# elfe3D: Modelling with the total electric field approach using finite elements in 3D

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Summary

The controlled-source electromagnetic method is a geophysical technique that detects variations in electric and magnetic material properties in the subsurface. The method is valuable for both environmental assessments and resource exploration. To evaluate electromagnetic data obtained over complex subsurface structures, precise three-dimensional numerical modeling software is required. This is particularly important for tasks related to survey design and for inversion routines that estimate subsurface models based on field data inputs. The forward modelling program `elfe3D` simulates synthetic data of frequency-domain controlled-source electromagnetic configurations for three-dimensional subsurface models. To optimise the balance between the size of the problems and the accuracy of the solutions, adaptive mesh refinement strategies are employed. The `elfe3D` program allows the user to define an arbitrary survey setup: The sensor locations, where the electric and magnetic field responses are calculated, can be placed at or below the subsurface, or in the air. This flexibility facilitates realistic modelling of surface-based, borehole and airborne controlled-source electromagnetic surveys.

Statement of need

Contemporary electromagnetic geophysical field investigations employ advanced measurement configurations designed to image complex subsurface structures. This context necessitates the development of flexible and manageable three-dimensional (3D) simulation software tailored for the evaluation of controlled-source electromagnetic data (Rochlitz et al., 2019). To address this task, `elfe3D` was developed to numerically calculate forward responses, i.e. electric and magnetic field components, for 3D subsurface models studied with frequency-domain controlled-source electromagnetic surveys (Figure 1). Compared to standard electromagnetic geophysical simulation software, `elfe3D` excels in flexibility regarding subsurface properties and geometries as well as survey settings, i.e. receivers can be arbitrarily placed in the modelling domain. Implemented adaptive mesh refinement approaches can automatically design problem-specific meshes and balance computational load and solution accuracy.

State of the field

Common strategies in electromagnetic modelling often avoid 3D simulations due to their substantial computational demands and the predominant focus tends to be on electrical resistivity models, as this material property is dominant at typical frequencies used in controlled-source electromagnetic surveys. The numerical techniques required to facilitate 3D simuations and their integration into controlled-source electromagnetic modelling code is currently a prominent area of academic research (Börner, 2010) and some related open-source codes

became available in recent years (Castillo-Reyes et al., 2018; Heagy et al., 2017; Rochlitz et al., 2019; Werthmüller et al., 2019). Objectives for designing these and other new electromagnetic forward modelling codes are to (i) enable modelling of complex subsurface settings (Rochlitz et al., 2019), (ii) enhance the accuracy of forward responses while minimising computational costs (Grayver & Kolev, 2015), (iii) optimise and understand the effects of model discretisation (Castillo-Reyes et al., 2023; Oldenburg et al., 2020; Werthmüller et al., 2021) and (iv) to develop efficient solvers (Weiss et al., 2023).
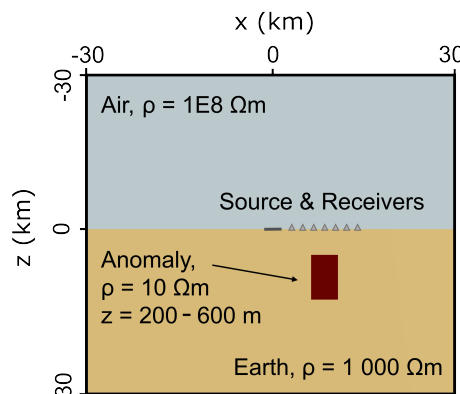
Step I: Model   **Step II:** Mesh
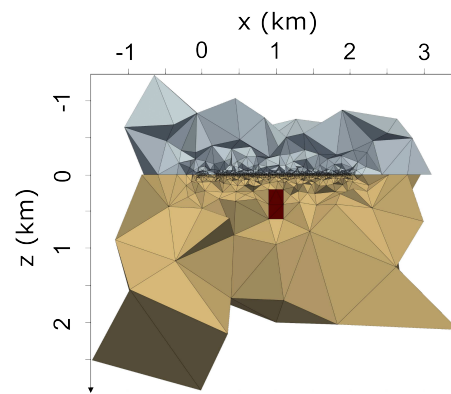
Step III: Field Responses obtained with elfe3D
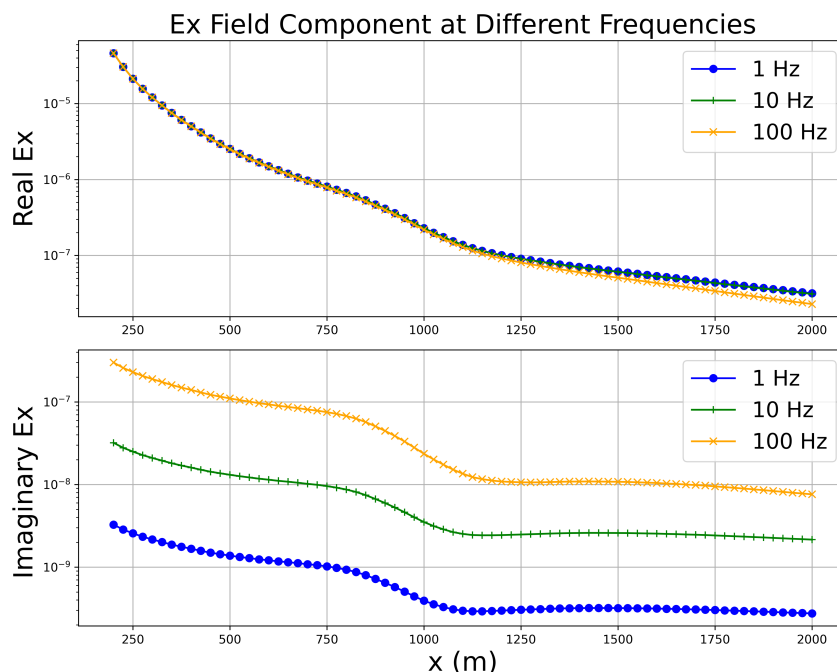
Figure 1: Key steps of the forward modelling procedure including the choice of a subsurface model and source-receiver setup (Step I; note that the subsurface anomaly and survey setup are enlarged in the image for better visibility), the meshing of the modelling domain (Step II; note that a slice through the inner modelling domain is displayed) and the calculation of field responses with elfe3D (Step III; note that only the electric field component in x-direction (Ex) is displayed). Figure adapted from PhD thesis: Rulff (2023).

