^*(n) \) a covariance matrix:

\[
J^*(n) = \begin{bmatrix} J(n) \\ P \\ R \end{bmatrix}
\]  

(2.45)

\[
\delta d^*(n) = \begin{bmatrix} \delta d(n) \\ \delta m(n) \\ \delta r(n) \end{bmatrix} = \begin{bmatrix} d(n) - d_{obs} \\ m(n) - m_{prior} \\ -Rm(n) \end{bmatrix}
\]  

(2.46)

\[
C^*(n) = \begin{bmatrix} C_{obs} & 0 & 0 \\ 0 & C_{prior} & 0 \\ 0 & 0 & C_R \end{bmatrix}
\]  

(2.47)

In the first equation of the Jacobian matrix (2.45), \( J(n) \) thus represents the Jacobian of the forward mapping; \( P \) is the constraint matrix on the a priori information and \( R \) is the roughness matrix. In Eq.(2.46), the data vector update \( \delta d^*(n) \) includes the distance \( \delta d(n) \) between the \( n \)th forward response \( d(n) \) and the observed data \( d_{obs} \), the distance \( \delta m(n) \) between the \( n \)th model update \( m(n) \) and a priori model vector \( m_{prior} \), and roughness of the \( n \)th model vector \( \delta r(n) = -Rm(n) \). The 3 blocks of the covariance matrix \( C^* \) contain the covariance on the observed data \( C_{obs} \), the covariance on the a priori information \( C_{prior} \) and the covariance on the roughness constraints \( C_R \). One can find more detailed matrix format and derivations in Auken and Christiansen (2004). No prior information was incorporated in the examples of this thesis. However, two types of constraints, horizontal and vertical, are enforced, and the roughness matrix \( R \), the roughness of the \( n \)th model vector \( \delta r(n) \), and the covariance on the roughness constraints \( C_R \) can therefore be further subdivided into two terms:
Methodology

\[
R = \begin{bmatrix} R_h \\ R_v \end{bmatrix}
\]  
(2.48)

\[
\delta r_{(n)} = \begin{bmatrix} -R_h \mathbf{m}_{(n)} \\ -R_v \mathbf{m}_{(n)} \end{bmatrix}
\]  
(2.49)

\[
C_R = \begin{bmatrix} C_{Rh} & 0 \\ 0 & C_{Rv} \end{bmatrix}
\]  
(2.50)

2.3.3 Time lapse inversion

In the time-lapse inversion scheme adopted in this study, two datasets \( \mathbf{d}_1 \) and \( \mathbf{d}_2 \) are inverted simultaneously to obtain the corresponding models \( \mathbf{m}_1 \) and \( \mathbf{m}_2 \) by constraining the model difference \( \delta \mathbf{m} = \mathbf{m}_2 - \mathbf{m}_1 \) (while \( \mathbf{d}_1 \) and \( \mathbf{d}_2 \) may differ in size, \( \mathbf{m}_1 \) and \( \mathbf{m}_2 \) are defined on identical meshes and have the identical size, such that their difference can be determined). Furthermore, in addition to the roughness constraint on individual models \( \mathbf{m}_1 \) and \( \mathbf{m}_2 \) roughness constraints are also applied to the model difference \( \delta \mathbf{m} \). Defining the whole inversion data and model vectors \( \mathbf{d} \) and \( \mathbf{m} \) in terms of the concatenation of individual vectors as \( \mathbf{d} = \begin{bmatrix} \mathbf{d}_1 \\ \mathbf{d}_2 \end{bmatrix} \) and \( \mathbf{m} = \begin{bmatrix} \mathbf{m}_1 \\ \mathbf{m}_2 \end{bmatrix} \), the objective function \( \Phi \) in our time-lapse inversion scheme consists of four terms:

\[
\Phi = \Phi_d (\delta \mathbf{d}) + \Phi_{TL} (\delta \mathbf{m}) + \Phi_{Rm} (\mathbf{r}) + \Phi_{Ru} (\delta \mathbf{r})
\]  
(2.51)

where:

\( \Phi_d, \Phi_{TL}, \Phi_{Rm}, \Phi_{Ru} \) represent the measures (i.e. the squared norms) of the data difference, model update, roughness of model, and model update, respectively. The three terms (\( \Phi_{TL}, \Phi_{Rm}, \Phi_{Ru} \)) represent the regularization of the inversion: in particular, the time-lapse term \( \Phi_{TL} \) measures and minimizes the distance between \( \mathbf{m}_1 \) and \( \mathbf{m}_2 \), i.e. the model update in the time-lapse inversion; the model roughness term \( \Phi_{Rm} \) minimizes the roughness of individual models; the measure \( \Phi_{Ru} \) minimizes the roughness of the model updates.

\( \delta \mathbf{d} = \mathbf{d} - \mathbf{d}_{obs} \) represents the difference between the forward response \( \mathbf{d} \) and the observed data \( \mathbf{d}_{obs} \); \( \delta \mathbf{m} = \mathbf{m}_2 - \mathbf{m}_1 \) symbolizes the model update between two models, i.e., model temporal variations; \( \mathbf{r} = -R_m \delta \mathbf{m} \) represents the model roughness through the roughness matrix \( R_m = \begin{bmatrix} R_{m_1} & 0 \\ 0 & R_{m_2} \end{bmatrix} \); \( \delta \mathbf{r} = -R_u \delta \mathbf{m} \) is the roughness of the model update.
The time-lapse inversion is performed iteratively by following the practice established inside AarhusInv (Auken et al., 2015). This approach is based on the Levenberg-Marquardt adaptive minimization scheme (Menke, 2018, Hanke, 1997), a weighted combination of the gradient descent method with the GN method. Norms different from L2 in Eq.(2.51) are implemented through the iteratively reweighted least-squares (IRLS) approach following (Farquharson and Oldenburg, 1998). The model vector \( \mathbf{m} \) is updated at the \( n + 1 \)th iterative step:

\[
\mathbf{m}_{n+1} = \mathbf{m}_n + \left[ \mathbf{J}_n^T \mathbf{C}_n^{-1} \mathbf{J}_n^* + \lambda_n \mathbf{I} \right]^{-1} \cdot \left[ \mathbf{J}_n^T \mathbf{C}_n^{-1} \delta \mathbf{d}_n^* \right]
\]  

(2.52)

Here, the damping parameter, \( \lambda_n \), iteratively reweights the gradient descent approach and the GN method by scaling the identity matrix \( \mathbf{I} \), \( \mathbf{J}_n^* \) includes the Jacobian matrix of different partial derivatives, the vector update \( \delta \mathbf{d}_n^* \) contains data, model roughness and model difference; and \( \mathbf{C}_n^{-1} \) is the covariance matrix of data uncertainty and model roughness, as follows:

\[
\mathbf{J}_n^* = \begin{bmatrix} \mathbf{J}_n^1 & \mathbf{I} \\ \mathbf{R}_m & \mathbf{R}_u \end{bmatrix}
\]  

(2.53)

\[
\delta \mathbf{d}_n^* = \begin{bmatrix} \delta \mathbf{d}_n \\ \delta \mathbf{m}_n \\ \delta \mathbf{r}_n \\ \delta \mathbf{r}_u \end{bmatrix} = \begin{bmatrix} \mathbf{d}_n - \mathbf{d}_{obs} \\ \mathbf{m}_{2(n)} - \mathbf{m}_{1(n)} \\ - \mathbf{R}_m \mathbf{m}_n \\ - \mathbf{R}_u \delta \mathbf{m}_n \end{bmatrix}
\]  

(2.54)

\[
\mathbf{C}_n^{-1} = \begin{bmatrix} \mathbf{C}_{obs}^{-1} & \mathbf{0} & \mathbf{W}_{TL(n)}^{-1} & \mathbf{C}_{TL}^{-1} \mathbf{W}_{TL(n)}^T & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{W}_{RL(n)}^{-1} & \mathbf{C}_{RL}^{-1} \mathbf{W}_{RL(n)}^T & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix}
\]  

(2.55)

In Eq.(2.53), \( \mathbf{J}_n = \begin{bmatrix} \mathbf{J}_1(n) & \mathbf{0} \\ \mathbf{0} & \mathbf{J}_2(n) \end{bmatrix} \) represents the Jacobian of the two acquisitions, translated from the forward mesh to the inversion mesh following Madsen et al. (2020) and Zhang et al. (2021); \( \mathbf{I} \) is the identity matrix; \( \mathbf{R}_m \) and \( \mathbf{R}_u \) are the roughness matrices on model and model update. In
Eq. (2.54), the data vector update $\delta \mathbf{d}^*_n$ includes the distance $\delta \mathbf{d}_n$ between the $n^{th}$ forward response $\mathbf{d}_n$ and the observed data $\mathbf{d}_{\text{obs}}$, the distance $\delta \mathbf{m}_n$ between the two models at the $n^{th}$ iteration, the roughness of the $n^{th}$ model vector $\mathbf{r}_n = -\mathbf{R}_m \mathbf{m}_n$ and the roughness of the model difference $n^{th}$ model vector $\delta \mathbf{r}_n = -\mathbf{R}_u \delta \mathbf{m}_n$. In Eq. (2.55), the covariance matrix $\mathbf{C}^*$ is defined in terms of the covariance on the observed data $\mathbf{C}_{\text{obs}}$, the time-lapse covariance on the model difference $\mathbf{C}_{TL}$ and the covariance on the roughness constraints $\mathbf{C}_{R_m}$ and $\mathbf{C}_{R_u}$. The elements of $\mathbf{C}_{\text{obs}}$ indicates the noise level in the data, while the elements of $\mathbf{C}_{TL}$, $\mathbf{C}_{R_m}$ and $\mathbf{C}_{R_u}$ control the constraint strength from the model side. All four matrices are diagonal, thus the data errors have no linkage between each other. In Eq. (2.55), the matrices $\mathbf{W}_{TL}(n)$, $\mathbf{W}_{R_m}(n)$ and $\mathbf{W}_{R_u}(n)$ are the IRLS re-weighting matrices that allows to define norms in the objective function different from the L2. In particular, for a given model vector $\mathbf{x}$ (equal to either $\delta \mathbf{m}$, $\mathbf{r}$ or $\delta \mathbf{r}$) and a given measure functional $\Phi(\mathbf{x}) = \sum_{i=1}^{\text{size}(\mathbf{x})} \varphi(x_i)$, the matrices $\mathbf{W}_{\eta}$ (where $\eta = TL$ or $R_m$ or $R_u$) are linked to the measure $\Phi$ and the covariance matrices $\mathbf{C}_{\eta}$ following (Farquharson and Oldenburg, 1998):

\[
\mathbf{W}_{\eta_{ii}} = \frac{\sqrt{\mathbf{C}_{\eta_{ii}}}}{2\chi_i} \varphi'(x_i)
\]

The stopping criterion of the iterative procedure in Eq. (2.51) is implemented on the total misfit $\mathcal{X}$, defined as:

\[
\mathcal{X} = \left( \frac{\Phi_d(\delta \mathbf{d}) + \Phi_{TL}(\delta \mathbf{m}) + \Phi_{R_m}(\mathbf{r}) + \Phi_{R_u}(\delta \mathbf{r})}{N_d + N_{TL} + N_{R_m} + N_{R_u}} \right)^{\frac{1}{2}}
\]

\[
= \left( \frac{N_d \chi_d^2 + N_{TL} \chi_{TL}^2 + N_{R_m} \chi_{R_m}^2 + N_{R_u} \chi_{R_u}^2}{N_d + N_{TL} + N_{R_m} + N_{R_u}} \right)^{\frac{1}{2}}
\]

In which:

$N_d$, $N_{TL}$, $N_{R_m}$, $N_{R_u}$ represent the number of data points, the number of time-lapse constraints, and the number of roughness constraints on model and model update.

$\chi_d = \left( \frac{\delta \mathbf{d}^T \mathbf{C}_{\text{obs}}^{-1} \delta \mathbf{d}}{N_d} \right)^{\frac{1}{2}}$ represents the data misfit.
\[ X_{TL} = \left( \frac{\delta m^T W_{TL}^T C_{TL}^{-1} W_{TL} \delta m}{N_{TL}} \right)^{\frac{1}{2}} \] represents the time-lapse model penalty.

\[ X_{Rm} = \left( \frac{r^T W_{Rm}^T C_{Rm}^{-1} W_{Rm} r}{N_{Rm}} \right)^{\frac{1}{2}} \] represents the roughness model penalty.

\[ X_{Ru} = \left( \frac{\delta r^T W_{Ru}^T C_{Ru}^{-1} W_{Ru} \delta r}{N_{Ru}} \right)^{\frac{1}{2}} \] represents the roughness model difference penalty.

The matrices \( W_\eta \) (where \( \eta = TL \) or \( R_m \) or \( R_u \)) are linked to the measure \( \Phi \) and the covariance matrices \( C_\eta \) as:

\[ W_{\eta_{ii}} = \sqrt{\frac{C_{\eta_{ii}}}{x_i^2} \varphi(x_i)} \]  

(2.58)

The inversion is carried out in logarithmic data and model spaces. The forward response \( d_{(n)} \) of Eq.(2.54) and the Jacobian calculation \( J_{(n)} \) of Eq.(2.53) are computed for 3D TEM data following the routine devised by Xiao et al. (2020). The inversion process is terminated when the variation of the total misfit between two consecutive iterations is smaller than a defined threshold (e.g. 1%).

**Asymmetric minimum support MS norm for time-lapse model difference**

In this study, the measure of the model difference \( \Phi_{TL}(\delta m) \) in the objective function of Eq.(2.51) is defined in terms of a minimum support (MS) functional, instead of the classic L2 measure. While the L2 measure penalizes the sum of the squared difference of the components of the vector \( \delta m = m_2 - m_1 \), the MS functional penalizes the number of components \( \delta m_i = m_{2,i} - m_{1,i} \) that differ “significantly”, to favor compact time-lapse changes. Researchers have proposed different solutions for defining the significance of parameter difference in MS functionals for their applications (Last and Kubik, 1983, Zhdanov et al., 2006a, Ajo-Franklin et al., 2007, Carbajal et al., 2012, Kim and Cho, 2011, Zhdanov and Tolstaya, 2004, Vignoli et al., 2012, Fiandaca et al., 2015). In particular, Fiandaca et al. (2015) proposed a definition of generalized asymmetric MS, which is an easy-to-tune regulation to find globally optimal compatibility between data and model variation. The analytical expression of the functional is expressed:

\[ \varphi_{MS} = \alpha^{-1} \left[ (1 - \beta) \cdot \frac{(x_i^2 / \sigma_i^2)^{p_1}}{(x_i^2 / \sigma_i^2)^{p_1} + 1} + \beta \cdot \frac{(x_i^2 / \sigma_i^2)^{p_2}}{(x_i^2 / \sigma_i^2)^{p_2} + 1} \right] \]  

(2.59)
\[ \beta = \frac{(x_i^2/\sigma_i^2)^{\max(p_1,p_2)}}{(x_i^2/\sigma_i^2)^{\max(p_1,p_2)} + 1} \]  

where \( x_i = \delta m_i \) represents the difference of the \( i \)th component of the model difference and \( \alpha, p_1, p_2 \) and \( \sigma_i \) represent the MS settings.

The norm settings have the following meaning:

The setting \( \sigma_i \) symbolizes the threshold value that defines the “significance” of a parameter change because \( \sigma_i \) represents the transition point in the minimum support functional: \( \delta m_i \ll \sigma_i \) gives a zero penalty in the objective function, i.e. \( \varphi_{MS}(\delta m_i) = 0 \); \( \delta m_i \gg \sigma_i \) gives the maximum penalty \( \varphi_{MS}(\delta m_i) = \alpha^{-1} \); \( \delta m_i = \sigma_i \) represent the transition point at which half penalty \( \varphi_{MS}(\delta m_i) = 0.5 \cdot \alpha^{-1} \) is reached. It is expressed typically as a fixed fraction (10% - 30%) of the expected relative parameter (e.g. resistivity) variation, which can be estimated from either prior information of underlying temporal changes or a standard (e.g. L2) time-lapse inversion. In this study \( \sigma_i = 0.1 \) is used, both in the synthetic and field examples.

The setting \( \alpha \) controls the maximum penalty, and hence the relative weight of data and model reassures in the objective function and affects the size of time-lapse changes. Let’s define \( N_{transitions} \) as the expected number of model parameters that differ “significantly” (i.e. above the transition point \( \delta m_i = \sigma_i \)) in time-lapse inversion. Fiandaca et al. (2015) suggests using \( \alpha \) values bigger than \( \alpha = \frac{N_{transitions}}{N_{TL}} \), such that in Eq.(2.57) \( \chi_{TL} < 1 \). Actually, contrary to Fiandaca et al. (2015), in this study \( N_{TL} \gg N_d \), and the risk of over-regularizing the inversion through the time-lapse constraint is significant. Consequently, the field data are analyzed for different \( \alpha \) values (ranging from \( \alpha = 1 \) to \( \alpha = 1000 \)), in order to study explicitly the dependence of inversion results on the balance between time-lapse constraints and data misfit in the objective function. Only one value (\( \alpha = 1 \)) is used in the synthetic examples.

The settings \( p_1 \) and \( p_2 \) control the shape of \( \varphi_{MS} \) before and after the transition point \( \delta m_i = \sigma_i \) (the sharpness of the transition increases with \( p \)), and determine how the focusing depends on the other settings \( \sigma \) and \( \alpha \). In this study, I use the values that give the weaker overall dependence of the focusing on \( \sigma \) and \( \alpha \) suggested by Fiandaca et al. (2015), i.e. \( p_1 = 1.35 \) and \( p_2 = 2 \).
3. Results, Paper 1: Fast 2.5d and 3d inversion of transient electromagnetic surveys using the octree-based finite element method

3.1 Introduction

In the last two decades, various numerical 3D TEM modeling algorithms have been presented using multiple numerical methods (Zhdanov et al., 2006b, Commer et al., 2015, Haber et al., 2002, Um et al., 2010). However, the 3D inversion of TEM data is a massive computational challenge. The standard industry routine for TEM inversion is to perform 1D inversions (Auken and Christiansen, 2004, Vignoli et al., 2015, Viezzoli et al., 2008, Brodie and Fisher, 2008), rapid approximations or a combination of both (Christiansen et al., 2016). In recent years, several strategies have been reported in the literature to alleviate the 3D TEM inversion problem more effectively, such as considering sensitivity within the footprint (Cox et al., 2012), using the direct solvers (Oldenburg et al., 2013), and domain decomposition (Yang et al., 2013). Even so, it remains a computationally expensive task to realize a large-scale multi-dimensional inversion for TEM surveys.

Here, I present a 3D inversion scheme and a 2.5D inversion scheme through an octree finite element modeling and a multi-mesh approach. The non-uniform meshing is only adapted in the regions where fine resolution is needed to represent complex geometry features and capture large field variations, such as areas close to the transmitter and receiver or places including a conductivity discontinuity. The meshing can effectively reduce the number of unknowns in the linear system to be solved (Horesh and Haber, 2011), and achieve computational savings on the process of forward modeling and Jacobian calculation. The multi-mesh approach decouples the forward mesh and inversion mesh, which decomposes the survey domain using a local mesh at each sounding for forward calculation and a full-survey model mesh for inversion. The 2.5D solution is based on a 3D modeling and an assumption on the symmetry of the modeling, in terms of source and boundary conditions, which allows us to almost halve the computation cost for both forward responses and Jacobian calculations compared to the complete 3D solution.
I verify the effectiveness of the algorithm through two numerical experiments using the towed transient electromagnetic (TEM) system (Auken et al., 2019). The first example presents 3D and 2.5D forward responses of resistive and conductive half-space models against 1D responses. Following this, I present a performance analysis comparing against 3D tetrahedral results. The second numerical example shows synthetic inversion results of a 3D valley model from 1D, 2.5D, and 3D algorithms. Finally, I present inversions of field data that demonstrate the advantages of our implementations.

3.2 Numerical experiments

3.2.1 Validation

I validate the implementations through a half-space problem, comparing the responses with 1D computations (Auken et al., 2015). The homogenous half-space model is calculated for resistivities of 10 and 400 Ωm, and the air resistivity is defined as $10^6$ Ωm. I designed the octree mesh to meet a target of 3% accuracy at the receiver position, resulting in a 3D forward mesh with 17,100 DoF and a 2.5D forward mesh with 12,200 DoF. The smallest cell at the receiver is $0.5m \times 0.5m \times 0.5m$, while the size of the largest cell at the boundary is $1024m \times 1024m \times 1024m$.

