elfe3D
Modelling with the total electric field approach using finite elements in 3D
User manual

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1 About

`elfe3D` is a 3D forward modelling code that simulates electric and magnetic field responses from frequency-domain controlled-source electromagnetic setups. It uses tetrahedral meshes and first-order finite-element approximations. `elfe3D` was validated in [6].

To balance problem sizes and solution accuracy, adaptive mesh refinement approaches are implemented. They are based on error estimators obtained by calculating face jumps in the normal current density, the tangential magnetic field and residuals and combined with amplitude-dependent weights. Also, global mesh quality improvement (q-refinement) can be applied during the refinement procedure. See [6, 1, 5] for details.

`elfe3D` is designed in modern `Fortran` and uses shared-memory parallelisation with `OpenMP`. It uses a direct solver to solve the system of equations. Variable model parameters are isotropic electric resistivities and magnetic permeabilities. Extended line or loop sources are modelled along element edges.

A first version of `elfe3D` was developed by Paula Rulff with contributions from Laura Maria Buntin and Thomas Kalscheuer at Uppsala University from 2018-2023. The code development was financed by the Smart Exploration project (European Union's Horizon 2020 funding, grant agreement No. 775971).

A modified version of `elfe3D` is implemented in the inversion software `emilia` [4, 3, 2, 7] available upon request for purely academic purposes from Thomas Kalscheuer (thomas.kalscheuer@geo.uu.se).

Further developments of `elfe3D` by Paula Rulff, now at Delft University of Technology, are ongoing. Suggestions for improvements are welcome via p.rulff@tudelft.nl.

1.1 Theory

Please have a look at pages 26-30 in [5].

1.2 Implementation

Please have a look at pages 34-40 in [5].

2 Getting Started

2.1 Installation

`elfe3D` can be compiled with `gfortran` or `ifort`. The provided Makefile is based on `gfortran` compilation. `gfortran` should be part of your system in Gnu compiler collection (gcc). Also, `OpenBLAS` and `make` packages are required. The latest compilation was performed on Ubuntu 22.04.
The following steps guide you through the `elfe3D` compilation:

- `tetgen`: The open source mesh generator `tetgen` must be installed. It can be downloaded from `https://wias-berlin.de/software/index.jsp?id=TetGen&lang=1` or directly installed via typing in your terminal:

  ```
  $ sudo apt install tetgen
  ```

  If you would like to run the provided example model, you can create the mesh input files in your `elfe3D`/in folder with

  ```
  $ tetgen -pq1.3kAaen CSEM_input_model.poly
  ```

- `MUMPS` is an open source direct solver available at `https://mumps-solver.org`. Read the MUMPS documentation for installation instructions! Link the `MUMPS` routines in your Makefile.
  Short example of `MUMPS_5.7.3` compilation:

  ```
  $ tar zxvf MUMPS_5.7.3.tar.gz
  $ cd MUMPS_5.7.3
  $ cp Make.inc/Makefile.debian.SEQ Makefile.inc
  $ make all
  ```

  Copy the following files, `MUMPS` is your `MUMPS` folder and `elfe3D` is your `elfe3D` folder:

```
$ cp MUMPS/libseq/mpif.h elfe3D/elfe3D/.
$ cp MUMPS/include/zmumps_root.h elfe3D/elfe3D/.
$ cp MUMPS/include/zmumps_struc.h elfe3D/elfe3D/.
```

- Modify your makefile as appropriate. At least, adjust LIBDIR in the `elfe3D` Makefile:

```
$ LIBDIR = /path/to/your/MUMPS_5.7.3/lib
```

- Compile `elfe3D` in your `elfe3D` folder by typing in your terminal:

```
$ make all
```

- Run `elfe3D` with

```
$ ./elfe3d
```

2.2 Input files

Input files for `elfe3D` are located in
`elfe3D`/in

- `elfe3D_input.txt`: This is the most important input file. It contains model and mesh refinement information as well as specifications for in and output files. `elfe3D_input.txt` must contain the following keywords:
  - solver: Followed by an integer. The only option that is currently available is option 2: `MUMPS`.
  - model_size: Define the following below keyword model_size
    minimum x,y,z coordinates of model
    maximum x,y,z coordinates of model
  - num_freq: Followed by an integer that specifies the number of frequencies. List the actual frequencies in the lines below.
  - num_rec: Followed by an integer that specifies the number of receivers. List the receiver coordinates in the lines below.