Special code capabilities

In `elfe3D`, three special functionalities are combined. These features address the above-mentioned objectives i-iii and, in summary, distinguish `elfe3D` from other available codes:

1. **Variable Magnetic Permeability**: In traditional 3D electromagnetic forward modeling algorithms, magnetic permeability and dielectric permittivity are typically not considered variable model parameters. This oversight is often due to the relatively minor contrasts in these properties compared to conductivity contrasts prevalent in most geological environments at frequencies in the Hz- to kHz-range. However, it is well documented that mineralised zones and metallic infrastructure (Heagy & Oldenburg, 2023) may exhibit pronounced contrasts in magnetic permeability relative to their host rocks. Dielectric permittivities influence only high-frequency data in very resistive environments (Kalscheuer et al., 2008). Consequently, in `elfe3D`, magnetic permeability is treated as a variable model parameter, in conjunction with electrical resistivity. Rulff et al. (2021) present a numerical test example with magnetic anomalies.

2. **Automatic Mesh Refinement**: The refinement approach implemented in `elfe3D` is inspired by Ren et al. (2013) and Grayver & Kolev (2015). It aims to achieve an optimal balance between the accuracy of the solutions at specified areas of interest and the overall size of the computational problem. This is accomplished through a goal-oriented mesh refinement strategy, specifically tailored for models characterised by variable electrical conductivity and magnetic permeability. The goal-oriented mesh refinement strategy including an adjoint problem formulation and the utilised error estimation approaches are detailed in Rulff et al. (2021).

3. **Perfect Electric Conductors**: `elfe3D` incorporates a methodology for approximating highly conductive infrastructures within the model, such as steel-cased wells that are frequently encountered in exploration contexts. These structures are modeled as perfect electric conductors (Um et al., 2020), utilising an approach similar to boundary conditions. Within the computational domain, this formulation enforces the electric field to zero at mesh edges corresponding to the perfect electric conductors. Castillo-Reyes et al. (2023) provide details on the perfect electric conductor implementation and application.

Target audience

The program `elfe3D` is designed for geophysicists who want to:

- Plan controlled-source electromagnetic experiments and require a tool for conducting numerical feasibility studies.
- Generate problem-specific tetrahedral meshes for controlled-source electromagnetic settings, which can be utilised in other simulation environments.
- Integrate the code into their inversion frameworks.
- Further develop the code.