3.2.2 Performance comparison with the tetrahedral implementation

I present a comparison of the octree 3D and 2.5D implementations and the 3D tetrahedral implementation shown in Zhang et al. (2021) in terms of the running time and memory usage. The 3D octree algorithm requires 20 s for the forward response, which is less than 1/3 of running time on a 3D tetrahedral scheme. The 2.5D octree algorithm further speeds up the process by another factor of two. As for memory usage, the 3D octree modeling and Jacobian calculation needs 1/3 of the tetrahedral, and 2.5D octree further reduces it to nearly a half of the 3D octree one.

3.2.3 Synthetic examples

For synthetic inversions, I designed an idealized 3D model, consisting of a 10 Ωm buried valley structure embedded in a 100 Ωm homogeneous background (Fig. 3.1-a). I carried out a 3D inversion and a 1D voxel inversion (Christensen et al., 2017) for the whole survey, and a 2.5D inversion on two profiles. As shown in Fig. 3.1, the 1D inversion does not recover the upper branch of the model, but the 3D inversion is able to image both the valley branches, although with poor resolution on the lower branch. I further compare the 1D, 2.5D, and 3D inversion results along two
profiles (Fig. 3.2). The superior performance, in terms of model recovery, of the 2.5D inversion along one profile compared to the other, is a direct consequence of the degree of model symmetry, i.e. almost 2D or highly 3D, along the profile.

Figure 3.1 The 3D octree inversion for a valley model using the tTEM system. (a) 3D view of the conductive valley, with a section plane at a depth of 25m. (b) Soundings’ layout above the valley, with 20m distance in the x-direction and 10 m distance in the y-direction. Line A and B are the profiles inverted in 2.5D and shown in Fig. 3.2. (c) Two used driving directions of the tTEM system. (d) 1D inversion result of the resistivity model section. (e) 3D inversion result of the resistivity model section. (f) Colorbar of sections d and e. The dotted white lines in sections (d) and (e) represent the extension of the valley.
Figure 3.2 Model and inversion result at two profiles of the valley model. (a) True model of profile A. (b) 3D inversion result of profile A. (c) 2.5D inversion result of profile A. (d) 1D inversion result of profile A. (e) True model of profile B. (f) 3D inversion result of profile B. (g) 2.5D inversion result of profile B. (h) 1D inversion result of profile B.

3.3 Field example

I used the data collected in Javngyde, Denmark, where the high heterogeneity makes the site a good example to validate our 3D and 2.5D inversion algorithms. I performed a 3D inversion of the entire subset with 200 soundings and selected a 24-sounding profile for the 2.5D inversion. All the inversions were given a homogeneous starting model of 100 $\Omega$m. The total data misfits of the 3D full survey, the 2.5D profile, and the 1D inversion are 1.2, 0.9, and 0.8, respectively. According to the geology background, I can see the significant differences are present in the imaging of the conductive anomalies between the 1D inversion and 2.5D/3D inversions (Fig. 3.3). These differences are similar to the ones found in the analysis of the inversions of the synthetic model. I, therefore, follow the multi-dimensional inversion results for geological interpretations.
Figure 3.3 3D (a), 2.5D (b) and 1D (c) inversion result and corresponding sounding misfit (d) at the profile L. The white dashed lines in (a), (b), (c) represent 1D DOI.

3.4 Conclusion

I have presented two implementations of modeling and inversion using an octree-based finite element method in 3D and 2.5D of TEM data. The octree technique locally refines the mesh, which reduces the degree of freedom efficiently resulting in a lower computational cost for forward modeling and Jacobian calculation. With a mirror approach, I built a 2.5D algorithm using an octree mesh, which additionally improves efficiency of the inversion scheme. The multi-mesh approach
Results, Paper 1: Fast 2.5d and 3d inversion of transient electromagnetic surveys using the octree-based finite element method provides a flexible link between the local forward meshes and one inversion model space, successfully avoiding fine inversion mesh refinements without sacrificing forward accuracy.

The applicability of the proposed algorithms was demonstrated through a synthetic example with a 3D valley structure and a field example. Based on the inversion results, I conclude that our 3D and 2.5D octree-based inversion schemes for TEM data can resolve complicated subsurface structures. I expect the implementation to play a bigger role in the TEM applications for engineering and environmental problems.
4. Results, Paper 2: Three-dimensional time-lapse inversion of transient electromagnetic data, with an application at an Icelandic geothermal site

4.1 Introduction

Time-lapse inversion of resistivity has been used for inferring temporal changes in the subsurface for different environmental and engineering problems such as groundwater mapping (Doetsch et al., 2012), seawater intrusion delineation (Ogilvy et al., 2009), soil moisture assessment (Farzamian et al., 2021), gas sequestration (Auken et al., 2014), geothermal system monitoring (Peacock et al., 2013), and oil production (Orange et al., 2009). With different inversion strategies and regularizations, time-lapse inversion, has been actively studied and applied in the field of electrical resistivity tomography (ERT) for more than two decades (Bièvre et al., 2021, LaBrecque and Yang, 2001). Moreover, it has gradually been applied to inductive methods such as magnetotelluric (Rosas-Carbajal et al., 2015) and controlled source electromagnetic method (Bretaudeau et al., 2021), which show superior sensitivity to conductive structures, with respect to ERT.

Nonetheless, to the best of my knowledge, time-lapse inversion has never been applied to TEM data, despite the fact that the TEM method is widely used in near-surface resistivity distribution mapping. This is probably due to the specific challenges associated with TEM time-lapse inversions: i) data collection with consistent acquisition layouts (geometries, locations, etc.) is complicated with a moving measurement such as in airborne EM, but also with ground-based EM where the exact geometry and location of the transmitter loop can be cumbersome to reproduce identically without leaving the set-up at the site; ii) TEM surveys may result in different data density due to the unexpected coupling to man-made infrastructures in different time-lapse acquisition steps, or limitations in accessibility; iii) 3D TEM inversion, best suited for retrieving localized time-lapse changes, requires intensive computational capacity in terms of both time consumption and memory cost.

I address these issues with the development of a new TEM time-lapse inversion scheme in which: i) forward and Jacobian computations are carried out in 3D through the octree-based finite element method; ii) the multi-mesh approach (Zhang et al., 2021) is used to decouple the forward/Jacobian mesh and inversion mesh so that the same inversion mesh can be used at different
time-lapse steps despite possible variations in acquisition layouts; iii) the calculation burden in the modeling process is effectively alleviated owing to the domain decomposition strategy (Yang et al., 2013), which uses a local mesh for individual soundings; iv) datasets acquired at different time-lapse steps are inverted simultaneously, using the asymmetric generalized MS norm for time-lapse constraints, to obtain compact time-lapse changes.

4.2 Numerical experiments

To investigate the transition resolution of the implementation and the dependence on data density given by the 3D sensitivity, I designed two sets of synthetic examples, with coarse and dense acquisition layouts, respectively (Fig. 4.1 and Fig. 4.2). A 3D conductive anomaly is designed embedded in a resistive two-layered background media, the values chosen were representative of the resistivity background values of the field case illustrated in the next section. The horizontal extension of the 3D anomaly grows from the first measurement to the second measurements to simulate the time-lapse changes. I modelled the response of a central-loop WalkTEM system (Nyboe et al., 2010) with a $50 \times 50 \text{m}^2$ transmitter coil.

![Figure 4.1 Model sections and resistivity ratios of independent and time-lapse inversion results using the coarse acquisition layout. Black dots on the top sections represent the sounding positions.](image-url)
Figure 4.2 Model sections and resistivity ratios of independent and time-lapse inversion results using the dense acquisition layout. Black dots on the top sections represent the sounding positions.

I performed both independent and time-lapse inversion. The synthetic example shows that the 3D sensitivity of the TEM measurements allows us to retrieve time-lapse changes with an acquisition layout that does not entirely cover the conductive anomaly. However, significantly better results are achieved with increased data coverage. Furthermore, compared to an independent inversion, the time-lapse inversion scheme significantly improves the retrieval of time-lapse changes, with sharper anomaly boundaries and a more homogenous background.

4.3 Field example

The new inversion algorithm is applied to a field example, consisting of two TEM datasets collected at a geothermal power plant with a one-year interval, to build a baseline model. Two datasets have a different number of soundings, due to the different amount of inductive coupling evidenced by the local infrastructures. The datasets have a gap in the domain of interest after coupling removal. The independent TEM inversion result was verified by a 2D inversion result of ERT data acquired (Fig. 4.3). Due to the poor data coverage, the time-lapse inversion results were investigated by varying the weight of the time-lapse constraints on the inversion objective function to better interpret the focusing effect of the asymmetric minimum support norm (Fig. 4.4). All inversions carried out with the new time-lapse algorithm gave much more focused time-lapse changes, when compared to independent inversions.
Results, Paper 2: Three-dimensional time-lapse inversion of transient electromagnetic data, with an application at an Icelandic geothermal site

Figure 4.3. SW-NE profiles of 2020 3D TEM inversion and 2D ERT inversion, where the datasets were both collected in 2020. Black dots on the top sections represent the TEM sounding positions’ projection.

Figure 4.4 SW-NE inversion model sections for 2019 data (left column) and 2020 data (middle column), as well as 2020/2019 resistivity ratios (right column). Rows from top to bottom show time-lapse inversions with increasing $\alpha$ values and independent inversions. Black dots on the top sections represent the TEM sounding positions’ projection.
4.4 Conclusion

I have developed a new algorithm to carry out time-lapse inversion of TEM data with three features designed for improving applicability and robustness, i.e.: (1) a 3D octree-based forward and sensitivity computation, which allows the algorithm to be also applied when the sounding distances in the acquisition layout are larger than the horizontal extension of background resistivity variations and time-lapse changes; (2) a multi-mesh approach for forward and inversion computations, such that the same inversion mesh is applicable even in the presence of variations in the acquisition layouts; (3) a focusing of time-lapse changes by the use of the asymmetric minimum support norm.

I tested the new algorithm on both synthetic and field data. The study showed that the implementation allows to handle a dataset with different acquisition layouts and to study the data influence on the inversion results in detail, considerably increasing the robustness of the interpretation. This new implementation will help increase the applicability of the TEM method in time-lapse monitoring and in applications in which data coverage is limited by the presence of infrastructures and the sounding location cannot be repeated exactly.
5. Results, Paper 3: 3D inversion of an integrated ground-based and waterborne TEM survey

5.1 Introduction

Nowadays, many TEM systems are developed for improved manoeuver flexibility and acquisition efficiency (Auken et al., 2019, Aigner et al., 2021, Sørense and Auken, 2004), which enables us to do measurements in different environments -- airborne, ground-based, or waterborne (Christensen and Halkjær, 2014, Maurya et al., 2020, Christiansen et al., 2021). An integrated survey, a combination of different systems, can in some cases be a valuable solution as different systems may offer a superior resolution by focusing at different depths or various areas, according to the geologic settings. For instance, combining airborne and ground-based measuring is helpful to obtain a full resolution in both shallow and deep regions since the depth of investigation (DOI) (Christiansen and Auken, 2012) depends on instrument characteristics such as the loop size and the current amplitude. In addition, when the focal area covers both onshore and offshore landscapes (Bücker et al., 2021), either airborne survey is adopted, or a combination of ground-based and waterborne measurement is required. In this work, I only study the case of the latter, an integrated survey with ground-based and waterborne systems in coastal area. However, it should be noted that the presented solution is ready to be applied for general integrated surveys on other environmental or engineering problems.

Two problems are prominent to invert TEM data in coastal surveys: i) the strong conductivity contrast between seawater and/or lithologies affected by high salinity and freshwater lithologies in a coastal environment results in strong 2D and 3D effects in the data; ii) the utilized ground-based and waterborne (or airborne) TEM systems result in different footprints, which makes it complicated to combine the inversion model space and incorporate the 2D/3D effects present in the boundary of different geological settings. Thus, a standard 1D inversion framework cannot resolve sub-surface structures correctly. To address the issues of multi-dimensional effects that exist in the data, and the merging of inversion between different TEM systems, I adopt a 3D multi-mesh inversion scheme (Xiao et al., 2020). This approach makes better use of TEM data above the 2D/3D anomalies, and obtains a consistent subsurface resistivity model with the data collected by multiple systems.

5.1.1 Two TEM systems

The research was based on of onshore and offshore data collected at a contaminated coastal area. The onshore data was collected by the tTEM (Auken et al., 2019) and the offshore data was
collected by the FloaTEM (Christiansen et al., 2021). The data along the coast was highly underfitting after a standard 1D spatially constrained inversion (Viezzoli et al., 2009). Since the measurements are conducted in a coastal area with highly conductive subsurface, only the high moment (Sørense and Auken, 2004) pulse is used for both systems. Besides, to increase the shallow depth of investigation due to the slow diffusion at the surface saline water, the number of transmitter coil turns in the FloaTEM system was increased to three. The FloaTEM system is operated in an aquatic environment, the conductivity is measured and echo-sounder data is obtained automatically with depth information to the river/lake/sea bed, which serves as prior information for the starting model of inversions.

5.1.2 Mesh design

Figure 5.1 Illustration of the octree mesh refinement for a three-layered (1/4/100 Ωm) model with thickness of 4 m and 28m, respectively. a) shows a normal halfspace meshing while b) show a refined mesh for highly conductive and thin top-layer. c) shows a close-up of the mesh in a) at the end of the fine mesh, laterally, and d) shows a similar close-up just below the transmitter.
TEM methods are highly sensitive to conductors. When a survey is carried out on saline water, the eddy currents diffuse horizontally for a long time instead of moving downwards, which results in a shallow vertical resolution. Hence, for a measurement on saline water, the mesh elements in the seawater layer must be refined to describe both rapid field variations near the system. At the same time, they must also cover large horizontal footprints for the lateral extension of the eddy currents with time. Aiming for a numerical accuracy in the forward response of 4%, these models, with highly conductive overburden, require a dense refinement of up to hundreds of meters (Fig. 5.1). As a consequence, it will increase the number of unknowns dramatically and thus increase the computational cost. Besides, since the tTEM and FloaTEM systems have different configurations, the mesh densities are designed separately to have as few unknowns as possible while meeting the accuracy standard.

5.2 Numerical experiments

To demonstrate the importance of using 3D (or 2.5D) simulation, I designed a three-layer 3D synthetic model to simulate a coastal environment (Fig. 5.2). Selecting a profile (the solid red line), I computed the 1D/3D response and calculated the difference between responses. The difference (Fig. 5.2-a) increases when the sounding location is closer to the seawater-land interface and reaches the maximum, approximately 400%, right above the interface, where strong 2D effects are present. Additionally, it shows around a 10% response difference from the 1D response (a combination of 3D effects and numerical error) when the sounding is 40 m away from the interface.

In the 1D inversion (Fig. 5.3), it is noticed that the FloaTEM soundings close to the transition area have the poorest fits, whereas the tTEM soundings have a satisfying misfit, despite that the 1D modeling error not being minor. The 3D inversion, however, not only results in a lower total misfit, but also produces a similar data agreement for the land-based and waterborne data. As for the result, I observe that 1D inversion cannot recover the water depth and produce a conductive pant leg in the high-resistivity layer. In contrast, the 3D inversion recovers fairly accurate resistivities and layer boundaries without the pant leg. Overall, the modeling and inversions of this synthetic model offer us a new perspective to see the multi-dimensional effects in the TEM surveys across a shoreline.
Figure 5.2 The response difference of 1D and 3D forward modeling on a coastal model: 

- a) Response difference between 1D forward and 3D forward against 3D response; 
- b) Coastal model illustration, where the iTEM and FloaTEM soundings are symbolized by black and grey dots, respectively; 
- c) Measurement layout; 
- d) iTEM (black) and FloaTEM (gray) measurement layout; 
- d) Response curves of selected soundings for both iTEM (solid lines) and FloaTEM (dashed lines) in 1D (blue) and 3D (red).
5.3 Field example

The coastal survey was conducted to pinpoint the interface between the sand unit and the till to identify pathways for the pollution. The FloaTEM data collected near the interface could not be fitted by a 1D inversion, however the 3D inversion performed better with much lower data misfits. Besides, even though the 1D inversion presents a lower (1D) misfit for the tTEM data, the recovered
model contains errors likely driven by 3D effects. For instance, the 1D response has an average of ~72% difference from 3D response. As for the model retrieval (Fig. 5.4), I evaluate it in three aspects: i) Both the 1D model and the 3D model indicate a highly conductive water layer (0.3-0.5 Ωm) with similar resolution, which is well-aligned with the measured value of 0.4 Ωm. ii) I look into the match against the available boreholes. The transition to the more resistive till layer (~20 Ωm) is only aligned with the reported sand-clay interface from boreholes in the 3D result. In particular, the thickness of the saline sand layer gradually increases from the shoreline to the sea. The 1D results show that the interface is 2-3 meters shallower than what is observed in the boreholes. iii) I calculate the formation factor of the 1D/3D inversion models within the range of sand layer referring to borehole, which is saturated with saline pore-water. Following Archie’s law (Archie, 1942) and dividing the sediment resistivity by the seawater resistivity, we find out that 1D inversion results in a formation factor of 20, while 3D inversion predicts the value as ~4-5. Published lab measurements of saline sand rock properties (Frings et al., 2011; Kadhim et al., 2013), indicate that sand units with a cementation exponent of 1.5, a tortuosity factor of 1, and a porosity of 0.4, the formation factor should be approximately 4. Therefore, the 3D result gives a more reasonable estimate on the resistivity.
5.4 Conclusion

The study investigated the 2D and 3D effects present in coastal-near TEM applications, where data was collected with both on-shore and off-shore measurements. The FloaTEM data along the shoreline was highly under-fitting after a 1D inversion. I addressed this issue by applying the classic
Results, Paper 3: 3D inversion of an integrated ground-based and waterborne TEM survey

3D inversion scheme developed in Paper I. This scheme entails: i) a 3D octree-based modeling allows an accurate simulation of electromagnetic fields in a multi-dimensional environment with strong conductivity contrast; ii) a multi-mesh approach provides the flexibility to invert datasets collected with different system configurations simultaneously through one inversion mesh, while maintaining different meshes for the individual soundings for forward modeling and Jacobian computation. The saline environment requires a particularly refined mesh to explain the eddy currents’ duration.

Based on the synthetic model and field example results, I conclude that a 3D inversion enables more accurate information about the subsurface structures for these highly 2D/3D affected data and at a much higher computation cost.
6. Conclusion and outlook

6.1 Conclusion

This thesis presents a general solution for 3D inversion of TEM data. The study firstly developed a 3D and 2.5D inversion scheme, using the octree-based finite element method for modeling and the multi-mesh approach for inversion. Based on this, I investigated the 3D time-lapse inversion of TEM data using the minimum support norm, which generates focused temporal variations. Finally, I demonstrated that our code can handle an integrated survey dataset measured by land and waterborne systems in a coastal area, where the existing strong 3D effects could not be interpreted by 1D inversion. The results are organized into three papers, summarized below.

In Paper I, a fast 3D and 2.5D inversion scheme of TEM data are presented. The modeling of two implementations uses an octree-based finite element method, which reduces the computational cost for forward modeling and Jacobian calculation by local refinement only in the domain of interest. Compared to similar tetrahedral implementations, this 3D modeling code is approximately three times faster and uses only 1/3 of the memory. Based on this, I further built a 2.5D inversion scheme with a mirror approach, which improves the inversion efficiency in terms of memory cost and computing time by another factor of two. In particular, the model space of 3D inversion is a regular structured voxel mesh, while in 2D the model spaces are sections that follow the acquisition lines. The multi-mesh approach is another highlight of my implementations, where the forward and Jacobian mesh of each sounding is linked with the entire inversion model space through an interpolation function. The method successfully avoids dense inversion mesh refinements and provides a flexible way to enforce spatial constraints and incorporate prior information.

I have demonstrated the algorithms on both synthetic 3D valley structure and a field example, and compared 3D, 2.5D, and 1D inversions in terms of section results and computational expense. The 3D inversion result showed substantial differences from the 1D inversion, while the resolving power of 2.5D inversion is expectedly in between but uses fewer resources. When choosing 3D or 2.5D inversion, I suggest one should first consider the geological setting and the data collection layout and then make the compromise between model resolution and computational cost.

In Paper II, I proposed a 3D time-lapse inversion algorithm of TEM data using the asymmetric minimum support norm. In practice, it is challenging to carry out TEM surveys at the same position or covering areas with infrastructure underground. Therefore, I used the multi-mesh
approach to invert the whole survey area regardless of specific sounding locations and include 3D sensitivity to keep general footprints for time-lapse inversion. Furthermore, the minimum support norm allows us to take the smoothness of temporal variation into consideration in the objective function.