- output_E_file: Specify the path and filename of the output file for electric field components behind this keyword. The output file will contain the frequencies and real and imaginary electric field components in the following order: frequency — Ex — Ey — Ez
- output_H_file: Specify the path and filename of the output file for magnetic field components behind this keyword. The output file will contain the frequencies and real and imaginary magnetic field components in the following order: frequency — Hx — Hy — Hz
- source_type: Followed by an integer. Several options are implemented. If you specify the source corners in the `source.txt` file, you can choose either option 6 (segmented line source) or option 7 (segmented loop source). Coordinates of source start and end-points can also be specified below this keyword.
- current_direction: Followed by an integer that specifies the current direction. Line source: current in positive direction (0), current in negative direction (1). Loop source: clockwise current (0), anticlockwise current (1).
- source_moment: Followed by a number that specifies the source moment $m = Idl$
- PEC_present: Followed by an integer that specifies the presence of a perfect electric conductor (PEC). See [1] for more information. No PEC present (0), PEC present (1).
- num_PEC: Followed by the number of PECs with start and end coordinates below.
- model_file_name: Specify the path and filename of the model input file, without file name extension, but with a . at the end.
- maxRefSteps: Followed by an integer that specifies the maximum number of mesh refinement steps. Set to 0 for forward simulations for several frequencies without mesh refinement.
- maxUnknowns: Followed by an integer that specifies the maximum number of unknowns for the mesh refinement.
- betaRef: threshold for the number of elements to be refined
- accuracyTol: accuracy tolerance < 1

  - vtk: Followed by an integer that specifies if `yourmodel.vtk` files should be written during the refinement (1), set to 0 for forward simulations only without refinement.
  - errorEst_method: Method for error estimation. residuals (1), residuals and face jumps J (2), residuals and face jumps J and H (3), face jumps J (4), face jumps H (5), face jumps J & H (6)
  - refStrategy: Refinement strategy. Constant quality factor (0), maxRefSteps-1 on low-quality mesh, last step high-quality mesh (1), increasing quality factor (2), increasing quality factor on mesh with detailed subsurface anomaly (-T and -d option added) (3)

- `yourmodel.poly`: The required model files can be generated with the mesh generator `tetgen` described in the `tetgen` manual. Region numbers have to be specified in the input model file (`.poly` file), receiver locations must be within small elements and edges must be placed along the source cable locations. No node or edge markers are required. `yourmodel.node`, `yourmodel.edge`, `yourmodel.ele`, `yourmodel.neigh` and `yourmodel.vtk` files are expected as input files.

- `regionparameters.txt`: This file specifies the model parameters within the model regions. The following is an example for a model with three different regions (eleattr): air (1), half space (2) and a conductive anomaly (3) and their resistivities (rho), relative magnetic permeabilities (`mu_r`) and relative electric permittivities (`epsilon_r`). (`epsilon_r`) is currently not used in the forward simulations.

```
# eleattr
3
# eleattr rho mu_r epsilon_r
1 100000000.0 1.0  0.0
2 100.0       1.0  0.0
3 10.0        1.0  0.0
```

- `source.txt`: This file specifies the number and locations of source corner points. For a straight line source, it contains only start and endpoints as e.g.

```
2
-50.0 0 0
50.0 0 0
```

2.3 Example

You find an examplary 3D CSEM resistivity model in
`elfe3D`/in
Information about the model are in
`elfe3D`/in/readme_CSEM_input_model.txt

3 Citation

If you publish results generated with `elfe3D`, please give credit to the `elfe3D` developers by citing:

Paula Rulff, Laura M Buntin, Thomas Kalscheuer, Efficient goal-oriented mesh refinement in 3-D finite-element modelling adapted for controlled source electromagnetic surveys, Geophysical Journal International, Volume 227, Issue 3, December 2021, Pages 1624–1645, https://doi.org/10.1093/gji/ggab264

and refer to the `elfe3D` the version you used using the ZENODO DOI:
Link to Zenodo DOI

Do not forget to acknowledge MUMPS and tetgen developers!

4 License

Bibliography

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[5] Paula Rulff. *Three-dimensional forward modelling and inversion of controlled-source electromagnetic data using the edge-based finite-element method*. PhD thesis, Uppsala University, 2023.

[6] Paula Rulff, Laura M Buntin, and Thomas Kalscheuer. Efficient goal-oriented mesh refinement in 3D finite-element modelling adapted for controlled-source electromagnetic surveys. *Geophysical Journal International*, 227:1624–1645, 2021. doi: 10.1093/gji/ggab264.

[7] Paula Rulff and Thomas Kalscheuer. 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*, 2024.