Workflow overview

Isotropic electric resistivities and magnetic permeabilities are variable, but element-wise constant, model parameters arranged in a tetrahedral mesh generated with TetGen (Si, 2015). The mesh files must be provided as input to `elfe3D` along with a start file specifying survey parameters such as frequencies, receiver and source positions, etc. Line or loop sources are represented along the edges of the mesh elements.

The physical behavior of electromagnetic fields is described by Maxwell's equations, which serve as the foundation for the curl-curl equation in terms of the total electric field $\mathbf{E}$ that `elfe3D` is solving:

$$\nabla \times \frac{1}{\mu} \nabla \times \mathbf{E} - i\omega \frac{1}{\rho} \mathbf{E} - \omega^2 \epsilon \mathbf{E} = i\omega \mathbf{J}_p \quad \text{in} \quad \Omega,$$

where Ω is the computational domain, ω is the angular frequency, ρ the electrical resistivity, ε the dielectric permittivity and μ the magnetic permeability. A time dependence $e^{-i\omega t}$ is assumed and $\mathbf{J}_p$ describes the source term. Dirichlet boundary conditions are imposed on the outer domain boundaries.

This governing equation is discretised with linear vector finite-element shape functions (Jin, 2014). Developed using modern Fortran, elfe3D leverages vectorisation and shared-memory parallelism and employs a direct method, the MUMPS solver (Amestoy et al., 2001), for solving the system of equations. At the end of the workflow (Figure 1), the synthetic data, that is the electric and magnetic field components in Cartesian space, are calculated from the solution $\mathbf{E}$ and written to output files.

Development history and ongoing research

The underlying code of elfe3D was developed between 2018-2023 and validated in Rulff et al. (2021). This initial code is implemented in the inversion software emilia (Kalscheuer et al., 2008, 2010, 2015) to enable 3D controlled-source electromagnetic inversion (Rulff, 2023; Rulff & Kalscheuer, 2024). Adaptively refined meshes and parts of the synthetic data reported in Castillo-Reyes et al. (2023) were generated with elfe3D. The program is currently used and extended to design surface-to-borehole controlled-source electromagnetic surveys for geothermal applications (Rulff et al., 2024).

Acknowledgements

Availability

Version 1.0.0 of elfe3D is freely available under the Apache License, Version 2.0. The source code, along with documentation, an example and reference solutions, is hosted at https://github.com/emsig/elfe3D/tree/main. Further developments of elfe3D are ongoing. Collaboration and community feedback are welcome.

References

Amestoy, P. R., Duff, I. S., L'Excellent, J.-Y., & Koster, J. (2001). A fully asynchronous multifrontal solver using distributed dynamic scheduling. *SIAM Journal on Matrix Analysis and Applications*, *23*(1), 15–41. https://doi.org/10.1137/s0895479899358194

Börner, R.-U. (2010). Numerical modelling in geo-electromagnetics: Advances and challenges. *Surveys in Geophysics*, *31*(2), 225–245. https://doi.org/10.1007/s10712-009-9087-x

Castillo-Reyes, O., de la Puente, J., & Cela, J. M. (2018). PETGEM: A parallel code for 3D CSEM forward modeling using edge finite elements. *Computers & Geosciences*, *119*, 126–136. https://doi.org/10.1016/j.cageo.2018.07.005

Castillo-Reyes, O., Rulff, P., Schankee, E., & Adrian, U. (2023). Meshing strategies for 3d geo-electromagnetic modeling. *Computational Geosciences*. https://doi.org/10.1007/s10596-023-10247-w

Grayver, A. V., & Kolev, T. V. (2015). Large-scale 3D geoelectromagnetic modeling using parallel adaptive high-order finite element method. *Geophysics*, *80*(6), E277–E291. https://doi.org/10.1190/GEO2015-0013.1

Heagy, L. J., Cockett, R., Kang, S., Rosenkjaer, G. K., & Oldenburg, D. W. (2017). A framework for simulation and inversion in electromagnetics. *Computers and Geosciences*, *107*, 1–19. https://doi.org/10.1016/j.cageo.2017.06.018

Heagy, L. J., & Oldenburg, D. W. (2023). Impacts of magnetic permeability on electromagnetic data collected in settings with steel-cased wells. *Geophysical Journal International*, *234*(2), 1092–1110. https://doi.org/10.1093/gji/ggad122

Jin, J. (2014). *The finite element method in electromagnetics* (3rd ed.). Wiley-IEEE Press.