I demonstrated the validity of the implementations through two synthetic models and a field case. In the synthetic experiments, I investigated the influence of data density. I showed that the time-lapse inversion scheme could deliver much more focused changes with good retrieval of model resistivity and shape delineation, compared to independent inversions. The field example, with two TEM datasets collected in 2019 and 2020 close to a geothermal plant, showed that the 3D sensitivity allows good imaging of the subsurface resistivity distribution despite the poor data coverage, as evidenced by its agreement with an ERT profile acquired at the site. Additionally, by tuning the asymmetric minimum support norm, I studied the focusing effect of the time-lapse inversions and identified the likely data-driven model changes between 2019 and 2020.

In Paper III, I investigated the 2D and 3D effects that are present in TEM applications in a coastal environment, where data is collected by both on-shore and off-shore surveys. The developed algorithms from Paper I were used for two reasons: i) the 3D octree-based modeling simulates electromagnetic fields more accurately in a multi-dimensional environment with strong conductivity contrast; ii) the multi-mesh approach inverts datasets collected with different systems simultaneously through one inversion mesh, while maintaining local forward meshes with different model discretization according to the configuration for individual soundings.

In the synthetic coastal model, I showed that there are significant difference between the forward responses calculated by a 1D and 3D forward code. The comparison of inversion results using 1D and 3D solutions further demonstrates that the 3D inversion reproduced the model more accurately with no particular artifacts and a low data misfit. Finally, I studied the 1D and 3D inversion results of an actual coastal survey, using knowledge gained through the synthetic examples. The 3D inversion yielded much lower data misfits in the interface area than 1D inversion. Moreover, the 3D inversion results were in better agreement with previously published petrophysical data and they more accurately characterized the particular transition from sand to clay verified by the existing borehole data.

Overall, the implementations of 3D inversion have advanced the interpretation of TEM data with improved efficiency. The classic 3D inversion offers some versatility as it can be applied easily
to various platforms or surveys using different system configurations. The time-lapse inversion will help in increasing the applicability of TEM method in time-lapse monitoring. Based on the study of synthetic examples and field cases, I have demonstrated the utility of the developed 3D inversion schemes. I expect a routine application for TEM explorations in the near future.

6.2 Outlook

6.2.1 3D inversion for production size

Although this thesis provides significant work towards realizing an automatic full-scale 3D inversion, there is plenty of room for future work. Firstly, rigorous GPS recording of transmitter and receiver location facilitates following data processing, especially for offset TEM systems, since the configuration setting strongly impacts the 3D modeling response. Then, subsequent robust data processing would guarantee the quality of input data and therefore improve inversion convergence.

For large-scale inversions, model updates are a cumbersome process. Thus, splitting the inversion area into several regions and carrying out inversion in blocks can be an option, such that at least three benefits are gained: i) minimizing the matrix to a reasonable size and less ill-posed, so the equation is less demanding for the solver; ii) performing the parallelization on different platforms; iii) setting up a proper starting model and applying spatial constraints.

The calculation of the forward response and Jacobian is the most time-consuming section during inversion. An innovative mesh-free method would be revolutionary, for example, machine learning to predict the 3D forward response and Jacobian calculation with physical constraints.

6.2.2 Improve mesh generation for cases in extreme conditions

Currently, a general mesh is set up for all the cases. However, in some cases such as the examples presented in Paper 3, where a highly conductive body presents in the top surface, dense refinement is required to describe and capture field variations. Thus, a residual-based posteriori error estimator and more robust adaptive meshing strategies for problem-adapted discretization should be taken into account for further improvement.

6.2.3 Differentiate effects from induced polarization (IP), 3D bodies, and a mix of the two

Although the majority of TEM inversion approaches focus solely on resistivity, in many cases data are influenced by IP phenomena (Grombacher et al., 2021). Even though it is more difficult to account for IP effects, such data contains additional information of petro-physical and hydrological
properties of the subsurface. Due to the non-uniqueness of inversion in nature, it can happen that the inversion may treat the IP information as 3D effects, or vice versa. Therefore, a greater understanding of the basic theory of IP in different geological settings, from 1D to 3D, is needed. Simultaneously, the instrument should record the responses more precisely, with more advanced noise suppression. Unravelling the exact nature of IP and 3D effects, and modeling them accurately will surely provide a wealth of information to better tackle hydrological problems.


Rosas-Carbajal, M., Linde, N., Peacock, J., Zyserman, F.I., Kalscheuer, T. & Thiel, S., 2015. Probabilistic 3-D time-lapse inversion of magnetotelluric data: application to an enhanced...


Appendix 1: Paper I

Title: Fast 2.5D and 3D inversion of transient electromagnetic surveys using the octree-based finite element method

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Fast 2.5D and 3D Inversion of transient electromagnetic surveys using the octree-based finite element method

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Abstract

Two efficient implementations of three-dimensional (3D) and two-and-a-half-dimensional (2.5D) modeling and inversion are presented to be applicable to large-scale transient electromagnetic method (TEM) explorations. The key novel features are: (1) forward response and Jacobian calculations are implemented using the octree-based finite element method, (2) a mirror approach is used to build a 2.5D inversion scheme for further efficiency, and (3) a flexible link between the forward mesh and inversion model is applied on both 3D and 2.5D schemes based on the voxel formulation. We compare the performance of the new implementations with 3D modeling using tetrahedral meshes, with respect to speed and memory requirements. The 3D octree algorithm requires less than 1/3 of running time compared with a 3D tetrahedral scheme for equivalent accuracy. The 2.5D octree algorithm further speeds up the process by reducing the running time by another factor of two. The inversion uses the Levenberg-Marquart approach minimizing the least squares criterion.
of the objective function. We demonstrate the utility of our inversion approach on a synthetic example and a field example. In the synthetic example, the 3D octree inversion result showed superior resolution of a 3D anomaly compared to a one-dimensional (1D) result, while the 2.5D inversion result was, expectedly, between the 1D and 3D results, but with favorable computing expenses compared to the full 3D solution. The field dataset contained 200 soundings and we performed a 3D inversion on the full survey. A 24-sounding section was then selected for the 2.5D inversion. The 2.5D inversion result shows similar resistivity features as the 3D inversion result at the selected profile. Hence, we conclude that the presented implementations are capable of handling fairly large TEM surveys on modern computational platforms. This could be smaller subsets of production size surveys where 2D and 3D effects are pronounced.

**Introduction**

Over the past decades, TEM modeling and inversion has developed significantly (Auken *et al.*, 2017), supplemented by a continued improvement in instrumentation and a steady growth in computing capabilities. The common industry routine for TEM inversion is to perform either unconstrained layered inversions (Brodie and Fisher, 2008) or constrained 1D inversions (Auken and Christiansen, 2004, Vignoli *et al.*, 2015, Viezzoli *et al.*, 2008). Also, various forms of rapid approximations (Christensen, 2016, Fullagar *et al.*, 2015) or combinations with accurate and approximate solutions (Christiansen *et al.*, 2016) are often utilized. The constrained solutions provide a spatially smooth model, whereas the inherent limitations in the 1D assumption make it challenging or impossible for them to accurately describe complex 2D or 3D geological structures. These heterogeneities increase the complexity of eddy current patterns, which are commonly found in natural circumstances making a 1D assumption non-applicable such as mineral exploration (Yang and Oldenburg, 2012) and even in complicated aquifer structures (Maurya *et al.*, 2020). In the last
two decades, various numerical 3D TEM modeling algorithms have been presented using the integral equation method (Zhdanov et al., 2006), the finite difference method (Commer et al., 2015), the finite volume (FV) method (Haber et al., 2002) and the finite element (FE) method (Um et al., 2010). The 3D inversion of TEM data is a massive computational challenge. Firstly, the time-domain data from one receiver contains tens of time gates spanning several decades in time, and the forward problems needs to be solved twice for each iteration during the inversion, one time for the forward and the other for the Jacobian. Secondly, hundreds of thousands of TEM soundings are commonly collected in one survey. In recent years, a number of strategies are reported in the literature in order to solve the 3D TEM inversion problem more effectively. Cox et al. (2012) introduces the ‘footprint’ concept in the time domain data, where only elements close to the system with significant data impact are considered for sensitivity calculation; Oldenburg et al. (2013) demonstrates that the performance of direct solvers outrun traditional iterative solvers; Yang et al. (2013) uses local meshes to decompose the inversion domain into small problems. Even so, it remains a computationally expensive task to realize a large-scale multi-dimensional time-domain inversion for TEM surveys. Here, we present a 3D inversion scheme and a 2.5D inversion scheme through octree finite element modeling, and a multi-mesh approach, which decomposes the survey domain using a local mesh at each sounding for forward calculation and a full-survey model mesh for inversion. We will refer this strategy as the domain decomposition.

The computation of the TEM forward response and Jacobian calculation accounts for the bulk of the time cost in a 2D and 3D inversion scheme, and we therefore seek to achieve computational savings on this process through non-uniform meshing. Local refinement only adapted in the regions where fine resolution is needed to represent complex geometry features and capture large field variations, such as areas close to the transmitter and receiver or places including a conductivity discontinuity, can effectively reduce the number of unknowns in the linear system to be solved.
(Horesh and Haber, 2011). Compared to unstructured grids adopted to 3D EM modeling programs using either the FE method (Um, 2011, Ansari and Farquharson, 2014, Schwarzbach et al., 2011) or the FV solution (Jahandari and Farquharson, 2014), octree meshes are easier to construct and the resulting system is often better conditioned and the number of cells remains reasonable for numerical computing (McMillan et al., 2018). The earliest application in the EM field using octree meshes was done by Haber and Heldmann (2007), who demonstrated the advantage of octree discretization using the FV for Maxwell’s equations. Grayver and Kolev (2015) also showed that considerable computational savings can be achieved on magnetotelluric inversion problems. Haber and Schwarzbach (2014) did a finite volume solution for TEM on octree meshes, but to our knowledge, there is no TEM inversion solution using octree-meshes with the finite element method. Furthermore, we have not, so far, seen any direct performance comparison over different implementations using different non-uniform meshes. We therefore present two octree-based solutions, and a performance comparison with a tetrahedral-based solution in this paper.

2.5D inversion was once a preferred solution, when the computing power was less than today (Allers et al., 1994, Mitsuhata et al., 2002) and was challenging to complete a 3D inversion for multiple soundings, especially for time-domain datasets. Traditionally, the 2.5D algorithms were based on the 2.5D formulations of Maxwell’s equations (Yu and Haber, 2012, Wilson et al., 2006, Abubakar et al., 2008), which compute the response of a 3D source from a 2D geoelectric model using different numerical methods. In this study, we followed a different approach, easily generalized to any problem in which the 3D solution is available. Specifically, we developed a 2.5D algorithm based on a 3D modeling mesh halved through the 2D xz plane passing through receiver and transmitter (i.e. along the moving direction for towed or airborne systems). Assumptions on the symmetry of the modeling, in terms of source and boundary conditions, allow us to almost halve the
degrees of freedom (DoF) in the linear system for both forward responses and Jacobian calculations, and thereby achieve a 2 times speed-up in our 2.5D inversion compared to the complete 3D solution.

Decoupling between the modeling mesh and inversion mesh combined with the domain decomposition strategy offers flexibility to design a local modeling mesh for each sounding and a regional inversion mesh for the survey. Madsen *et al.* (2020) uses two separate meshes for forward modeling and inversion to solve the direct current and induced polarization problem. Bo *et al.* (2021) also applies this decoupling method and uses two tetrahedral meshes with different densities for forward modeling and Jacobian calculation to accelerate a 3D TEM inversion. In this study, we apply the decoupling of the inversion mesh and the forward modeling mesh to octree-based forward modeling. This enables the utilization of a regular inversion model grid while maintaining the advantages of non-uniform nature of the octree mesh in the forward modeling.

The goal of this paper is to present two highly efficient TEM inversion schemes that can be applied to any TEM system, airborne, land-based, or on water. The inversion schemes are using the octree-based finite element method for forward modeling with the second order backward Euler method (Butcher and Goodwin, 2008): the multi-mesh approach with domain decomposition for inversion, and a mirror approach for the 2.5D inversion. In the next section, methodology, we describe the finite element discretization using octree meshes for the TEM forward and Jacobian calculation, as well as a brief description of our inversion scheme. Then under results, we verify the effectiveness of the algorithm through two numerical experiments using the towed transient electromagnetic (tTEM) system (Auken *et al.*, 2019). The first example presents 3D and 2.5D forward responses of both resistive and conductive half-space models against 1D responses. Following this, we present a performance analysis comparing against 3D tetrahedral results. The second example shows synthetic
inversion results of a 3D valley model from 1D, 2.5D and 3D algorithms. Finally, we present inversions of field data that demonstrate the advantages of our approaches.

Methodology

Forward Modeling

Forward problem formulation

Assuming that the media is linear, isotropic and homogeneous and electrical properties are independent on time, pressure and temperature, the time-domain forward problem allows the derivation from quasi-static Maxwell's equations and can be formulated as a diffusion equation in terms of the electrical field as a function of space, \( \mathbf{r} \), and time, \( t \), \( \mathbf{e}(\mathbf{r}, t) \):

\[
\nabla \times \nabla \times \mathbf{e}(\mathbf{r}, t) + \mu \sigma(\mathbf{r}) \frac{\partial \mathbf{e}(\mathbf{r}, t)}{\partial t} = - \frac{\partial \mathbf{j}_s(t)}{\partial t} \tag{1}
\]

where \( \mathbf{r} \in \Omega, \ t \in (0,T) \), \( \mathbf{j}_s \) is the electric current density, \( \sigma \) the electric conductivity, and \( \mu \) the magnetic permeability. The initial conditions are given as:

\[
\mathbf{e}(\mathbf{r}, 0) = \mathbf{e}_0(\mathbf{r}) \tag{2}
\]

When the modeling domain is big enough and boundary effects are negligible, we can apply the homogeneous Dirichlet boundary condition:

\[
\mathbf{e}(\mathbf{r}_\partial, t) = 0 \tag{3}
\]

The initial boundary value problem can be discretized in time using the second order backward Euler method (Butcher and Goodwin, 2008):

\[
\frac{de(t)}{dt} = - \frac{1}{2\Delta t} [3e(t) - 4e(t - \Delta t) + e(t - 2\Delta t)] \tag{4}
\]
and spatially using the vector FE method (Jin, 2015), for field $\mathbf{e}$ at any position:

$$\mathbf{e} = \sum_{i=1}^{12} N_i e_i$$

(5)

where $e_i$ denotes the tangential field along the $i$th edge and $N_i$ are the vector interpolation functions (i.e. shape functions) at the edges.

Combining the equations of all the elements at all time gates, a linear sparse system of equations is therefore yielded as

$$\mathbf{K} \mathbf{e}(\mathbf{r}, t) = \mathbf{b}$$

(6)

where the right-hand side $\mathbf{b}$ is a source term, and $\mathbf{K}$ is a symmetric stiffness matrix:

$$\mathbf{K} = \begin{pmatrix}
A^1 & A^2 & A^3 \\
B^2 & A^2 & A^3 \\
C^3 & B^3 & A^3 \\
\vdots & \vdots & \vdots \\
C^{n_t - 2} & B^{n_t - 2} & A^{n_t - 2} \\
C^{n_t - 1} & B^{n_t - 1} & A^{n_t - 1} \\
C^{n_t} & B^{n_t} & A^{n_t}
\end{pmatrix}$$

(7)

where $n_t$ denotes the number of time steps, and $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ at $k$th element are

$$A^k = 3Q^k + 2\Delta t S^k$$

(8)

$$B^k = -4Q^k$$

(9)

$$C^k = Q^k$$

(10)

$$Q^k = \iiint \sigma^k N^k \cdot N^k dV^k$$

(11)

$$S^k = \iiint \frac{1}{\mu} (\nabla \times N^k) \cdot (\nabla \times N^k) dV^k$$

(12)
Since the problem is designed for local meshes (Yang et al., 2013), the matrix associated with each time gate is quite small, and in this case direct solvers are favorable as the matrix factorization can be shared when the time steps are in the same length (Oldenburg et al., 2013).

The time derivative of the vertical magnetic induction, i.e. the simulated system response \( d_{sys} \), will be obtained from the electrical field \( \mathbf{e} \) through Faraday’s law, followed by multiplication of the interpolation matrix \( \mathbf{L} \):

\[
\begin{align*}
\mathbf{d}_{sys} &= \mathbf{Le} = \mathbf{L}_t \mathbf{L}_s \mathbf{e} \\
\end{align*}
\]

\( \mathbf{L}_t \) denotes the linear interpolation matrix in time domain according to the actual time gates, and \( \mathbf{L}_s \) represents the interpolation matrix in space domain at the location of receivers.

**Hanging nodes**

Octree mesh generation is a spatial partition topology which recursively subdivides a cell into eight blocks (see Figure 1) until a stopping criterion is met (Frey and George, 2007); for example, in our case, the criterion is the volume of the cell. Firstly, we divide the model uniformly in all directions, and set the level of these ancestor cells as zero. Based on this basic skeleton, we set several nested regions from the model margin to the center where the transmitter is located. Elements in each region are refined to different levels, with the refinement increasing from the outer regions to the inner ones. The level, or subdivision times, of each cell is stored as a tree structure. The more refined, the higher level the cell will be. One stand-out feature of mesh gradation management is that the level difference between adjacent cells may not exceed 1. And hanging nodes appear when two adjacent cells do not share the same level (Legrain et al., 2011). Two types of hanging nodes can be noted as shown in the Figure 1: hanging nodes on the edges and hanging nodes on the faces (Grayver, 2015), which require special treatment when we compose the system matrix.
Appendix 1: Paper I

Figure 1. Octree mesh illustration, where the filled circles denote hanging nodes on edges and the open circles denote hanging nodes on faces

We need to handle the added parameters from the edges associated to hanging nodes, to ensure the compatibility of the finite element approximation and the continuity of the finite element fields even on the interface. Our solution is inspired by the work of Bielak et al. (2005), who selects the added parameters and treats them using a properly weighted constraint during the stiffness matrix assembly process in equation (7).

Based on the classic FE solution $\mathbf{e}$ as equation (5), the field definition in the octree-based FE is extended as

$$
\mathbf{e} = \sum_{i_1=1}^{12-n_h} \mathbf{N}_{i_1} e_{i_1} + \sum_{i_2=1}^{n_h} \mathbf{N}_{i_2} \left( \sum_{j=1}^{n_{ed}} d_{j}^{i_2} \cdot \phi_j^{i_2} \right)
$$

where $n_h$ represents the number of edges with hanging nodes, $d_j^{i_2}$ are fields on the edges of lower-level master cell that associated to the added parameters, $\phi_j^{i_2}$ denotes the enrichment function applied on the added parameters, and $n_{ed}$ is the number of related edges. Given the property of edge element and all the elements are regular, we define the enrichment function as
\[
\phi^{iz}_j = \begin{cases} 
1 & \text{on the edge, } n_{ed} = 1 \\
(1/2,1/2) & \text{on the face, } n_{ed} = 2 
\end{cases}
\]  

(15)

Note that when the hanging node is on the face, two parallel edges on the face share the contribution equally, as the field varies linearly in the normal direction to the vector. In general, the main idea of our approach is to redefine the shape function of edges at the hanging nodes by linear combinations of the previous shape functions, similarly to Grayver (2015).

Therefore, the fields at the edges associated with hanging nodes can be expressed by the edges from master cells, and the dimension size of the stiffness matrix is always smaller than the number of physical edges.

2.5D solution: the mirror approach

During a TEM survey, it is common that the transmitter, either in offset configuration or in a central loop configuration, is geometrically symmetric. Here we take the tTEM system (Auken et al., 2019) as an example to illustrate the principle of the mirror approach which is the base of our 2.5D implementation. We assume that the resistivity model has variations in the x and z directions and is symmetric in y direction. The x-direction is defined by a line passing through the center of the transmitter and the receiver. In this condition, the magnetic fields on the xy plane are symmetric, with values mirrored from the left side to the right side of the xz plane, and has no y component along the xz plane, because of the system and 2D model symmetry. No y component of the magnetic field in the xz plane means that the electric field has zero x and z components on the plane, because of Faradays law. These are exactly the Dirichlet boundary condition we set in the 3D modeling on the outer faces of the forward mesh.
Figure 2. Mirror approach illustration, where the red rectangle symbolizes the transmitter of TEM system (the size of the transmitter is 4m × 2m) and the red dot symbolizes a dipole receiver. a) Magnetic field on the bisector plane; b) Octree forward mesh in the 2.5D inversion.

Consequently, if we remove a flank of the original 3D model according to the bisector of the system (see Figure 2) as well as the transmitter, and we apply the Dirichlet boundary condition on all mesh outer faces including the mirroring xz plane, we will obtain a forward modeling equivalent to the full problem in which the resistivity is defined in the entire mesh, left and right of the xz plane mirroring plane. Defining the model in the half mesh and using a resistivity model in the half mesh that does not change along the y direction, we obtain a pseudo 2.5D solution to the problem, using a 3D implementation with proper source definition and boundary conditions.

An analogous point of view is the one that looks at the stiffness matrix of the problem. If we take equation (6) with a size of 4*4 matrix (4 unknowns) as an example, the original 3D system matrix would be:
\[
K_{11}e_1 + K_{12}e_2 + K_{13}e_3 + K_{14}e_4 = b_1 \\
K_{21}e_1 + K_{22}e_2 + K_{23}e_3 + K_{24}e_4 = b_2 \\
K_{31}e_1 + K_{32}e_2 + K_{33}e_3 + K_{34}e_4 = b_3 \\
K_{41}e_1 + K_{42}e_2 + K_{43}e_3 + K_{44}e_4 = b_4
\]  

(16)

With the symmetric conditions of fields and the information of cells from the mirror approach, namely:

\[
e_1 = e_2 \\
e_3 = e_4 \\
K_{i1} = K_{i2}, \ (i \in 1,4) \\
K_{i3} = K_{i4}, \ (i \in 1,4)
\]

and equation (16) in the half mesh will be

\[
K_{11}e_1 + K_{13}e_3 = b_1/2 \\
K_{21}e_1 + K_{23}e_3 = b_2/2
\]

(18)

In this manner, half of the cells can be saved from computation without the accuracy being affected. To achieve this, we simply need to use only half of the transmitter as the source input, since the entire system still follows the same physical law on half of the 3D forward mesh. Consequently, this is de-facto mathematical optimization, where the 2.5D problem is characterized as a 3D source on a mirrored model using a 3D octree mesh.

**Jacobian calculation**

The Jacobian is the matrix of sensitivities with size \(N_d\) (the number of data) by \(N_e\) (the number of elements), and each element in the matrix reflects the contribution to the response of conductivity at this point (Christensen, 2014). We calculate the Jacobian in an explicit backward stepping scheme (Börner, 2010) through adjoint forward modeling. This methodology is applied to both the 3D and 2.5D inversion, since we calculate the Jacobian in the octree mesh firstly and then interpolate to the inversion model mesh, as illustrated in Figure 3.
Let us define the Jacobian matrix for each step, \( n \), as:

\[
J^n = \frac{\partial d^n_{sys}}{\partial m}
\]  

(19)

The derivative of equation (6) with respect to model parameters \( m \) will be:

\[
\frac{\partial e}{\partial m} = K^{-1}G
\]  

(20)

where

\[
G = -\frac{\partial K}{\partial m} e
\]  

(21)

Combing the interpolation matrix \( L \) in equation (13), the Jacobian matrix is derived to:

\[
J^T = G^T K^{-T} L^T
\]  

(22)

If we define a vector \( V = K^{-T} L^T \), then we have the adjoint modeling equation:

\[
K^TV = L^T
\]  

(23)

Solving the equation (23) through the backward propagation from the last time step, we have the temporary vector \( V \). We thus obtain the Jacobian through the relation:

\[
J^T = G^T V.
\]  

(24)

**Multi-mesh approach**

The definition of model parameters and forward meshes is obtained by adapting the approach of Christensen et al. (2017) and Madsen et al. (2020) with domain decomposition. Domain decomposition breaks the full-survey forward problem into small tasks at the soundings, minimizing the computing expenses without sacrificing modeling accuracy. Specifically, we used two sets of
separate octree meshes for forward modeling and Jacobian calculation at each transmitter, where we compute the forward response from equation (6) and the Jacobian from equation (24) using the adjoint modeling method.

We designed one voxel mesh for the full-scale model update in the inversion, where the model parameters are defined in two different ways for 3D and 2.5D inversions (see Figure 3). In 3D, the parameters are determined on the nodes of a 3D regular structured mesh, with uniform node spacing in $x$ and $y$ direction and log-increasing node spacing in $z$ direction. In 2.5D, the parameters are specified on the nodes of 2D sections, which follow the acquisition lines, with uniform node spacing along lines and log-increasing vertical spacing. The inversion model parameters are linked to the center of the forward mesh elements through interpolation with an inverse distance function:

$$\mathbf{m} = f(\mathbf{M}) = \mathbf{F} \cdot \mathbf{M}$$  \hspace{1cm} (25)

where the vector $\mathbf{m}$ represents the values of model parameters in the forward mesh elements, and $\mathbf{M}$ holds the resistivity values at the voxel nodes in the inversion mesh. $\mathbf{F}$ is an interpolation matrix with weights, which merely rely on the relative distances between the forward mesh elements with the model nodes used for interpolation.

Since the interpolation function is a linear operation, and applying the chain rule for derivatives, so that

$$\frac{\partial \mathbf{d}}{\partial \mathbf{M}_i} = \sum_j \frac{\partial \mathbf{d}}{\partial \mathbf{m}_j} \frac{\partial \mathbf{m}_j}{\partial \mathbf{M}_i} = \sum_j \frac{\partial \mathbf{d}}{\partial \mathbf{m}_j} F_{j,i}$$  \hspace{1cm} (26)

we therefore write the Jacobian on the model mesh mapping from Jacobian mesh as:

$$\mathbf{J}_M = \mathbf{J}_m \cdot \mathbf{F}^T$$  \hspace{1cm} (27)
where the $J_M$ is the Jacobian of the inversion model space, the voxel mesh, and $J_m$ is the Jacobian computed in the forward mesh through equation (24).

![Diagram](image)

*Figure 3. Relation between forward/Jacobian mesh (green) and inversion model mesh (orange). a) 2.5D inversion: 3D octree mesh and 2D inversion section. b) 3D inversion: 3D octree mesh and 3D inversion mesh.*

This multi-mesh approach, with model parameters defined on the regular meshes and forward/Jacobian computations carried out on octree meshes, one for each transmitter, allows for minimizing computation time and resource requirements whilst maintaining an inversion model space well suited for inversion. In this fashion, enforcing vertical and horizontal constraints for the inversion becomes easily applicable, as well as incorporating other prior knowledge, when present.

**Inversion**

For inversion, we adopted the framework from AarhusInv (Auken et al., 2015), which provides means for minimizing a general multi component objective function

\[
Q(m) = \frac{Q_{obs}(m) + Q_{prior}(m) + Q_{reg}(m)}{N_{obs} + N_{prior} + N_{reg}}
\]

(28)
where each component of the objective function describes the norm misfit of the solution with respect to the observed data, prior information and regularizing constraints, respectively ($N_{obs}$, $N_{prior}$ and $N_{reg}$ being the number of data, number of prior constraints and number of roughness constraints).

In our algorithm, the objective function is minimized iteratively following the rules of the Levenberg-Marquardt adaptive minimization scheme (Menke, 2018, Hanke, 1997), which combines the gradient descent method with the Gauss-Newton (GN) method, for getting the optimal convergence rate. Hence, the $n + 1$th iterative model update vector $\mathbf{m}$ becomes:

$$
\mathbf{m}_{n+1} = \mathbf{m}_n + \left[ \mathbf{J}'(n)^T \mathbf{C}'^{-1}(n) \mathbf{J}'(n) + \lambda(n) \mathbf{I} \right]^{-1} \cdot \left[ \mathbf{J}'(n)^T \mathbf{C}'^{-1}(n) \delta \mathbf{d}'(n) \right] \quad (29)
$$

Here, the damping parameter $\lambda(n)$ is regenerated at each step, which determines the contribution amount of the gradient descent and the GN method on the current iteration by scaling the identity matrix $\mathbf{I}$; $\mathbf{J}'(n)$ denotes the Jacobian matrix of partial derivatives; $\delta \mathbf{d}'(n)$ is the data vector update and $\mathbf{C}'(n)$ a covariance matrix:

$$
\mathbf{J}'(n) = \begin{bmatrix} \mathbf{J}(n) \\ \mathbf{P} \\ \mathbf{R} \end{bmatrix} \quad (30)
$$

$$
\delta \mathbf{d}'(n) = \begin{bmatrix} \delta \mathbf{d}(n) \\ \delta \mathbf{m}(n) \\ \delta \mathbf{r}(n) \end{bmatrix} = \begin{bmatrix} \mathbf{d}(n) - \mathbf{d}_{obs} \\ \mathbf{m}(n) - \mathbf{m}_{prior} \\ -\mathbf{Rm}(n) \end{bmatrix} \quad (31)
$$

$$
\mathbf{C}'(n) = \begin{bmatrix} \mathbf{C}_{obs} & 0 & 0 \\ 0 & \mathbf{C}_{prior} & 0 \\ 0 & 0 & \mathbf{C}_R \end{bmatrix} \quad (32)
$$

In the first equation of the Jacobian matrix (30), $\mathbf{J}(n)$ thus represents the Jacobian of the forward mapping; $\mathbf{P}$ is the constraint matrix on the priori information and $\mathbf{R}$ is the roughness matrix. In equation (31), the data vector update $\delta \mathbf{d}'(n)$ includes the distance $\delta \mathbf{d}(n)$ between the $n^{th}$ forward
response $d_{(n)}$ and the observed data $d_{obs}$, the distance $\delta m_{(n)}$ between the $n^{th}$ model update $m_{(n)}$ and a priori model vector $m_{prior}$, and roughness of the $n^{th}$ model vector $\delta r_{(n)} = -Rm_{(n)}$. The 3 blocks of the covariance matrix $C'$ contain the covariance on the observed data $C_{obs}$, the covariance on the a priori information $C_{prior}$ and the covariance on the roughness constraints $C_{R}$. One can find more detailed matrix format and derivations in Auken and Christiansen (2004). No prior information was incorporated in the examples of this paper. However, two types of constraints, horizontal and vertical, are enforced, and the roughness matrix $R$, the roughness of the $n^{th}$ model vector $\delta r_{(n)}$, and the covariance on the roughness constraints $C_{R}$ can therefore be further subdivided into two terms:

$$R = \begin{bmatrix} R_h \\ R_v \end{bmatrix}$$

(33)

$$\delta r_{(n)} = \begin{bmatrix} -R_h m_{(n)} \\ -R_v m_{(n)} \end{bmatrix}$$

(34)

$$C_{R} = \begin{bmatrix} C_{Rh} & 0 \\ 0 & C_{Rv} \end{bmatrix}$$

(35)

**Verification**

The presented algorithms have been implemented using the programming language Fortran 2003. The mesh generation, forward modeling, and Jacobian calculation are all devised from scratch, which built into an existing GN inversion scheme (Auken et al., 2015). For solving the system equation (6), we employed the solver Pardiso (Schenk and Gärtner, 2004) directly from the intel MKL library. To better harness the modern computing architectures and accelerate the process, OpenMP was used to perform parallelization over sounding domains. All the following numerical experiments were run on 2.60GHz Xeon Gold 6132 CPUs.
Forward modeling

![Forward modeling diagram](image)

*Figure 4. tTEM system configuration scheme, where the size of the transmitter is 4m×2m and the dipole receiver locates 9.44m from the transmitter loop center.*

To demonstrate the effectiveness of our implementations, we conducted a numerical test on a half-space problem, comparing the responses with 1D computations (Auken *et al.*, 2015). The homogenous half-space model is calculated for resistivities of 10 and 400 Ωm, and the air resistivity is defined as 10⁶ Ωm. The tTEM system, which consists of a 4m × 2m transmitter and a receiver located 9.44m away from the transmitter loop center, is simulated as shown in Figure 4. We designed the octree mesh to meet a target of 3% accuracy at the receiver position, resulting in a 3D forward mesh with 17,100 DoF and in a 2.5D forward mesh with 12,200 DoF. The smallest cell at the receiver is 0.5m × 0.5m × 0.5m, while the size of the largest cell at the boundary is 1024m × 1024m × 1024m. The source waveform was simulated by a linear turn-off of the current from 1ns to 5ns. The responses were compared to the impulse response in the time range from 1μs to 10ms.
Figure 5. The 2.5D and 3D octree-based hexahedral forward modeling accuracy for a $10/400$ $\Omega m$ halfspace model using the tTEM system. (a) Forward responses. (b) Relative difference compared to corresponding 1D response. Positive and negative responses for the $10$ $\Omega m$ case are shown with different colours, indicated with the signs (+) and (−) in the legend.

Figure 5-a illustrates the homogenous half-space responses with a late time sloping rate of $-5/2$ for all the models; Figure 5-b provides a relative error comparison between the octree-based solutions and the 1D solution. The overall relative error is under 3% for all cases, except the early responses of 10 $\Omega m$ halfspace as the blue and red solid line shown, which was caused by the sign change in the early time of conductive surface. It is possible to achieve an even smaller error margin (less than 1%) as long as the meshing is dense enough to represent tiny field variabilities. However, 3% we deem sufficient when considering the noise level in production EM data.
Appendix 1: Paper I

Performance comparison with the tetrahedral implementation

Table 1. Performance and computing cost of forward (Fwd) response and the first iteration (1st) for one local mesh.

<table>
<thead>
<tr>
<th></th>
<th>Octree-3D</th>
<th>Tetrahedra-3D</th>
<th>Octree-2.5D</th>
</tr>
</thead>
<tbody>
<tr>
<td>DoF/Edge number</td>
<td>17,200/27,500</td>
<td>40,000/40,000</td>
<td>12,100/18,400</td>
</tr>
<tr>
<td>Fwd/time(s)</td>
<td>20</td>
<td>72</td>
<td>8</td>
</tr>
<tr>
<td>Inv(1st)/time(s)</td>
<td>90</td>
<td>374</td>
<td>29</td>
</tr>
<tr>
<td>Fwd/memory(MB)</td>
<td>244</td>
<td>678</td>
<td>138</td>
</tr>
<tr>
<td>Inv(1st)/memory(MB)</td>
<td>615</td>
<td>1,300</td>
<td>362</td>
</tr>
</tbody>
</table>

Table 1 presents a comparison, in terms of the running time and memory usage, of the Octree 3D and 2.5D implementations and the 3D tetrahedral implementation presented in Bo et al. (2021). For one local mesh, of which the discretization attains the accuracy of 3% compared to 1D response, the tetrahedral method requires 40,000 edges, while the octree 3D mesh has around 17,200 DoF with 27,500 physical edges. The 2.5D mesh yields 12,100 edges, which accounts for 2/3 of the 3D octree mesh. The immediate consequence of the DoF is the computing expense. The 3D octree algorithm requires 20s for the forward response, which is less than 1/3 of running time on a 3D tetrahedral scheme. The 2.5D octree algorithm further speeds up the process by reducing the running time by another factor of two. As for memory usage, the 3D octree modeling and Jacobian calculation needs 1/3 of the tetrahedral, and 2.5D octree further reduces it to nearly a half of the 3D octree one.

Synthetic Inversions

For synthetic inversions, we designed an idealized 3D model, consisting of a 10 Ωm buried valley structure embedded in a 200 Ωm homogeneous background. The valley model stretches from
15m to 40m vertically, with one branch uplifting. It is 130m wide in the y direction, and extends infinitely in the x direction (see Figure 6-a). The model was designed such that the valley structure varies both horizontally and vertically. In this example, as shown in Figure 6-b, we modelled 204 soundings over a 200 m x 160 m area in order to cover the valley. The soundings have the interval distance of 20m in x direction, and 10m in y direction, roughly resembling typical field data collection.

Figure 6. The 3D octree inversion for a valley model using the tTEM system. (a) 3D view of the conductive valley, with a section plane at the depth of 25m. (b) Soundings’ layout above the valley, with 20m distance in x direction and 10 m distance in y direction. Line A and B are the profiles inverted in 2.5D and shown in Figure 7. (c) Two used driving directions of the tTEM system. (d) 1D inversion result of the resistivity model section. (e) 3D inversion result of the resistivity model section. (f) Colorbar of sections d and e. The dotted white lines in sections (d) and (e) represent the extension of the valley.
Figure 7. Model and inversion result at two profiles of the valley model. (a) True model of profile A. (b) 3D inversion result of profile A. (c) 2.5D inversion result of profile A. (d) 1D inversion result of profile A. (e) True model of profile B. (f) 3D inversion result of profile B. (g) 2.5D inversion result of profile B. (h) 1D inversion result of profile B.

Each local mesh of 3D or 2.5D inversions had the same size/discretization used in the modeling accuracy example, but contrary to the accuracy example, the tTEM current waveform and system response (Auken et al., 2019) were fully modeled, convolving the impulse response with the waveform and the system filters. This was done for the two system moments, with low moment times from $4.14 \times 10^{-6}$ s to $11.6 \times 10^{-5}$ s and high moment times from $1.14 \times 10^{-5}$ s to $9.01 \times 10^{-4}$ s, where all timing is referenced against the beginning of the turn-off.
The stopping criterion for all the inversions is based on the total misfit: the inversion stops when the change in the total misfit of the inversion (equation (28)), is smaller than 1%. The same starting model was used as well for all inversions, in this case a homogeneous 100 $\Omega m$ halfspace.

For the 3D modeling and inversion, the line directions of the tTEM systems are all x-wise, as indicated by A on Figure 6-c. It took 13 iterations and 14.8h on 10 CPUs to complete the 3D inversion, with a final total misfit of 0.60. The peak memory usage for this inversion was 44 GB. A 1D voxel inversion, which used the same model space but 1D forward and Jacobian computations (Christensen et al., 2017), was carried out on the same data for comparison: it took 8 iterations and 137s to end up with a total misfit of 1.06.

Figures 6-d and 6-e show a xy slice at 25m depth of the 3D and 1D inversion models, respectively. The 1D inversion does not recover the upper branch of the model, but the 3D inversion is able to image both the valley branches, although with poor resolution on the lower branch.

To compare with 2.5D inversion results, we made two profiles, which are illustrated in Figure 6-b, where Profile A consists of 12 soundings along the x direction (at y=130m), and Profile B consists of 17 soundings is in the y direction B (at x=60m). For the 2.5D inversion, it is required that the inversion plane is aligned with the driving direction. Consequently, when generating the data and inverted Profile A, the system was assumed driving in the x direction, while driving in the y direction for Profile B, as described in Figure 6-c. The sounding layout is the same regardless of the driving direction.

We carried out the 2.5D inversions of Profile A and Profile B and the key inversion numbers are listed in the Table 2. The data misfit is calculated as $\sqrt{\frac{Q_{obs}(m)}{N_{obs}}}$. From the table, we can see that the memory usage increases linearly with the number of soundings. With perfect scaling of the OpenMP
parallelization, the running times for one iteration in Table 2 should be identical for Profile A and Profile B, because we used one thread for each sounding. A sub-optimal scaling was obtained, with a 20% increase of running time per sounding with 17 threads instead of 12.

<table>
<thead>
<tr>
<th></th>
<th>Profile A (12 Threads)</th>
<th>Profile B (17 Threads)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Peak Memory (MB)</strong></td>
<td>4,200</td>
<td>6,000</td>
</tr>
<tr>
<td><strong>Running time, total (s)</strong></td>
<td>871</td>
<td>1342</td>
</tr>
<tr>
<td><strong>Iterations</strong></td>
<td>10</td>
<td>13</td>
</tr>
<tr>
<td><strong>Data misfit</strong></td>
<td>0.66</td>
<td>0.69</td>
</tr>
</tbody>
</table>

Table 2. Resources and performance comparison for 2.5D inversion on Profile A and B

Figure 7 presents the synthetic models and 1D, 2.5D and 3D inversion results along Profile A (left column) and B (right column). Figure 7-a shows the model along Profile A, with the uplifting branch of the valley that expands 120m horizontally and from 10m to 35m in depth. Figure 7-b presents a xz slice of the 3D inversion model of Figure 6, which clearly delineates the shape of the branch, but with an underestimation of resistivity at the bottom of the anomaly. Figures 7-c and 7-d show the 2.5D and 1D inversions, respectively. Both inversions have a worse recovery of the anomaly, compared to the 3D inversion. This is expected also for the 2.5D inversion, because the anomaly is elongated along the profile direction, with strong model variations along the y direction perpendicular to the profile, which is a violation of the 2D assumption.

In the right panels of Figure 7, Profile B shows two conductive blocks (Figure 7-e), i.e. the cross sections of the valley branches. Figure 7-f presents a yz slice of the 3D inversion model of Figure 6 along Profile B, while Figure 7-g and 7-h show the 2.5D and 1D inversions, respectively.
The 3D inversion in Figure 7-f is able to image both the branches, with better resolution on the shallower, bigger branch (similarly, the deeper branch is imaged poorer also in Figure 6-e). In this case also the 2.5D inversion gives good results, with good imaging of both valley branches, while the 1D inversion is not able to distinguish the branches, resulting in a single merged anomaly with wrong shape. The superior performance, in terms of model recovery, of the 2.5D inversion along Profile B compared to Profile A, is a direct consequence of the fact that the model is almost 2D along Profile B, but highly 3D along Profile A.