Kalscheuer, T., Blake, S., Podgorski, J. E., Wagner, F., Green, A. G., Muller, M., Jones, A. G., Maurer, H., Ntibinyane, O., & Tshoso, G. (2015). Joint inversions of three types of electromagnetic data explicitly constrained by seismic observations: results from the central Okavango Delta, Botswana. *Geophysical Journal International*, *202*(3), 1429–1452. https://doi.org/10.1093/gji/ggv184

Kalscheuer, T., Garcia Juanatey, M. de los A., Meqbel, N., & Pedersen, L. B. (2010). Non-linear model error and resolution properties from two-dimensional single and joint inversions of direct current resistivity and radiomagnetotelluric data. *Geophysical Journal International*, *182*(3), 1174–1188. https://doi.org/10.1111/j.1365-246X.2010.04686.x

Kalscheuer, T., Pedersen, L. B., & Siripunvaraporn, W. (2008). Radiomagnetotelluric two-dimensional forward and inverse modelling accounting for displacement currents. *Geophysical Journal International*, *175*(2), 486–514. https://doi.org/10.1111/j.1365-246X.2008.03902.x

Oldenburg, D. W., Heagy, L. J., Kang, S., & and, R. C. (2020). 3D electromagnetic modelling and inversion: A case for open source. *Exploration Geophysics*, *51*(1), 25–37. https://doi.org/10.1080/08123985.2019.1580118

Ren, Z., Kalscheuer, T., Greenhalgh, S., & Maurer, H. (2013). A goal-oriented adaptive finite-element approach for plane wave 3-d electromagnetic modelling. *Geophysical Journal International*, *194*(2), 700–718. https://doi.org/10.1093/gji/ggt154

Rochlitz, R., Skibbe, N., & Günther, T. (2019). CustEM: Customizable finite-element simulation of complex controlled-source electromagnetic data. *Geophysics*, *84*(2), F17–F33. https://doi.org/10.1190/geo2018-0208.1

Rulff, P. (2023). *Three-dimensional forward modelling and inversion of controlled-source electromagnetic data using the edge-based finite-element method* [PhD thesis, Uppsala University]. https://urn.kb.se/resolve?urn=urn:nbn:se:uu:diva-514339

Rulff, P., Buntin, L. M., & Kalscheuer, T. (2021). Efficient goal-oriented mesh refinement in 3D finite-element modelling adapted for controlled-source electromagnetic surveys. *Geophysical Journal International*, *227*, 1624–1645. https://doi.org/10.1093/gji/ggab264

Rulff, P., Drijkoningen, G., Bortolotti, M., & Slob, E. (2024). Optimal placement of capacitive electrodes in a borehole for monitoring purposes in geothermal applications. *26th EM Induction Workshop*.

Rulff, P., & Kalscheuer, T. (2024). Research note: A comparison between normalized controlled-source electromagnetic field components and transfer functions as input data for three-dimensional non-linear conjugate gradient inversion. *Geophysical Prospecting*. https://doi.org/10.1111/1365-2478.13488

Si, H. (2015). TetGen, a delaunay-based quality tetrahedral mesh generator. *ACM Trans. Math. Softw.*, *41*(2). https://doi.org/10.1145/2629697

Um, E. S., Kim, J., & Wilt, M. (2020). 3D borehole-to-surface and surface electromagnetic modeling and inversion in the presence of steel infrastructure. *Geophysics*, *85*, E139–E152. https://doi.org/10.1190/geo2019-0034.1

Weiss, M., Neytcheva, M., & Kalscheuer, T. (2023). Iterative solution methods for 3D controlled-source electromagnetic forward modelling of geophysical exploration scenarios. *Computational Geosciences*, *27*, 81–102. https://doi.org/10.1007/s10596-022-10182-2

Werthmüller, D., Mulder, W. A., & Slob, E. C. (2019). emg3d: A multigrid solver for 3D electromagnetic diffusion. *Journal of Open Source Software*, *4*(39), 1463. https://doi.org/10.21105/joss.01463

Werthmüller, D., Rochlitz, R., Castillo-Reyes, O., & Heagy, L. (2021). Towards an open-source landscape for 3-d CSEM modelling. *Geophysical Journal International*, *227*(1), 644–659. https://doi.org/10.1093/gji/ggab238