Field example

Javngyde is a headwater catchment located in Jutland, Denmark, where the landscape was mainly formed during the Weichselian glaciation (Houmark-Nielsen, 2004). The general surface soil of the catchment is low-medium resistive clay-till, while some areas are dominated by freshwater and meltwater sandy deposits (Jakobsen et al., 2011). Some clayey glaciotectonic thrust structures are present in the area (Kim et al., 2019), and the high heterogeneity makes the site a good example to validate our 3D and 2.5D inversion algorithms. In 2017, 61% of the catchment area was surveyed with tTEM. This specific dataset (see Figure 8) is a small subset of the entire dataset and it consists of 200 soundings, distributed over 9 lines oriented in a NW-SE direction with ~10m sounding spacing along the lines and 25m line spacing. The tTEM data was processed following the procedures described in Auken et al. (2019).

First, we performed a 3D inversion of the entire subset, and then Profile L was selected for 2.5D inversion based on the 3D inverted model. Profile L holds 24 soundings. The 3D inversion of the full survey run in 12.5 hours on 10 CPUs, and the peak memory usage was 42 GB. The 2.5D inversion of profile L took 24 minutes and 6 GB on 12 CPUs. We also performed a 1D voxel inversion of this profile as a reference.
Appendix 1: Paper I

All the inversions were given a homogeneous starting model of 100 Ohm. The total data misfits of the 3D full survey, the 2.5D profile and the 1D profile are 1.2, 0.9, and 0.8 respectively.

Figure 9 presents a section of the 3D inversion model along Profile L, together with the 2.5D and the 1D inversions. The Depth of Investigation (DOI) is also displayed on the section following (Christiansen and Auken, 2012). The misfits of the soundings along the profile are shown in Figure 9-(d). Overall, all the misfits are under 2, with higher misfit for the 3D inversion, which however is a part of full survey inversion.

Figure 8. Map of the survey and measurement locations
As shown in Figure 9, all the inversion results have a 10m thick medium-high resistive surface layer. According to the geology background, we interpret it as sand and gravel glacial deposits. Below 10m, clayey glaciotectonic thrust structures are evident, but significant differences are present in the imaging of the conductive anomalies between the 1D inversion and 2.5D/3D inversions. In the northwest (left) part of the profile, 1D shows an almost continuous conductive anomaly at 20m depth,
contrary to the 2.5D and 3D inversions, which image two clearly distinct anomalies. Furthermore, the 1D inversion finds a deep conductive anomaly at 60 m depth, not present in the other inversions. These differences are rather similar to the ones found in the analysis of the inversions of the synthetic model of Profile B in Figure 7, where 1D inversion has a hard time imaging the two valley branches separately. We therefore follow the multi-dimensional inversion results and interpret the south-east conductive area as a clayey thrust structure. Though the computing complexity of the 2.5D inversion is notably smaller, the inversion result is quite similar to the 3D inversion section, making it a valuable tool for inverting TEM data in complex geology, especially where the main structure directions are perpendicular to the data collection direction.

**Conclusion**

We have presented two implementations of modeling and inversion using an octree-based finite element method in 3D and 2.5D of TEM data. The octree technique offers an elegant manner to locally refine the mesh to represent geological features and capture field variations, which reduces the degree of freedom efficiently resulting in a lower computational cost for forward modeling and Jacobian calculation. With a mirror approach, we built a 2.5D algorithm using an octree mesh, which additionally improves efficiency of the inversion scheme. Specifically, the 3D FE modeling using octree meshes is approximately three times faster than the tetrahedral implementations and uses only one-third the memory. The 2.5D implementation reduces the computing time and memory use by another factor of two.

Another highlight of our implementations is the flexible link between the forward mesh and inversion model space. In particular, the 3D and 2.5D inversion models are defined in structured meshes, linked through an interpolation to the forward meshes in a domain decomposition strategy, successfully avoiding fine inversion mesh refinements without sacrificing forward accuracy.
The applicability of the proposed algorithms was demonstrated through a synthetic example with a 3D valley structure and a field example. The synthetic experiment illustrated that 3D inversion can validly recover the anomaly with proper size and conductivity. The 2.5D inversion result approached the true model with faster speed and smaller computing expenses, as long as no strong variations in resistivity were present perpendicularly to the profile. On the contrary, 1D inversion could not delineate the correct shape of the 3D anomaly. The field example showed good agreement between 3D and 2.5D inversion, but with a substantial difference from a 1D inversion result. Hence, we conclude that the 3D and 2.5D octree-based inversion schemes for TEM data can resolve complicated subsurface structures. The choice between 3D and 2.5D inversion will depend on the geological environment and the data collection layout, but should also consider the trade-off between model resolution and computational cost.
Reference


Title: Three-dimensional time lapse inversion of transient electromagnetic data, with application at an Icelandic geothermal site

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Three-dimensional time lapse inversion of transient electromagnetic data, with application at an Icelandic geothermal site

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Abstract

Transient electromagnetics (TEM) is an efficient non-invasive method to map electrical conductivity distribution in the subsurface. This paper presents an inversion scheme for three-dimensional (3D) TEM time-lapse data using a generalized minimum support norm and its application to monitor conductivity changes over time. In particular, two challenges for time-lapse TEM applications are addressed: i) the survey repetition with slightly different acquisition layouts, as it would happen without leaving the acquisition set-up at the site or with moving acquisition systems, like in airborne surveys; ii) non-optimal data coverage above the time-lapse anomalies, for instance due to the presence of infrastructure that limit the acquisition layout because of coupling. To address these issues, we developed a new TEM time-lapse inversion scheme with the following features: (1) a multi-mesh approach for model definition and forward computations, which allows for seamless integration of datasets with different acquisition layouts; (2) 3D sensitivity calculation during the inversion, which allows retrieving conductivity changes in-between TEM soundings; (3)
simultaneous inversion of two datasets at once, imposing time-lapse constraints defined in terms of a generalized minimum support norm, which ensures compact time-lapse changes.

We assess the relevance of our implementations through a synthetic example and a field example. In the synthetic example, we study the capability of the inversion scheme to retrieve compact time-lapse changes despite slight changes in the acquisition layout, as well as the effect of data coverage on the retrieval of time-lapse changes. Results from the synthetic tests are used for interpreting field data, which consists of two TEM datasets collected in 2019 and 2020 at the Nesjavellir high-temperature geothermal site (Iceland), within a monitoring project of H\textsubscript{2}S sequestration. Furthermore, the field example is used to illustrate the effect of the trade-off between data misfit and time-lapse constraints in the inversion objective function, through the use of the tuning settings of the generalized minimum support norm. Based on the results from both the synthetic and real cases, we show that our implementation of 3D time-lapse inversion has a robust performance for TEM monitoring.

Key words: Time lapse inversion, Transient electromagnetic (TEM), three-dimensional (3D)

**Introduction**

Time-lapse inversion of resistivity has been used for inferring temporal changes in the subsurface for different environmental and engineering problems such as groundwater mapping (Doetsch *et al.*, 2012, Singha *et al.*, 2015), seawater intrusion delineation (Falgàs *et al.*, 2009, Ogilvy *et al.*, 2009, Vann *et al.*, 2020), soil moisture assessment (Blanchy *et al.*, 2020, Farzamian *et al.*, 2021), gas sequestration (Doetsch *et al.*, 2015, Auken *et al.*, 2014), geothermal system monitoring (Hermans *et al.*, 2015, Peacock *et al.*, 2013), and oil production (Orange *et al.*, 2009, Shantsev *et al.*, 2020).
Time-lapse strategies can be roughly divided into three categories: i) difference inversion (Ajo-Franklin et al., 2007, Bretaudeau et al., 2021, Carbajal et al., 2012, LaBrecque and Yang, 2001) and ratio inversion (Daily et al., 1992), which take the difference/ratio of the observed data as data input and invert for model differences, allowing an efficient suppression of the systematic noise and lowering of the computational dimensionality; ii) cascaded inversion (Miller et al., 2008, Oldenborger et al., 2007), which inverts the datasets sequentially based on the previous inversion result; iii) simultaneous inversion of two (or multiple) datasets with constrained models (Hayley et al., 2011, Kim et al., 2009).

Results of difference/ratio and cascaded inversions are highly influenced by the model used as reference, and inversion artifacts can easily propagate from the reference model to the difference/sequent model; furthermore, difference/ratio inversion requires a rigorously matching acquisition setup, which is not always achievable due to budget reasons (instrument cost) and/or risk of instrument damage by weather and/or animals. On the contrary, simultaneous inversion treats all time steps in the inversion equivalently, so it is less prone to artifact propagation from one model to another, and the acquisition setup may vary among acquisitions; furthermore, in iterative inversion schemes it allows the models of the time steps to ‘communicate’ after each iteration, and therefore avoids models being updated in significantly different inversion paths. However, the computational expense is multiplied, since the size of data space and model space are proportional to the number of time lapse steps.

Time-lapse inversion strategies differ significantly also because of the different regularization schemes applicable to the time-lapse constraints. In this regard, Carbajal et al. (2012) compared the performance of the classic L2 norm for time-lapse constraints, which penalizes the squares of parameter variations between time-lapse steps, to the minimum support (MS) norm (Portniaguine and
Zhdanov, 1999, Zhdanov et al., 2006b), which penalizes the number of inversion cells that vary, regardless of the magnitude of parameter variations. However, MS norms are usually difficult to tune, which led Fiandaca et al. (2015) to develop two generalizations of the MS norm for time-lapse inversion, the symmetric and asymmetric generalized minimum support norms, which give good performance in focusing time-lapse changes with easy-to-tune norm settings.

Time-lapse inversion, with different inversion strategies and regularizations, has been actively studied and applied in the field of electrical resistivity tomography (ERT) for more than two decades (Bièvre et al., 2021, Karaoulis et al., 2014, Kim et al., 2009, LaBrecque and Yang, 2001, Lesparre et al., 2017), and gradually applied in some other inductive methods such as magnetotelluric (Carbajal et al., 2012, Rosas-Carbajal et al., 2015) and controlled source electromagnetic method (Bretaudeau et al., 2021, Hoversten and Schwarzbach, 2021, Shantsev et al., 2020), which show superior sensitivity to conductive structures.

Nonetheless, to the best of our knowledge, time-lapse inversion has never been applied to TEM data, despite the fact that the TEM method is widely used in near surface resistivity distribution mapping (Auken et al., 2017). This is probably due to the specific challenges associated with TEM time-lapse inversions: i) data collection with consistent acquisition layouts (geometries, locations, etc.) is complicated with a moving measurement such as in airborne EM, but also with ground-based EM where the exact geometry and location of the transmitter loop can be cumbersome to reproduce identically without leaving the set-up at the site; ii) TEM surveys may result in different data density due to the unexpected coupling to man-made infrastructure in different time-lapse acquisition steps, or limitations in accessibility; iii) 3D TEM inversion, best suited for retrieving localized time-lapse changes, requires intensive computational capacity in terms of both time consumption and memory cost.
We address these issues with the development of a new TEM time-lapse inversion scheme in which: i) forward and Jacobian computations are carried out in 3D through the octree-based finite element method; ii) the multi-mesh approach (Zhang et al., 2021) is used to decouple the forward/Jacobian mesh and inversion mesh, so that the same inversion mesh can be used at different time-lapse steps despite possible variations in acquisition layouts; iii) the calculation burden in the modelling process is effectively alleviated owing to the domain decomposition strategy (Yang et al., 2013), which uses a local mesh for individual soundings; iv) datasets acquired at different time-lapse steps are inverted simultaneously, using the asymmetric generalized MS norm for time-lapse constraints, in order to obtain compact time-lapse changes.

The following sections of the paper are organized as follows: the principle of the TEM forward and inverse problems are described in the next section, together with the asymmetric MS norm. Then, we present a synthetic model, designed with sophistication equivalent to the field case, in order to illustrate the relevance of our implementation, compared to an independent inversion. In this section, we also discuss the impact of data density on both independent and time-lapse inversion performance. Following, the new inversion algorithm is applied to a field example, consisting of two TEM datasets collected with a one-year interval, in the purpose of building a baseline model before a monitoring experiment of H$_2$S sequestration at the Nesjavellir geothermal power plant in Iceland, within the GEMGAS (Geo-Electrical Monitoring of H2S Gas Sequestration) project (Lévy et al., 2020).

**Theory**

**Forward response**

The time-domain forward problem is formulated as a boundary-value problem, deriving from Maxwell’s equations:
\[ \nabla \times \mathbf{e}(\mathbf{r}, t) = -\mu_0 \frac{\partial \mathbf{h}(\mathbf{r}, t)}{\partial t} \] (1)

and

\[ \nabla \times \mathbf{h}(\mathbf{r}, t) - \frac{\partial \mathbf{D}(\mathbf{r}, t)}{\partial t} = \mathbf{j}(\mathbf{r}, t) + \mathbf{j}_s(t). \] (2)

where the electric field \( \mathbf{e}(\mathbf{r}, t) \), magnetic field intensity \( \mathbf{h}(\mathbf{r}, t) \), the dielectric displacement \( \mathbf{D}(\mathbf{r}, t) \) and the current density \( \mathbf{j}(\mathbf{r}, t) \) are functions of space, \( \mathbf{r} \in \Omega \), and time, \( t \in (0, T) \); \( \mu_0 \) is the magnetic permeability of free space and \( \mathbf{j}_s \) denotes the current source.

With the quasi-static approximation (displacement currents \( \frac{\partial \mathbf{D}}{\partial t} = 0 \)), the use of Ohm’s law for current density \( \mathbf{j} = \sigma \mathbf{E} \), where \( \sigma \) represents the electric conductivity), and the assumption that the media is isotropic and non-magnetizable and that electrical properties are independent on time (so induced polarization is neglected), the electrical field \( \mathbf{e}(\mathbf{r}, t) \) obeys a diffusion equation:

\[ \nabla \times \nabla \times \mathbf{e}(\mathbf{r}, t) + \mu_0 \sigma(\mathbf{r}) \frac{\partial \mathbf{e}(\mathbf{r}, t)}{\partial t} = -\frac{\partial \mathbf{j}_s(t)}{\partial t} \] (3)

We solve Eq. (3) following the method proposed by Xiao et al. (2020), where the equation is discretized in time domain using the second order backward Euler method (Butcher and Goodwin, 2008) and in space domain using the finite element (FE) method (Jin, 2015).
Figure 1. Multi-mesh approach illustration: local octree mesh (black) is used for forward response and Jacobian calculation at each sounding, and structured mesh (grey) is used for inversion model update.

Furthermore, the multi-mesh approach introduced by Zhang et al. (2021) is applied for decoupling the forward/Jacobian meshes’ inversion mesh (Fig.1): individual meshes are used for each sounding as local meshes for forward/Jacobian calculations (octree meshes in this study, whilst tetrahedral meshes are used in Zhang et al. (2021)), while a full-scale regular mesh that covers all the soundings is used as the inversion mesh. The model parameters in the regular inversion mesh are defined on the mesh nodes with uniform node spacing in horizontal direction and log-increasing node spacing in vertical direction (Christensen et al., 2017), and the resistivity values in the cells of the forward meshes are obtained from the values of the inversion mesh through an interpolation with an inverse distance function (Madsen et al., 2020).

The advantage of this method is three-fold for time-lapse TEM inversions. Firstly, the computational complexity is minimized whilst the forward accuracy is maintained, owing to the domain decomposition. Secondly, it eases the process to enforce spatial constraints for the inversion
or to incorporate prior knowledge, thanks to the regularity of the inversion mesh. Last, it overcomes the challenge of data repetition with matching layouts, providing the flexibility that surveys at different time-lapse steps can be carried out at different locations within the research area.

**Inversion**

In the time-lapse inversion scheme adopted in this study, two datasets $\mathbf{d}_1$ and $\mathbf{d}_2$ are inverted simultaneously, to obtain the corresponding models $\mathbf{m}_1$ and $\mathbf{m}_2$ by constraining the model difference $\delta \mathbf{m} = \mathbf{m}_2 - \mathbf{m}_1$ (while $\mathbf{d}_1$ and $\mathbf{d}_2$ may differ in size, $\mathbf{m}_1$ and $\mathbf{m}_2$ are defined on identical meshes and have identical size, such that their difference can be defined). Furthermore, in addition to the roughness constraint on individual models $\mathbf{m}_1$ and $\mathbf{m}_2$, roughness constraints are also applied on the model difference $\delta \mathbf{m}$. Defining the whole inversion data and model vectors $\mathbf{d}$ and $\mathbf{m}$ in terms of the concatenation of individual vectors as $\mathbf{d} = [\mathbf{d}_1 \mathbf{d}_2]$ and $\mathbf{m} = [\mathbf{m}_1 \mathbf{m}_2]$, the objective function $\Phi$ in our time-lapse inversion scheme consists of four terms:

$$\Phi = \Phi_d(\delta \mathbf{d}) + \Phi_{TL}(\delta \mathbf{m}) + \Phi_{Rm}(\mathbf{r}) + \Phi_{Ru}(\delta \mathbf{r})$$

where:

1. $\Phi_d$, $\Phi_{TL}$, $\Phi_{Rm}$, $\Phi_{Ru}$ represent the measures (i.e the squared norms) of the data difference, model update, roughness of model and model update, respectively. The model regularizations of the inversion are represented by the last three terms ($\Phi_{TL}$, $\Phi_{Rm}$, $\Phi_{Ru}$): in particular, the time-lapse term $\Phi_{TL}$ measures and minimizes the distance between $\mathbf{m}_1$ and $\mathbf{m}_2$, i.e. the model update in the time-lapse inversion; the model roughness term $\Phi_{Rm}$ minimizes the roughness of individual models; the measure $\Phi_{Ru}$ minimizes the roughness of the model updates.

2. $\delta \mathbf{d} = \mathbf{d} - \mathbf{d}_{obs}$ represents the difference between the forward response $\mathbf{d}$ and the observed data $\mathbf{d}_{obs}$; $\delta \mathbf{m} = \mathbf{m}_2 - \mathbf{m}_1$ symbolizes the model update between two models, i.e., model
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temporal variations; \( \mathbf{r} = -\mathbf{R}_m \mathbf{m} \) represent the model roughness through the roughness matrix

\[
\mathbf{R}_m = \begin{bmatrix}
\mathbf{R}_{m_1} & 0 \\
0 & \mathbf{R}_{m_2}
\end{bmatrix};
\]

\( \delta \mathbf{r} = -\mathbf{R}_u \delta \mathbf{m} \) is the roughness on the model update.

The time-lapse inversion is performed iteratively, by following the practice established inside AarhusInv (Auken et al., 2015), which is based on the Levenberg-Marquardt adaptive minimization scheme (Menke, 2018, Hanke, 1997), a weighted combination of gradient descent method with the Gauss-Newton (GN) method. Norms different from L2 in Eq.(4) are implemented through the iteratively reweighted least-squares (IRLS) approach following (Farquharson and Oldenburg, 1998).

The model vector \( \mathbf{m} \) is updated at the \( n + 1 \)th iterative step:

\[
\mathbf{m}_{n+1} = \mathbf{m}_n + \left[ \mathbf{G}^T_{(n)} \mathbf{C}^{-1}_{(n)} \mathbf{G}_{(n)}^* + \lambda_{(n)} \mathbf{I} \right]^{-1} \cdot \left[ \mathbf{G}^T_{(n)} \mathbf{C}^{-1}_{(n)} \delta \mathbf{d}_{(n)}^* \right] 
\]

(5)

Here, the damping parameter, \( \lambda_{(n)} \), iteratively reweights the gradient descent approach and the GN method by scaling the identity matrix \( \mathbf{I} \), \( \mathbf{G}^*_{(n)} \) includes the Jacobian matrix of different partial derivatives, the vector update \( \delta \mathbf{d}_{(n)}^* \) contains data, model roughness and model difference; and \( \mathbf{C}^{-1}_{(n)} \) is the covariance matrix of data uncertainty and model roughness, as follows:

\[
\mathbf{G}^*_{(n)} = \begin{bmatrix}
\mathbf{G}_{(n)} \\
\mathbf{I} \\
\mathbf{R}_m \\
\mathbf{R}_u
\end{bmatrix}
\]

(6)

\[
\delta \mathbf{d}^*_{(n)} = \begin{bmatrix}
\delta \mathbf{d}_{(n)} \\
\delta \mathbf{m}_{(n)} \\
\mathbf{r}_{(n)} \\
\delta \mathbf{r}_{(n)}
\end{bmatrix} = \begin{bmatrix}
\mathbf{d}_{(n)} - \mathbf{d}_{obs} \\
\mathbf{m}_{2(n)} - \mathbf{m}_{1(n)} \\
-\mathbf{R}_m \mathbf{m}_{(n)} \\
-\mathbf{R}_u \delta \mathbf{m}_{(n)}
\end{bmatrix}
\]

(7)
\[
C_{(n)}^{-1} = \begin{bmatrix}
C_{obs}^{-1} & 0 & 0 \\
0 & W_{TL(n)}^{T}C_{TL}^{-1}W'_{TL(n)} & 0 \\
0 & 0 & W_{Rm(n)}^{T}C_{Rm}^{-1}W'_{Rm(n)} \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
W_{Rm(n)}^{T}C_{Rm}^{-1}W'_{Rm(n)} & 0 & 0 \\
W_{Ru(n)}^{T}C_{Ru}^{-1}W'_{Ru(n)} & 0 & 0
\end{bmatrix}
\] (8)

In Eq.(6), \( G_{(n)} = \begin{bmatrix} G_{1(n)} & 0 \\ 0 & G_{2(n)} \end{bmatrix} \) represents the Jacobian of the two acquisitions, translated from the forward mesh to the inversion mesh following Madsen et al. (2020) and Zhang et al. (2021); \( I \) is the identity matrix; \( R_m \) and \( R_u \) are the roughness matrices on model and model update. In Eq.(7), the data vector update \( \delta d_{(n)} \) includes the distance \( \delta d_{(n)} \) between the \( n^{th} \) forward response \( d_{(n)} \) and the observed data \( d_{obs} \), the distance \( \delta m_{(n)} \) between the two models at the \( n^{th} \) iteration, the roughness of the \( n^{th} \) model vector \( r_{(n)} = -R_m m_{(n)} \) and the roughness of the model difference \( n^{th} \) model vector \( \delta r_{(n)} = -R_u \delta m_{(n)} \). In Eq.(8), the covariance matrix \( C^* \) is defined in terms of the covariance on the observed data \( C_{obs} \), the time-lapse covariance on the model difference \( C_{TL} \) and the covariance on the roughness constraints \( C_{Rm} \) and \( C_{Ru} \). The elements of \( C_{obs} \) indicates the noise level in the data, while the elements of \( C_{TL} \), \( C_{Rm} \) and \( C_{Ru} \) control the constraint strength from the model side. All four matrices are diagonal, thus the data errors have no linkage between each other. In Eq.(8), the matrices \( W_{TL(n)}', W_{Rm(n)}' \) and \( W_{Ru(n)}' \) are the IRLS re-weighting matrices that allows to define norms in the objective function different from the L2. In particular, for a given model vector \( x \) (equal to either \( \delta m \), \( r \) or \( \delta r \)) and a given measure functional \( \Phi(x) = \sum_{i=1}^{\text{size}(X)} \varphi(x_i) \), the matrices \( W_{\eta} \) (where \( \eta = TL \) or \( R_m \) or \( R_u \)) are linked to the measure \( \Phi \) and the covariance matrices \( C_{\eta} \) following (Farquharson and Oldenburg, 1998):
The stopping criterion of the iterative procedure in Eq. (4) is implemented on the total misfit $\chi$, defined as:

$$
\chi = \left( \frac{\Phi_d(\delta d) + \Phi_{TL}(\delta m) + \Phi_{R_m}(r) + \Phi_{R_u}(\delta r)}{N_d + N_{TL} + N_{R_m} + N_{R_u}} \right)^{\frac{1}{2}}
$$

(10)

In which:

1. $N_d$, $N_{TL}$, $N_{R_m}$, $N_{R_u}$ represent the number of data points, the number of time-lapse constraints, and the number of roughness constraints on model and model update.

2. $\chi_d = \left( \frac{\delta d^T C^{-1}_{\text{obs}} \delta d}{N_d} \right)^{\frac{1}{2}}$ represents the data misfit.

3. $\chi_{TL} = \left( \frac{\delta m^T W_{TL}^T C^{-1}_{TL} W_{TL} \delta m}{N_{TL}} \right)^{\frac{1}{2}}$ represents the time-lapse model penalty.

4. $\chi_{R_m} = \left( \frac{r^T W_{R_m}^T C^{-1}_{R_m} W_{R_m} r}{N_{R_m}} \right)^{\frac{1}{2}}$ represents the roughness model penalty.

5. $\chi_{R_u} = \left( \frac{\delta r^T W_{R_u}^T C^{-1}_{R_u} W_{R_u} \delta r}{N_{R_u}} \right)^{\frac{1}{2}}$ represents the roughness model difference penalty.

The matrices $W_{\eta}$ (where $\eta = TL$ or $R_m$ or $R_u$) are linked to the measure $\Phi$ and the covariance matrices $C_{\eta}$ as:

$$
W_{\eta,i} = \sqrt{\frac{C_{\eta,i}}{\chi_i^2}} \varphi'(x_i)
$$

(11)
The inversion is carried out in logarithmic data and model spaces. The forward response $d_{(n)}$ of Eq. (3) and the Jacobian calculation $G_{(n)}$ are computed for 3D TEM data following the routine devised by Xiao et al. (2020). The inversion process is terminated when the variation of the total misfit between two consecutive iterations is smaller than a defined threshold (e.g. 1%).

**Asymmetric minimum support norm for time-lapse model difference**

In this study, the measure of the model difference $\Phi_{TL}(\delta m)$ in the objective function of Eq.(4) is defined in terms of a MS functional, instead of the classic L2 measure. While the L2 measure penalizes the sum of the squared difference of the components of the vector $\delta m = m_2 - m_1$, the MS functional penalizes the number of components $\delta m_i = m_{2,i} - m_{1,i}$ that differ “significantly”, in order to favor compact time-lapse changes. Researchers have proposed different solutions for defining the significance of parameter difference in MS functionals for their applications (Last and Kubik, 1983, Zhdanov et al., 2006a, Ajo-Franklin et al., 2007, Carbajal et al., 2012, Kim and Cho, 2011, Zhdanov and Tolstaya, 2004, Vignoli et al., 2012, Fiandaca et al., 2015). In particular, Fiandaca et al. (2015) proposed a definition of generalized asymmetric MS, which is an easy-to-tune regulation to find globally optimal compatibility between data and model variation. The analytical expression of the functional is expressed:

$$
\varphi_{MS} = \alpha^{-1} \left[ (1 - \beta) \cdot \frac{(x_i^2 / \sigma^2_i)^{p_1}}{(x_i^2 / \sigma^2_i)^{p_1} + 1} + \beta \cdot \frac{(x_i^2 / \sigma^2_i)^{p_2}}{(x_i^2 / \sigma^2_i)^{p_2} + 1} \right] 
$$

$$
\beta = \frac{(x_i^2 / \sigma^2_i)^{\max(p_1,p_2)}}{(x_i^2 / \sigma^2_i)^{\max(p_1,p_2)} + 1}
$$

where $x_i = \delta m_i$ represents the difference of the $i^{th}$ component of the model difference and $\alpha$, $p_1$, $p_2$ and $\sigma_i$ represent the MS settings.

The norm settings have the following meaning:
(1) The setting $\sigma_i$ symbolizes the threshold value that defines the “significance” of a parameter change, because $\sigma_i$ represents the transition point in the minimum support functional: $\delta m_i \ll \sigma_i$ gives zero penalty in the objective function, i.e. $\varphi_{MS}(\delta m_i) = 0$; $\delta m_i \gg \sigma_i$ gives the maximum penalty $\varphi_{MS}(\delta m_i) = \alpha^{-1}$; $\delta m_i = \sigma_i$ represent the transition point at which half penalty $\varphi_{MS}(\delta m_i) = 0.5 \cdot \alpha^{-1}$ is reached. It is expressed typically as a fixed fraction (10% - 30%) of the expected relative parameter (e.g. resistivity) variation, which can be estimated from either prior information of underlying temporal changes, or a standard (e.g. L2) time-lapse inversion. In this study $\sigma_i = 0.1$ is used, both in the synthetic and field examples.

The setting $\alpha$ controls the maximum penalty, and hence the relative weight of data and model reassures in the objective function, and affects the size of time-lapse changes. Let’s define $N_{transitions}$ as the expected number of model parameters that differ “significantly” (i.e. above the transition point $\delta m_i = \sigma_i$) in time-lapse inversion. Fiandaca et al. (2015) suggests to use $\alpha$ values bigger than $\alpha = \frac{N_{transitions}}{N_{TL}}$, such that in Eq.(10) $\chi_{TL} < 1$. Actually, contrary to Fiandaca et al. (2015), in this study $N_{TL} \gg N_d$, and the risk of over-regularizing the inversion through the time-lapse constraint is significant. Consequently, the field data are analyzed for different $\alpha$ values (ranging from $\alpha = 1$ to $\alpha = 1000$), in order to study explicitly the dependence of inversion results on the balance between time-lapse constraints and data misfit in the objective function. Only one value ($\alpha = 1$) is used in the synthetic examples.

(2) The settings $p_1$ and $p_2$ control the shape of $\varphi_{MS}$ before and after the transition point $\delta m_i = \sigma_i$ (the sharpness of the transition increases with $p$), and determine the way in which the focusing depends on the other settings $\sigma$ and $\alpha$. In this study, we use the values that give the weaker overall dependence of the focusing on $\sigma$ and $\alpha$ suggested by Fiandaca et al. (2015), i.e. $p_1 = 1.35$ and $p_2 = 2$.

Numerical experiments
In an attempt to investigate the transition resolution of the implementation and the dependence on data density given by the 3D sensitivity, we designed two sets of synthetic examples: coarse and dense acquisition layouts, with xy sounding distances of 300 m and 150 m, respectively. The resistive background media is an idealized two-layered model with a 1000 Ωm top layer (thickness is 50 m) underlain by a 100 Ωm homogeneous half space, in accordance with the resistivity background values of the field case illustrated in the next section.

A 3D conductive anomaly with a resistivity of 4 Ωm and a thickness of 50 m is embedded in the second layer, and its horizontal extension grows from 320 m x 300 m in the first measurement to 460 m x 300 m in the second measurements (black and grey dashed lines in Fig. 2), to simulate the time-lapse changes. The 300 m sounding interval in the x and y directions of the coarse acquisition results in 16 soundings, in order to cover the anomaly properly. The dense acquisition halves the distance and requires 35 soundings in total as shown in Fig. 2. In addition, since it is difficult to ensure soundings from different surveys to meet the same positions, we simulate the soundings with slight xy displacements (black and grey solid lines in Fig. 2 indicate the TEM transmitter positions).
Figure 2. Coarse and dense acquisition layouts. The black rectangles represent the layout in the first measurement and the grey ones represent the second measurement. The dashed lines symbolize the top view of the 3D anomaly in the first (black) and second (grey) measurement. The red lines represent the position of the profile along which the inversion results are shown.

We modelled a central-loop WalkTEM system (Nyboe et al., 2010) with a $50 \times 50 \, m^2$ transmitter coil, convolving the impulse response with the waveform, bandwidth of the receiver coil and low pass filter of the electronics. Two system moments, with low moment gate center times from $9.19 \times 10^{-6} \, s$ to $6.78 \times 10^{-4} \, s$ and high moment gate center times from $2.07 \times 10^{-5} \, s$ to $1.22 \times 10^{-2} \, s$, were simulated with different shapes of the transmitted waveforms, in order to obtain both shallow imaging and deep penetration (Auken et al., 2019). We used the 3D finite element solver from Xiao et al. (2020) to generate the forward response, and the model space, using octree meshes, are refined locally in close proximity to the transmitter and receiver where the electric fields change rapidly. The forward domain was decomposed with one local mesh for each transmitter-receiver system (Xiao et al., 2020). The input data were contaminated with 3% of Gaussian noise for all time gates.

The stopping criterion for all inversions is based on the total misfit variation, the variation in the squared root of the objective function (eq.(10)), which is required to be smaller than 1% in our case. The same starting model was used for all inversions, which is a homogeneous $100 \, \Omega m$ halfspace. We conducted three inversions for each acquisition layout: two independent inversions (i.e. Model 1 and Model 2) and one time-lapse inversion. The number of iterations and the final data misfit of all the inversion jobs are listed in the Table 1. The inversions converged with similar data misfits and iteration number.

Table 1. Number of iterations/data misfits of the independent (Ind-) and time lapse (TL-) inversions with coarse and dense measurement layout.
Inversion results are shown along a W-E section at the middle of the models (as shown by the red in Fig. 2). Fig. 3 and Fig. 4 show the inversion results along the section for the coarse and dense acquisition layouts, respectively: the true resistivity distribution of the two model sections (section (a) and section (d)), the corresponding independent inversions (b and e) and time-lapse inversion sections (c and f); the third figure columns (g,h,i) are the resistivity ratios of the two model parameter vectors $(m_2/m_1)$ at the section. The dotted white lines symbolize the anomaly position. The inversion results in Fig. 3, i.e. with the coarse acquisition layout, show that the conductive body grows bigger over time, but it is hard to delineate the shape of the anomaly, especially for the Model 1. This behavior is better evidenced in the resistivity ratio sections: both independent and time-lapse inversion reveal the increasing conductive body in the right part of anomaly, but have difficulty resolving the changes in the left region. In addition, the connecting conductive (blue) changes in between are artifacts. The missing resolution in the left region is mainly caused by the poor data coverage compared to the size of the anomaly in Model 1, in which the conductive anomaly has no complete coverage by the soundings. However, the time-lapse inversion retrieves a more focused time-lapse image, with less inversion artifacts.

<table>
<thead>
<tr>
<th>Layout / Inversion</th>
<th>Ind-Model 1</th>
<th>Ind-Model 2</th>
<th>TL-Total</th>
<th>TL-Model 1</th>
<th>TL-Model 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse</td>
<td>10 / 1.01</td>
<td>10 / 1.00</td>
<td>10 / 1.26</td>
<td>- / 1.24</td>
<td>- / 1.27</td>
</tr>
<tr>
<td>Dense</td>
<td>12 / 1.04</td>
<td>11 / 1.20</td>
<td>9 / 1.26</td>
<td>- / 1.18</td>
<td>- / 1.33</td>
</tr>
</tbody>
</table>
Figure 3. Model sections and resistivity ratios of independent and time-lapse inversion results using the coarse acquisition layout. Black dots on the top sections represent the sounding positions.

Figure 4. Model sections and resistivity ratios of independent and time-lapse inversion results using the dense acquisition layout. Black dots on the top sections represent the sounding positions.

The resolution of the model anomaly improves significantly when we halve the sounding distance. In Fig. 4, the two models are recovered to a satisfactory level in both the independent...
inversions and the time-lapse inversion. However, the resistivity ratio highlights the lower quality of the independent inversions, where together with the two conductive blocky changes (blue) a resistivity increase and decrease are present all around the section. The ratio image of the time-lapse inversion has much clearer background and the anomaly boundary is sharper.

Overall, the 3D sensitivity of the TEM measurements allows us to retrieve time-lapse changes also with an acquisition layout that does not completely cover the conductive anomaly, although significantly better results are achieved with increased data coverage. Furthermore, the focusing scheme significantly improves the retrieval of time-lapse changes, with sharper anomaly boundaries and more homogenous background.

**Field example**

Geothermal gas re-injection is becoming a key step in mitigating air pollution caused by geothermal exploitation. Re-injected acid gases (mostly CO$_2$ and H$_2$S) are expected to mineralize, but monitoring mineralization processes in the subsurface are challenging. The GEMGAS project aims at testing the capability of several geophysical methods, including TEM, for monitoring the sequestration of a small-scale H$_2$S injection at the Nesjavellir power plant in Southwest Iceland (Lévy et al., 2020). H$_2$S injection is expected to trigger basaltic glass dissolution, resulting in the precipitation of pyrite and clay minerals, which should be reflected by changes in the electrical properties of the subsurface (Lévy et al., 2018, Lévy et al., 2019, Prikryl et al., 2018). Before the start of H$_2$S injection in January 2021, two sets of TEM and ERT data were collected in 2019 and 2020, in order to obtain a baseline model and evaluate the resistivity variability at the site (either natural or caused by power plant operations). Time-lapse inversion of these baseline datasets is the focus of this section, while post-injection monitoring are not addressed further in this article.
Figure 5. Map of Nesjavellir field site with measurement locations. Grey circles, black triangles, and red star represent the 2019, 2020 TEM, and borehole locations respectively. The dashed line indicates the location of an ERT profile acquired in 2020 and used for comparison. The red solid line represents the position of the profile along which the inversion results are shown. The yellow solid lines indicate the power plant infrastructures at the site.

The ground-based TEM data acquisition used the WalkTEM system, with a $50 \times 50 \, m^2$ transmitter coil. Data were acquired with two magnetic dipole moments, with low moment gate center times from $9.19 \times 10^{-6} \, s$ to $6.78 \times 10^{-4} \, s$ and high moment gate center times from $2.07 \times 10^{-5} \, s$ to $1.22 \times 10^{-2} \, s$. The same starting model, homogeneous $100 \, \Omega m$ halfspace, and stopping criterion, the total misfit variation smaller than $1\%$, are used for all inversions. The same spatial constraints are applied to both time lapse and independent inversions.

Fig. 5 shows the acquisition layout, with 20 soundings acquired in 2019 and 15 soundings in 2020, with no data coverage in the vicinity of the power plant infrastructure (yellow lines). The
different number of soundings is due to the different amount of inductive coupling evidenced in the 2020 TEM data, with more soundings completely removed during data processing in 2020. The coupling was caused not only by the power plant infrastructure, but also by metal fences present at the area and not shown in the map. Unfortunately, the area affected by coupling is also the area where H$_2$S injection is taking place. In the following, the inversion models will be shown in 3D view and along two profiles, shown in Fig. 5: the profile indicated by the red line, running close to the TEM soundings; the profile indicated by the dashed black line, along which ERT data have been acquired in 2020 (with electrode distance of 10 m).

This latter profile is shown in Fig. 6, in comparison with the ERT results. A similar resistivity pattern appears in both inversions, with a strong conductive anomaly around $x=1000$ m along the profile, in the vicinity of one of the injection well at Nesjavellir power plant (Lévy et al., 2020), where hot water (around 100°C) has been reinjected continuously for over ten years. However, differences are present when looking at the small-scale resistivity variations, due to the different data coverage and sensitivity of the ERT and TEM methods. It is interesting to note that the strong conductive anomaly lays mostly in-between TEM soundings but is nonetheless retrieved by the 3D inversion in a consistent manner with 2D ERT inversion.
Figure 6. SW-NE profiles of 2020 3D TEM inversion and 2D ERT inversion along the black dashed line in Fig. 5, where the datasets were both collected in 2020. Black dots on the top sections represent the TEM sounding positions’ projection.

The time-lapse inversion results are affected by the choice of the inversion setting $\alpha$ (eq. (12)) as discussed earlier. Here, we show the effect of changing $\alpha$ on the inversion results. Fig. 7 and Fig. 8 present the variation of data misfit as a function of $\alpha$ (as overall variation and sounding by sounding, respectively), while Fig. 9 and Fig. 10 show the inversion models in comparison with independent inversions (along the red profile of Fig. 5 or in 3D view, respectively).

Figure 7. The data misfit of the independent (Ind, dashed lines) and time lapse (TL, solid lines) inversions for 2019 data (blue lines), 2020 data (green lines) and total data (black lines) as a function of $\alpha$ values (Eq.(12)).
Fig. 7 tells us that the inversion of the 2019 dataset is weakly influenced by the weight of the time-lapse constraints in the objective function (i.e. by $\alpha$), while a significant influence appears on the 2020 data: with increasing $\alpha$, two significant drops in data misfit present at $\alpha = 10$ and $\alpha = 300$. Fig. 8 presents the data misfit differentiated by sounding and magnetic dipole moment for three $\alpha$-values. It highlights that the changes in data misfit occur in the 2020 high-moment data in the vicinity of the conductive anomaly and in the 2020 low-moment data in the north-east part of the survey. Again, the 2020 high-moment data in the vicinity of the anomaly are the data most affected by the inductive coupling at the site, with some soundings culled before inversion. Ideally, all coupled data have been culled, but with a sparse dataset a unique identification of coupled data is challenging and there might be small coupling effects remaining in some of these soundings. This means that the misfit changes might be due to not fully removed coupling.

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A2-22
Figure 8. Map of data misfit at individual soundings of time lapse (TL) inversions with different $\alpha$-values (Eq. (12)) and independent inversions, separate for moment (low and high) and acquisition year (2019 and 2020).

Figure 9. SW-NE inversion model sections for 2019 data (left column) and 2020 data (middle column), as well as 2020/2019 resistivity ratios (right column). Rows from top to bottom show time-lapse inversions with increasing $\alpha$ values (Eq. (12)) and independent inversions. Black dots on the top sections represent the TEM sounding positions’ projection.
Figure 10. The resistivity ratio and ratio volume within two thresholds $-\infty$-0.8 and 1.25-$\infty$ of time lapse inversions with different $\alpha$ value and the independent inversion.

Fig. 9 presents the sections of the 2019 and 2020 inversion models along the red line of Fig. 5, as well as the resistivity ratios of the 2020/2019 inversions, for both independent inversions and time lapse inversions at the three different $\alpha$-values (3, 30 and 300). All the inversion results present similar resistivity patterns, with the highly conductive body also shown in Fig. 6 lying mostly in the gap of TEM measurements (between 800m and 1200m along the profile). Nonetheless, slight differences in the shape of the conductive region, as well in the entire resistivity pattern, exist among inversions obtained with different settings. The resistivity ratio plots of Fig. 9 help significantly in quantifying the temporal changes over the two models: very few variations exist between the 2019 and 2020 models with the $\alpha = 3$ and $\alpha = 30$ TL inversions, while the $\alpha = 300$ TL inversion presents more differences, but always significantly more focused than independent inversions. This
is even more evident in Fig. 10, which presents the inversion ratio images in 3D view within two ratio thresholds: from \(-\infty\) to 0.8 for highlighting significant resistivity reductions; from 1.25 to \(\infty\) for highlighting significant resistivity increases. As in Fig. 9, the time lapse inversions with \(\alpha = 3\) and \(\alpha = 30\) present almost no variation, and the larger \(\alpha\) results in more changes in the inversion. However, in Fig. 10 it is shown more clearly than in Fig. 9 that the independent inversions present massive changes over the entire inversion volume, especially when looking at the resistivity increases in Fig. 10-h.

Looking at all inversion results obtained tuning the \(\alpha\) setting, i.e. the weight of the time-lapse constraints in the objective function, helps in the interpretation: increasing \(\alpha\), more and more variations in time-lapse inversion are allowed. So, starting from small \(\alpha\)-values, the most data-driven time-lapse changes start to appear, whilst bigger time-lapse changes occur when releasing \(\alpha\), together with an increase in volume of the anomalies already present with small \(\alpha\)-values. Consequently, the most data-driven time-lapse changes are the shallow resistivity increases in the North-East area of the survey and the resistivity increase in the South-West area at around 150 m depth (around 1800 m and 300 m in Fig. 9 i-j with \(\alpha = 3\) and \(\alpha = 30\) results).

Time-lapse changes appear in new areas of the survey, close to the gap between TEM soundings, only with \(\alpha = 300\): with this setting, a reduction in resistivity appears at intermediate-large depths in the 2020 model. This corresponds to a slight decrease in the data misfit in the TEM soundings in the North-East side of the gap, as shown in Fig. 8. Unfortunately, as already stated, this area of the survey is the one most affected by inductive coupling (this is actually the reason for the data gap), so a slight decrease in the data fit is not necessarily significant, considering that there is a risk of coupling contamination in the data. Furthermore, the synthetic experiments have shown that
when time-lapse changes occur in acquisition areas with low sounding coverage, the time-lapse change might be misplaced.

Consequently, at this stage of the research it is not possible to define clearly, only by TEM data, if a resistivity decrease occurred in the conductive anomaly, i.e. if the TL inversion with $\alpha = 300$ has to be preferred to the TL inversion with $\alpha = 30$. Even in the case in which the $\alpha = 300$ inversion is preferred, the position of the resistivity changes shown in the inversion has to be considered uncertain. However, despite the lack of complete univocity in the interpretation of the field results, the TL-inversions also convey the important message that it cannot be ruled out that there is no significant change in the subsurface structures. This outcome would have been much more difficult to conclude based on the independent inversions alone. Furthermore, the time-lapse inversion proposed in this study easily allows to handle a dataset with different acquisition layouts and to study the data influence on the inversion results in detail, considerably increasing the robustness of the interpretation.

**Conclusion**

We have developed a new algorithm to carry out time-lapse inversion of TEM data with three features designed for improving applicability and robustness, i.e.: (1) a 3D octree-based forward and sensitivity computation, which allows the algorithm to be applied also when the sounding distances in the acquisition layout are larger than the horizontal extension of background resistivity variations and time-lapse changes; (2) a multi-mesh approach for forward and inversion computations, such that the same inversion mesh is applicable even in the presence of variations in the acquisition layouts; (3) a focusing of time-lapse changes by the use of the asymmetric minimum support norm.
We tested the new algorithm on both synthetic and field data. The synthetic experiments modelled a growing 3D conductive anomaly hosted in a two-layer resistive background, captured by two sets of measurements carried out with slight variations in the sounding positions. Furthermore, two acquisition layouts were modelled: a dense one, with sounding spacing closer than the horizontal extension of the anomaly and a coarse one, in which the sounding spacing exceeded the anomaly extension. The results show that excellent recovery of time-lapse changes can be achieved with dense data coverage, and that with coarse, non-optimal acquisition density, it is possible to identify the occurrence of resistivity variations, but with misplacement of time-lapse changes. In all cases, the presented approach deliver much more focused changes with clear background, compared to independent inversions.

In the field example, we used two TEM datasets collected in 2019 and 2020 at the Nesjavellir power plant in Southwest Iceland within the GEMGAS project, in order to establish a baseline for monitoring an experiment of H2S sequestration, which started in 2021. Due to the coupling from local infrastructure, only very few soundings close to the injection area could be used. However, the 3D sensitivity of the new time-lapse algorithm allowed reasonably clear imaging of the subsurface resistivity distribution over the whole domain, as confirmed by the comparison of the inversion models of the TEM data and of the ERT data acquired at the site in 2020 within GEMGAS.

The time-lapse inversions of field data were carried out varying the weight of the time-lapse constraints (i.e. $\alpha$-value) on the inversion objective function, in order to better interpret the focusing effect of the asymmetric minimum support norm. All inversions carried out with the new time-lapse algorithm gave much more focused time-lapse changes, when compared to independent inversions. Furthermore, the various values used in tuning the asymmetric minimum support norm identified the likely data-driven model changes that occurred between 2019 and 2020.
This new implementation will help in increasing the applicability of TEM method in time-lapse monitoring, also in applications in which data coverage is limited by the presence of infrastructures and the sounding location cannot be repeated exactly.

**Acknowledgement**

This project was funded by the Icelandic Centre for Research (Rannis), Grant No. 198637-0611.

**Data availability**

Data can be made available by contacting the corresponding author. The time lapse inversion code has been implemented in the existing inversion software AarhusInv (hgg.au.dk), which is free for academic use.

**References**


Appendix 2: Paper II


Appendix 3: Paper III

Title: 3D inversion of an integrated ground-based and waterborne TEM survey

Plan to submit to *Geophysics*, In preparation
3D inversion of an integrated ground-based and waterborne TEM survey

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Abstract

The transient electromagnetic (TEM) method is an effective geophysical tool to characterize the resistivity distribution of the subsurface. With the instrumental advancements that have taken place, an integrated TEM survey combining different systems becomes possible to adapt to different settings (e.g. for land-based and waterborne surveys) or to obtain fuller resolution at different depth. This brings more complexity to the inversion for two key reasons. i) Multi-dimensional effects usually exist in the data from settings with strong conductivity contrasts, which cannot be fully interpreted by a one-dimensional (1D) inversion. ii) Different systems result in different sensitivity footprints, and it is a challenge to integrate them into one inversion model. A survey in a coastal area may encounter such problems. We address the issues using a previously developed three-dimensional (3D) inversion scheme for such problems. Firstly, a 3D octree-based forward modeling is used to describe the multi-dimensional environment and simulate the field diffusions more accurately. Secondly, decoupling between forward and inversion mesh is utilized to offer the flexibility to model each sounding independently with minimum computation cost regardless of their configuration difference.
This latter procedure still allows continuity of the earth model in the survey area during inversion. We have illustrated that a special refinement is required for meshing such models with thin highly conductive top layers. We studied the problem and validated the versatility of the method through a synthetic model and a field case, where both ground-based and waterborne systems are used in a coastal survey. In the synthetic example, we made a comparison to the 3D forward response over a synthetic coastal model, where 1D modeling had an approximate 400% error over the land-water interface, and a 6% error when the sounding is 40 m away from the interface. Additionally, the 3D inversion was shown to outperform the 1D inversion by fitting the data with a generally lower misfit and presenting a superior model retrieval. The field case further demonstrated that 3D inversion interprets the data more consistently, especially for the soundings collected in the transition area. For instance, the 3D inversion result is in better agreement with the existing borehole data. Based on the experiments, we demonstrate that 3D inversion should be considered for the multi-system survey to produce a more reliable earth model from the data.

**Introduction**

Quality and quantity of groundwater resources is one of the most pressing global environmental concerns. It is frequently reported that anthropogenic contamination from domestic and industrial waste threatens groundwater quality and the health of people (Abiriga et al., 2020, Panagos et al., 2013, Kjeldsen et al., 1998). In addition, seawater intrusion can also be problematic due to either over-extraction of freshwater from coastal aquifers or rising sea levels due to climate change (Kirsch, 2006). Therefore, tools for mapping the groundwater distribution, possible pollution, and saltwater intrusion threats, and monitoring temporal variations can provide valuable support for management. Hydro-chemical, numerical, and geophysical methods are commonly used for
groundwater investigation (Prajapati and Soni, 2020). Geophysical methods, such as electrical resistivity tomography (ERT), electromagnetic (EM) methods, and resistivity logging are commonly used to delineate the subsurface conductivity distribution, which is mainly controlled by porosity, salinity, water content, and mineralogy. These geophysical tools help illuminate the subsurface structures, and conditions, at spatial resolutions that would be prohibitively costly to achieve with drilling operations.

Among the geophysical methods, the transient electromagnetic (TEM) method offers an efficient and non-invasive option to obtain a better insight into aquifer systems by providing models of subsurface electrical conductivity. The method has been applied worldwide to groundwater-related problems for more than three decades (Goldman et al., 1991, Torres-Martinez et al., 2019), and it has become increasingly prevalent for providing knowledge of water resources and enhancing water security (El-Kaliouby, 2020, Li et al., 2021). Nowadays, many TEM systems are developed for improved maneuverability and acquisition efficiency (Auken et al., 2019, Aigner et al., 2021, Sørense and Auken, 2004). This allows for measurements in different environments – e.g. airborne, ground-based, or waterborne surveys (Christensen and Halkjær, 2014, Maurya et al., 2020, Christiansen et al., 2021). An integrated survey, i.e. a combination of different systems, can be a valuable solution in some cases as different systems may offer superior resolution by focusing at different sensitivity depths or different areas. For instance, combining airborne and ground-based measuring is helpful to obtain a full resolution in both shallow and deep regions since the depth of investigation (DOI) (Christiansen and Auken, 2012) depends on instrument characteristics such as loop size and current amplitude. In addition, when the area of interest covers both onshore and offshore landscapes (Bücker et al., 2021), either an airborne survey is adopted or a combination of ground-based and waterborne measurements are required. In this work, we study the case of the latter, an integrated survey with ground-based and waterborne systems in coastal area. However, it should be noted that the presented
solution is ready to be applied for general integrated surveys on other environmental or engineering problems such as groundwater mapping in delta areas and mineral explorations.

A one-dimensional (1D) modeling approach is the most common practice with inversion TEM measurements, this is because the approach is robust and often yields satisfying results for most cases assuming that the subsurface is quasi-1D. However, it is challenging to resolve the subsurface structures with little ambiguity if substantial two-dimensional (2D) or three-dimensional (3D) effects exist, even if there is a good agreement between predicted and measured data. For example, most salinity related anomalies ought to be modeled as 3D bodies due to the rapid lateral variations in geometry or their highly conductive nature in comparison to the surrounding subsurface. Rabinovich (1995) demonstrated the model and response distortions obtained in the edge region of a confined conductive body using 1D interpretation, giving rise to false-positive anomalies. Bauer-Gottwein et al. (2010) further showed that field data with salinity anomalies cannot be interpreted by simple 1D layered models; instead they use COMSOL (Multiphysics, 2008) to simulate a 3D TEM response and a trial-and-error procedure to obtain a resistivity model and thereby build a more intuitive hydrodynamic model. Therefore, a 3D modeling and inversion scheme will allow us to exploit the information carried in the TEM datasets more thoroughly and thereby obtain a more reliable subsurface model.

In addition to accurately resolving 3D geometries, another problem to tackle in the inversion of integrated TEM surveys is the inevitable mix of system geometries. Different system configurations result in different sensitivity footprints horizontally and vertically, which require respective model discretization for both forward and inverse modeling, if we invert the data in 3D. It becomes more complicated when the 2D/3D effects usually present in the boundary of different geological settings, where different systems are applied. The discussed problems are prominent in
coastal surveys for two reasons. i) Both ground-based and waterborne (or airborne) TEM systems are used to image the resistivity distribution below land and seawater. ii) The strong conductivity contrast between seawater and/or lithologies affected by high salinity and freshwater lithologies in a coastal environment results in strong 2D and 3D effects in the data. Thus, a standard 1D inversion framework cannot resolve subsurface structures correctly, which may be critical for accurately conceptualizing seawater intrusion problems.

To address the issues of multi-dimensional effects that exist in the data and the merging of data from different TEM systems, we adopt a 3D multi-mesh inversion scheme (Xiao et al., 2020). This scheme permits better utilization of TEM data above the 2D/3D anomalies and allows for a consistent resistivity model for the data collected by multiple systems. The research was initiated based on an observation that the onshore and offshore data, collected at a contaminated coastal area, were highly under-fitted along the coast when a standard 1D spatially constrained inversion was used (Viezzoli et al., 2009). Our study offers a new perspective to a multi-system TEM data inversion, and investigates the 2D and 3D effects that generally exist in TEM surveys crossing the land-sea boundary.

The paper is structured as follows: firstly, we briefly introduce the principle of TEM exploration, the 3D numerical methods, and the TEM systems used. Following this, we present a synthetic coastal model, with which we visualize how a 3D conductive anomaly affects the data space in a TEM survey and examine our solution to a 3D dual-system TEM problem. Then we present a field case with dual-system TEM data applied in a contaminated coastal area. Lastly, we summarize our paper.

Material and Methods
In a TEM measurement (Figure 1-a), an ungrounded transmitter loop is deployed with a static direct current, which generates a static primary magnetic field. Eddy currents are induced underneath when the primary magnetic field changes rapidly due to the current turn-off. The current density maximum moves downwards and outwards when the resistive bodies in the subsurface convert the current into heat as time passes. A receiver positioned in the center of the transmitter, or at an offset distance, records the voltage, i.e., the rate of change of the secondary magnetic field generated by these eddy currents. Therefore, the recorded signal reflects the conductivity information of the ground during the diffusion of the eddy currents.

**TEM Modeling and inversion**

Assuming that the media is isotropic, non-magnetizable, and that electrical properties are independent of time, the time-domain forward problem is formulated as a diffusion equation in terms of the electrical field $e(x, t)$:

$$\nabla \times \nabla \times e(x, t) + \mu \sigma(x) \frac{\partial e(x, t)}{\partial t} = - \frac{\partial j_s(t)}{\partial t}$$  \hspace{1cm} (1)

where the electric field $e(x, t)$, is a function of space, $x(x \in \Omega)$, and time, $t \in (0, T)$; $\mu$ is the magnetic permeability of free space, $\sigma$ denotes the electric conductivity, and $j_s$ denotes the current source. To model the TEM response in 3D, we used a previously developed solver (Xiao et al., 2020), where the Equation (1) was discretized in time using the second-order backward Euler method (Butcher and Goodwin, 2008) and spatially using the finite element method (Jin, 2015) with an octree meshing strategy.

For inversion, we adopted the Levenberg-Marquardt optimization scheme (Menke, 2018, Hanke, 1997) from AarhusInv (Auken et al., 2015), where a general multi-component objective function $Q$ is defined as:
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\[ Q(\mathbf{m}) = \frac{Q_{\text{obs}}(\mathbf{m}) + Q_{\text{reg}}(\mathbf{m})}{N_{\text{obs}} + N_{\text{reg}}} \]  

(2)

Each component of the objective function defines the norm misfit of the solution regarding the observed data, \( Q_{\text{obs}} \), and regularizing constraints, \( Q_{\text{reg}} \), both are evaluated for a given model, \( \mathbf{m} \):

\[
Q_{\text{obs}}(\mathbf{m}) = (f(\mathbf{m}) - \mathbf{d}_{\text{obs}})^{T}\mathbf{C}_{\text{obs}}^{-1}(f(\mathbf{m}) - \mathbf{d}_{\text{obs}})
\]

(3)

\[
Q_{\text{reg}}(\mathbf{m}) = (\mathbf{R}\mathbf{m})^{T}\mathbf{C}_{\text{R}}^{-1}(\mathbf{R}\mathbf{m})
\]

(4)

Where \( f(\mathbf{m}) \) is the forward solution of the model \( \mathbf{m} \), \( \mathbf{d}_{\text{obs}} \) is the observed data, and \( \mathbf{R} \) is the roughness matrix on the model. \( \mathbf{C}_{\text{obs}} \) is the covariance on the observed data and \( \mathbf{C}_{\text{R}} \) is the covariance on roughness constraints. And, \( N_{\text{obs}} \), \( N_{\text{prior}} \) and \( N_{\text{reg}} \) denote the corresponding number of observed data points, prior constraints, and roughness constraints.

The multi-mesh approach (Zhang et al., 2021) is employed in the scheme, which is advantageous in this dual-system ground-based and waterborne TEM inversion. Specifically, one regular mesh is used for the full-scale model update in the inversion. At the same time, the forward modeling and Jacobian calculation are computed based on the individual soundings, with one mesh description for each system. The link between the forward/Jacobian mesh and the inversion mesh is an inverse distance interpolation function (Madsen et al., 2020). Compared to the strategy of breaking into several blocks and inverting the datasets regionally, the benefits of applying the approach to a dual-system inversion are several: i) the survey area is decomposed into independent tasks in the modeling process, which allows us to design meshes with different density accordingly if different configurations are adopted, which minimize the computational complexity while maintain sufficient modeling accuracy; ii) one inversion mesh representing the whole survey area makes it easier to incorporate the 2D or 3D structures, this is especially important for coastal models, as the multi-dimensional effects present at
the shoreline – the boundary of land and seawater, beside which ground-based and waterborne systems are used separately for measurement.

**Instruments: tTEM and FloaTEM**

Two types of TEM instruments are used for the examples presented in the paper: ground-based tTEM (Auken *et al.*, 2019) and waterborne FloaTEM (Christiansen *et al.*, 2021). Both systems use offset configurations, which consist of a square transmitter loop and a receiver coil. The detailed parameters of the transmitter loop (Tx), the receiver coil (Rx), and the general geometry of the two systems are listed in the table of Figure 1-b. Both the tTEM and FloaTEM systems utilize a dual-moment operation (Sørense and Auken, 2004). However, since the measurements are conducted in a coastal area with a highly conductive subsurface, only the high moment pulse is collected for both systems. This is a 30 A current for the tTEM transmitter and 25 A for the FloaTEM transmitter. Besides, to increase the shallow depth of investigation due to the slow diffusion at the surface saline water, the number of transmitter coil turns in the FloaTEM system was increased to three. The FloaTEM system is operated in an aquatic environment, thus, water conductivity is measured, and echo-sounder data is obtained automatically with depth information to the river/lake/sea bed. The resistivity and bathymetry information will serve as prior information for the starting model of inversions.

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a) Towed TEM system

b) System parameters
Figure 1. Illustration of the tTEM and the FloaTEM system in a) and the key system parameters are listed in the table in b).

Modeling mesh design

TEM methods are highly sensitive to conductors. When a survey is carried out on saline water, the eddy currents diffuse horizontally in the water for a long time instead of moving downwards, which results in a shallow vertical resolution.

Here, we aim at a numerical accuracy in the forward response of 4%, to balance the accuracy with computational efficiency. In the cases where conductive structures are present in the top subsurface, additional mesh refinement is required to achieve sufficient numerical accuracy. This is contrary to the examples presented in Xiao et al. (2020), where no strong conductors were present, and no particular mesh refinement was needed. Hence, for measurements on saline water, the mesh elements in the seawater layer must be refined to describe both rapid field variations near the TEM system. At the same time, they must cover large horizontal footprints for the lateral extension of the eddy currents with time.

The shallow seawater layer provides additional computational challenges for 3D inversion. For a spatially stretched and locally refined meshing method, such as tetrahedral and octree meshes, fine mesh elements (cells) are typically added within the footprint, and the cells grow bigger further away from the system. Therefore, a pure layer is simulated as a 3D model with layered structure (Figure 2-a) up to a certain distance, where the influence of the resistivity transition is negligible (Figure 2-b). These types of models, with thin highly conductive features in the top layer, have two meshing challenges. i) The more conductive and thinner the overburden is, the finer the cells close to the system is required to capture relevant field variations. ii) It requires a dense refinement of up to hundreds of meters to make the ‘boundary effect’ coming from the conductive top layer negligible.
The actual amount depends on the conductivity and thickness of the overburden, but it will always increase the number of unknowns dramatically and thus increase the computational cost. For instance, to survey with the FloaTEM system on a layered model with a highly conductive body (e.g. 1 Ωm) in the top layer (e.g. thickness is 4 m), the smallest cell around the transmitter is 1m × 1m × 1m. The first layer needs to be refined with 4m × 4m × 4m cells out to approximately ±220 m in the x-direction from the transmitter loop center. The refinement easily causes ~373,000 unknowns for one local mesh, while a normal half-space only generates ~59,000 unknowns (Figure 2-c). Since the tTEM and FloaTEM systems have different configurations, the mesh densities are designed separately to have as few unknown parameters as possible while meeting the accuracy criteria.

![Image](image-url)

Figure 2. Illustration of the octree mesh refinement for a three-layered (1/4/100 Ωm) model with a thickness of 4 m and 28 m, respectively. a) shows a normal half-space meshing while b) shows a refined mesh for a highly conductive and thin top layer. c) shows a close-up of the mesh in a) at the end of the fine mesh, laterally, and d) shows a similar close-up just below the transmitter.
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Synthetic model

Modeling

We designed a three-layer 3D synthetic model to simulate a coastal environment (Figure 3-b) close to that of the field case model presented in the next section. The first layer consists of seawater in the east part and sandy soil, with brackish water in the west region (the thickness is 4 m), with a resistivity of 1 Ωm and 10 Ωm, respectively. The second layer has a higher resistivity of 100 Ωm and a thickness of 28 m. The bottom layer is a conductive half-space, with a resistivity of 4 Ωm. The simulated layout of sounding positions for the synthetic example can be seen in Figure 3-c. We simulate 6 lines of tTEM data on land and 7 lines of FloaTEM data on the sea, with a 10 m line distance and a N-S driving direction. Each line consists of 5 soundings, which results in a total of 65 soundings over 140 m x 70 m area. The section along the red line of Figure 3-c is shown in Figure 3-b.

The local mesh of soundings with the same configuration, either the tTEM or FloaTEM system, shares the same size/discretization. After testing the required meshing density, to obtain an accuracy with a maximum 4% error against the 1D response of a layered model, which holds only seawater (1 Ωm) at the first layer, one tTEM local mesh contains ~75,000 elements. In contrast, a FloaTEM local mesh requires ~140,000 elements. The tTEM system has 25 gates with gate center times distributed from $1.21 \times 10^{-5}$ s to $2.94 \times 10^{-4}$ s, and the FloaTEM system has 25 gates distributed from $4.71 \times 10^{-5}$ s to $2.83 \times 10^{-3}$ s. All timings are referenced against the beginning of the current turn-off of the system. The convolution of transmitter waveforms and the system filters were modeled following Auken et al. (2019).

We selected a profile perpendicular to the driving direction (refer to solid red line in Figure 3-c) consisting of 6 tTEM soundings and 7 FloaTEM soundings. We computed the 1D response from
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AarhusInv (Auken et al., 2015) and the 3D forward response from the forward solution (Xiao et al., 2020) and calculated the difference between responses, D:

$$D = \sum_{i=1}^{N_t} \left( \frac{f_{1D}^i - f_{3D}^i}{f_{3D}^i} \right) \times \frac{N_t}{N_t} \times 100\%$$  (5)

where $N_t$ is the number of time gates, $f_{1D}^i$ and $f_{3D}^i$ are forward responses for the $i$th time gate.

Panel a) of Figure 3 shows the difference between the forward responses calculated by the 1D and 3D algorithms. As shown, the difference increases when the sounding location is closer to the seawater-land interface and reaches the maximum, approximately 400%, right above the interface, where the strongest 2D effects are present. Under such circumstances, a recovered model from a 1D inversion will be geologically unreasonable even though with geophysically satisfactory in terms of the data fitting.

Panel d) presents the forward responses selected from the soundings along the section shown on Figure 4. For the sounding right above the transition interface (#7), the 1D modeling response is fully off the 3D response in early time, while in the late time, the responses show less discrepancy. As in the early time, the eddy currents occur primarily in a 2D environment, where the seawater-land interface with strong conductivity contrast is nearby, while in the late time, the eddy currents have moved outward and downward to the 1D-layered part of the model. The 1D response is thereby more similar to the 3D response. Sounding #2 and #10 are equally distanced from the land-water transition (distance=60 m). Both soundings agree well in the early times and show around a 10% response difference from the 1D response, this can be attributed to a combination of 3D effects and numerical deviations.
Above all, the modeling test has illustrated the large difference between a 1D response and a 3D response in the case of strong 2D effects from a coastline. It has therefore demonstrated the importance of using multi-dimensional (e.g. 3D or 2.5D, depends on the driving direction) simulation instead of 1D modeling in such an area, at least within the range of 50 m from the coastline.
Figure 3. The response difference of 1D and 3D forward modeling on a coastal model: a) Response difference between 1D forward and 3D forward against 3D response; b) Coastal model illustration, where the tTEM and FloaTEM soundings are symbolized by black and grey dots, respectively; d) tTEM(black) and FloaTEM(gray) measurement layout; d) Response curves of selected soundings for both tTEM (solid lines) and FloaTEM (dashed lines) in 1D (blue) and 3D (red)

Inversion

To prepare the input data for inversion, we assign noise $N$ to the individual data points of forward solution $f(m)$ at the time gates, $t$, in the following way: the noise consist of a uniform uncertainty of 3% and a background noise level that is relevant to the transmitter’s magnetic moment, $M$, which is calculated by:

$$
N = \sqrt{\left(3\%\right)^2 + \left(\frac{n_{bg} \cdot t^{-1/2}}{M \cdot f(m) \cdot t_0^{-1/2}}\right)^2}
$$

(6)

Where $n_{bg}$ is the background noise at $t_0$, which is set as $3 \times 10^{-10}$ V/m at 1 ms in our example. The Equation assumes log-gating, in which case the noise drops of as $t^{-1/2}$ as seen in Equation (6).

To compare the inversion performance of different dimensions, we carried out both 3D and 1D inversions, where both inversions used the same model space, i.e. a voxel mesh with the same spatial discretization. Particularly, the 1D voxel inversion followed the methodologies presented by Christensen et al. (2017). Since seawater's bathymetry and resistivity value is known during measuring, the starting model is set as a 10 $\Omega$m half-space except in the water column for 1D inversion. The 3D inversion calculation of this nearly-layered model with a strong high-conductivity contrast is costly as discussed above. We, therefore, use the 1D inversion results as the starting model for the 3D inversion. The stopping criterion for all the inversions is fulfilled in the case of a relative total misfit (Equation (2)) decrease dropping below 1%, relative to the last iteration. The misfit of the
forward response from the inverted model to the actual observed data is assessed with the error function
\[ e = \frac{\sqrt{Q_{\text{obs}(m)}}}{\sqrt{N_{\text{obs}}}}. \]

The 1D inversion completed the inversion with a total misfit of 1.8 after 12 iterations, which is somewhat outside the error-bars. When starting from this 1D model, the 3D inversion has an initial misfit of 7.1, a significant difference from the 1D misfit. It converges to a misfit of 0.2 after 10 iterations, which is well within the error-bars. The overall misfit maps of the two inversions are shown in Figure 4-e/f. The misfit of the 1D inversion presents an identical misfit of each row since this is strictly a 2D model. The FloaTEM soundings close to the transition area, have the poorest fits. It is interesting to notice that the onshore tTEM soundings have a satisfying misfit in the 1D inversion (generally less than 1), even though the 1D modeling error is always larger than 10% when the distance to the shoreline is shorter than 50 m, as shown in Figure 3. The 3D inversion, however, results in a lower total misfit and produces a similar data fit for the land-based and waterborne data.

Figures 4-c and 4-d show a result section perpendicular to the coastal line of 1D and 3D inversion, respectively. The outline of the true model section is illustrated in the subfigures by solid white lines. Two main phenomena can be observed from the 1D inversion result: firstly, the seawater layer is too thin compared to the true model, even though we started the inversion with correct properties; secondly, a conductive pant leg is stretching into the high-resistivity layer. This can be explained: i) as the curves shown in the Figure 3-d (e.g. #7), to generate a 1D response close to 3D response with the minimum misfit, the recovered 1D model should be more resistive than the true 1D model directly beneath that point; ii) the inversion of tTEM data is affected by the sensitivity contribution from the more conductive seawater since the true 3D data contains information from surrounding areas. In contrast, the 3D inversion starting model (i.e. 1D inversion result) did not include a layer to represent the correct water table, but recovered the true model substantially.
includes reasonably accurate resistivities and layer boundaries without the pant leg. The inversions of this synthetic model offer us a new perspective to see the multi-dimensional effects in the TEM surveys across a shoreline.

Figure 4. The 1D and 3D inversion of a coastal model: a) True model section 3D response; b) Starting model of 1D inversion; c) 1D inversion section (starting model of 3D inversion); d) 3D inversion section; e) 1D inversion misfit map; f) 3D inversion misfit map. The dotted white lines outline the structures of the true model. The dotted black lines symbolize the land-seawater interface, where the tTEM survey is conducted in the west region, and the FloaTEM survey is carried out in the East region. The solid red line indicates the section location of inversion results in subfigure (c) and (d).
Field Case

Geology and hydrogeology

In the 1950s and 1960s, an area at Himmark Beach in southern Denmark was used to deposit thousands of cubic-meters of chemical waste from industrial production (Figure 5). At the time it was done with the authorities' approval then and has now become one of the ten most polluted sites in Denmark. The local company, which is still in operation, has contributed to a governmental efforts to restore the area and contribute financially to investigations on how the pollution can be removed. The principal aim of these efforts was to characterize the pathways by which the pollution enters the sea. Specifically, there is a shallow sand layer underlain by a clay till which largely controls the water. Therefore, the principal goal is to map the interface between the sand unit and the till to identify pathways for the pollution. The survey contained ground-based tTEM measurements on land and FloaTEM measurements in the sea close to the shoreline.

The dataset shown in Figure 5 is a small subset of the survey, consisting of 18 tTEM soundings and 41 FloaTEM soundings. In general, the distance between lines is around 20 m and the distance between soundings is 5 m. We use a small subset to illustrate the problem. Larger subsets become difficult to handle due to the required dense refinement of the forward/Jacobian mesh, as discussed earlier. We chose this particular subset as the many boreholes drilled in the area can be used to validate the inversion results. The data processing follows Auken et al. (2019). Accurate location recording for the offset system is essential to simulate the response in 3D inversion, a few soundings in the tTEM dataset with irregular GPS-recordings were removed on this account.
Figure 5. A dual-system TEM survey with land (tTEM) and waterborne (FloaTEM) systems in a coastal area. The solid yellow line represents a profile crossing existing boreholes.
Figure 6. The result from the 1D and 3D inversions: a) 1D inversion misfit map; b) 3D inversion misfit map; c) 1D inversion profile of top 60 m; d) 3D inversion profile of top 60 m; e) 1D inversion profile of top 10 m with borehole information; f) 3D inversion profile of top 10 m with borehole information. The solid green line represents a profile along the existing boreholes (black stars). The black dashed lines represent the land-seawater boundary. The white dashed line represents the bathymetry based on measurements at the borehole locations.

As in the misfit map shown (Figure 6-a/b), the 1D inversion has difficulty fitting the FloaTEM data close the beach, but can give reasonable misfits for the tTEM data on land. However, the 3D inversion, presents a more satisfying image with much better fitting for the FloaTEM data along the
beach and a slightly higher misfit for tTEM data. According to the study from the synthetic example, we learn that the 3D effect still has more than 6% impact on the soundings 50 m away from the shoreline. If we apply this knowledge here, we can rationalize that even though the 1D inversion presents a lower (1D) misfit for the tTEM data, the recovered model contains errors driven by 3D effects in the data. Specifically, for these tTEM data, the 1D responses have an average of ~72% difference from 3D responses, as calculated using Equation (5).

Figure 6-c and Figure 6-d show sections with results of the 1D and 3D inversions for the top 60 m, along the green profile going through boreholes. In general, the 3D inversion result presents a more conductive environment within the top of 30 m. The 1D inversion indicates a conductive-resistive interface at a depth of 40 m, while the 3D inversion predicts a more uneven interface that is shallower on the sea-side. Moreover, what appears to be a 2D pant leg effect is noticed in the 1D profile, similar to the one reported in the inversion of the synthetic example in Figure 4.

As noted, the sand-till interface is of particular interest, panels e) and f) show close-up sections of only the top 10 m. As an initial consistency test for the inversion results, the resistivity model and measured seawater resistivity/depth were compared. The bathymetry information is missing in this area due to the GPS damage in this survey. Therefore, we use the elevation of the top of the boreholes as the water depth, which is illustrated as the white line in Figure 6-e and Figure 6-f. Both the 1D model and the 3D model indicate a highly conductive water layer (0.3-0.5 Ωm) with similar resolution, which is well-aligned with the measured value of 0.4 Ωm. Secondly, we can compare the layer matching in all the available boreholes. The top of the more resistive till layer (~20 Ωm) is only aligned with the borehole reported sand-clay interface for the 3D result. In particular, the thickness of the saline sand layer gradually increases from the shoreline to the sea. The 1D result shows that the conductive layer is 2-3 meters shallower than what is reported in the boreholes. This phenomenon
is also noticed in the synthetic example, where the bottom of seawater is recovered by some resistive media in the 1D inversion result. The sand-clay boundary in the onshore borehole is not identified by any of the inversion results, which is probably because the onshore sand is mixed with saltwater (and/or clay), which has a lower salinity than the sand beneath seawater, resulting in higher resistivity. Thirdly, we calculate the formation factor of the 1D/3D inversion models within the depth range of the sand layer observed in the boreholes, which is saturated with saline water. Following Archie’s law (Archie, 1942), we find a formation factor from the 1D result of 20, while the 3D inversion predicts the value as ~4-5. Published lab measurements of saline sand formation properties (Kadhim et al., 2013, Frings et al., 2011), indicate that for clean sand units with a cementation exponent of 1.5, a tortuosity factor of 1, and a porosity of 0.4, the formation factor should be approximately 4. Hence, the 3D result gives a more reasonable estimation of the resistivity in the sand layer.

Based on these observations, we conclude that a 3D inversion enables more accurate information about the subsurface structures for environments characterized by substantial 2D/3D variability. However, it should be noted that this is also at a much higher computation cost.

**Conclusion**

In this study, we investigated the 2D and 3D effects present in TEM surveys at a coastal site. From the onshore and offshore measurements we observed a high data misfit in the sea-land transition area when a standard spatially constrained 1D inversion of TEM data was used. We addressed this issue by applying a previously developed 3D inversion scheme. The features of the scheme entail: i) A 3D octree-based modeling approach, simulating electromagnetic fields more accurately in a multi-dimensional environment with strong conductivity contrast; ii) A multi-mesh approach, inverting datasets collected with different system configurations simultaneously through one inversion mesh,
while maintaining different meshes for the individual soundings for forward modeling and Jacobian computation. In combination, this multi-mesh octree setup minimizes the computation complexity while maintaining accuracy. In particular, a purposely refined mesh is designed for these types of model with thin, highly conductive overburden to keep the numerical error below 4%.

To investigate the impact of multi-dimensional effects, we designed a synthetic coastal model with both onshore (tTEM) and offshore (FloaTEM) measurements. We simulated the forward responses using a 1D and 3D forward code. The difference between the two responses was up to 400% above the land-sea interface on a sounding basis, and it drops off to approximate 6% when the systems are 40 m away from the interface. We further inverted these synthetic data using 1D and 3D solutions. The model resulting from the 1D inversion cannot fit the offshore data close to the shoreline but generally fits all onshore data nicely. The 1D result did not recover the water depth properly, even when the actual value was given as the initial model for the inversion. Furthermore, a clear pant leg effect appeared in the onshore tTEM survey area. The 3D inversion reproduced the model fairly accurately with no particular artifacts and a low data misfit.

Finally, we studied the 1D and 3D inversion results of a field case, where many of the results from the synthetic study were also present. The data collected near the interface could not be fitted by a 1D inversion, which was not a problem with the 3D inversion having much lower data misfits. Existing borehole data verified that the 3D inversion provided accurate characterization of a particular transition from sand to clay, which was the primary target of the investigation.

Acknowledgement
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Reference


Appendix 4: The finite element method equations (hexahedral)

As described in Section 3.1, the resulting elemental matrices of finite element discretization contain two fundamental integrals:

\[
E_{ij}^e = \iiint_{V_e} (\nabla \times N_i^e) \cdot (\nabla \times N_j^e) \, dV
\]  
\[
F_{ij}^e = \iiint_{V_e} N_i^e \cdot N_j^e \, dV
\]  

Where the finite element method defines the vector basis functions \( N \) on the edges of the element:

**Parallel to \( \xi \)-axis:** \( N_i^e (\xi, \eta, \zeta) = \frac{l_i}{8} (1 + \eta \xi)(1 + \zeta \xi) \nabla \xi \)  

**Parallel to \( \eta \)-axis:** \( N_i^e (\xi, \eta, \zeta) = \frac{l_i}{8} (1 + \xi \eta)(1 + \zeta \eta) \nabla \eta \)  

**Parallel to \( \zeta \)-axis:** \( N_i^e (\xi, \eta, \zeta) = \frac{l_i}{8} (1 + \xi \zeta)(1 + \eta \zeta) \nabla \zeta \)

<table>
<thead>
<tr>
<th>Edge</th>
<th>Node 1</th>
<th>Node 2</th>
<th>( \xi )</th>
<th>( \eta )</th>
<th>( \zeta )</th>
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<td>7</td>
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<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

Here the coefficients \( \xi_i, \eta_i, \zeta_i \) can referred the Table A4.1. And the number of nodes and edges are named after the illustration in Figure A4.1.

The curl of the basis function can therefore be derived to:
Appendix 4: The finite element method equations (hexahedral)

\[
\nabla \times \mathbf{N}_i^\zeta = \frac{l_i}{8} \left[ (\zeta_i + \eta_i \zeta) \nabla \zeta \times \nabla \xi + (\eta_i + \eta_i \zeta) \nabla \eta \times \nabla \xi \right]
\]

(6)

\[
\nabla \times \mathbf{N}_i^\eta = \frac{l_i}{8} \left[ (\xi_i + \zeta_i \xi) \nabla \xi \times \nabla \eta + (\zeta_i + \xi_i \zeta) \nabla \zeta \times \nabla \eta \right]
\]

(7)

\[
\nabla \times \mathbf{N}_i^\xi = \frac{l_i}{8} \left[ (\xi_i + \xi_i \eta) \nabla \xi \times \nabla \zeta + (\eta_i + \xi_i \eta) \nabla \eta \times \nabla \zeta \right]
\]

(8)

To calculate the integrals in Eq.(1) and Eq.(2), the calculation of volume \( dV \) in \( xyz \)-system (Cartesian system) can be transformed in \( \zeta \eta \zeta \)-system (FE system) as

\[
dV = dx dy dz = \begin{vmatrix}
\frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\
\frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\
\frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta}
\end{vmatrix} d\xi d\eta d\zeta
\]

(9)

And the expression for \( \nabla \xi, \nabla \eta, \nabla \zeta \) can be obtained by letting \( f = \xi, \eta \) and \( \zeta \), respectively.

\[
\begin{pmatrix}
\frac{\partial f}{\partial x} \\
\frac{\partial f}{\partial y} \\
\frac{\partial f}{\partial z}
\end{pmatrix} = \begin{vmatrix}
\frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\
\frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\
\frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta}
\end{vmatrix}^{-1} \begin{pmatrix}
\frac{\partial f}{\partial \xi} \\
\frac{\partial f}{\partial \eta} \\
\frac{\partial f}{\partial \zeta}
\end{pmatrix}
\]

(10)

Finally, the product of three one-dimensional Gauss-Legendre quadratures is used:

\[
\int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} f(\xi, \eta, \zeta) d\xi d\eta d\zeta = \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} \sum_{k=1}^{n_3} W_i W_j W_k f(\xi_i, \eta_j, \zeta_k)
\]

(11)

where \( n_1, n_2, \) and \( n_3 \) are the number of integration points along the \( \xi, \eta, \) and \( \zeta \) axes, respectively, \( W_i, W_j, \) and \( W_k \) are weighting factors, and \( \xi_i, \eta_j, \) and \( \zeta_k \) denote the integration points.