emg3d Documentation

Release 0.12.0

The emg3d Developers

User Manual

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Version: 0.12.0 ~ Date: 25 July 2020

A multigrid solver for 3D electromagnetic diffusion with tri-axial electrical anisotropy. The matrix-free solver can be used as main solver or as preconditioner for one of the Krylov subspace methods implemented in *scipy.sparse.linalg*, and the governing equations are discretized on a staggered Yee grid. The code is written completely in Python using the NumPy/SciPy-stack, where the most time- and memory-consuming parts are sped up through jitted numba-functions.

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More information

For more information regarding installation, usage, contributing, roadmap, bug reports, and much more, see

- Website: https://empymod.github.io,
- Documentation: https://emg3d.readthedocs.io,
- Source Code: https://github.com/empymod/emg3d,
- Examples: https://empymod.github.io/emg3d-gallery.

Features

- Multigrid solver for 3D electromagnetic (EM) diffusion with regular grids (where source and receiver can be electric or magnetic).
- Compute the 3D EM field in the complex frequency domain or in the real Laplace domain.
- Includes also routines to compute the 3D EM field in the time domain.
- Can be used together with the SimPEG-framework.
- Can be used as a standalone solver or as a pre-conditioner for various Krylov subspace methods implemented in SciPy, e.g., BiCGSTAB (*scipy.sparse.linalg.bicgstab*) or CGS (*scipy.sparse.linalg.cgs*).
- Tri-axial electrical anisotropy.
- Isotropic magnetic permeability.
- Semicoarsening and line relaxation.
- Grid-size can be anything.
- As a multigrid method it scales with the number of unknowns N and has therefore optimal complexity O(N).

Installation

You can install emg3d either via conda (preferred):

conda install -c conda-forge emg3d

or via pip:

pip install emg3d

Minimum requirements are Python version 3.7 or higher and the modules scipy and numba. Various other packages are recommended or required for some advanced functionalities (xarray, discretize, matplotlib, h5py, empymod, scooby). Consult the installation notes in the manual for more information regarding installation, requirements, and soft dependencies.

Citation

If you publish results for which you used *emg3d*, please give credit by citing Werthmüller et al. (2019):

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

All releases have a Zenodo-DOI, which can be found on 10.5281/zenodo.3229006.

See CREDITS for the history of the code.

10 Chapter 4. Citation

License information

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5.1 Getting started

The code emg3d ([WeMS19]) is a three-dimensional modeller for electromagnetic (EM) diffusion as used, for instance, in controlled-source EM (CSEM) surveys frequently applied in the search for, amongst other, groundwater, hydrocarbons, and minerals.

The core of the code is primarily based on [Muld06], [Muld07], and [Muld08]. You can read more about the background of the code in the chapter *Credits*. An introduction to the underlying theory of multigrid methods is given in the chapter *Theory*, and further literature is provided in the *References*.

5.1.1 Installation

You can install emg3d either via conda:

```
conda install -c conda-forge emg3d
```

or via pip:

```
pip install emg3d
```

Minimum requirements are Python version 3.7 or higher and the modules scipy and numba. Various other packages are recommended or required for some advanced functionalities, namely:

- xarray: For the Survey class (many sources and receivers at once).
- discretize: For advanced meshing tools (fancy mesh-representations and plotting utilities).
- matplotlib: To use the plotting utilities within discretize.
- h5py: Save and load data in the HDF5 format.
- empymod: Time-domain modelling (utils.Fourier).
- scooby: For the version and system report (emg3d.Report()).

If you are new to Python we recommend using a Python distribution, which will ensure that all dependencies are met, specifically properly compiled versions of NumPy and SciPy; we recommend using Anaconda. If you install Anaconda you can simply start the *Anaconda Navigator*, add the channel conda-forge and emg3d will appear in the package list and can be installed with a click.

Using NumPy and SciPy with the Intel Math Kernel Library (*mkl*) can significantly improve computation time. You can check if mkl is used via conda list: The entries for the BLAS and LAPACK libraries should contain something with mkl, not with openblas. To enforce it you might have to create a file pinned, containing the line libblas [build=*mkl] in the folder path-to-your-conda-env/conda-meta/.

5.1.2 Basic Example

Here we show a *very* basic example. To see some more realistic models have a look at the gallery. This particular example is also there, with some further explanations and examples to show how to plot the model and the data; see Minimum working example. It also contains an example without using discretize.

First, we load emg3d and discretize (to create a mesh), along with numpy:

```
>>> import emg3d
>>> import discretize
>>> import numpy as np
```

First, we define the mesh (see discretize. TensorMesh for more info). In reality, this task requires some careful considerations. E.g., to avoid edge effects, the mesh should be large enough in order for the fields to dissipate, yet fine enough around source and receiver to accurately model them. This grid is too small, but serves as a minimal example.

```
>>> grid = discretize.TensorMesh(
           [[(25, 10, -1.04), (25, 28), (25, 10, 1.04)],
>>>
           [(50, 8, -1.03), (50, 16), (50, 8, 1.03)],
>>>
           [(30, 8, -1.05), (30, 16), (30, 8, 1.05)]],
>>>
           x0='CCC')
>>> print (grid)
 TensorMesh: 49,152 cells
                    MESH EXTENT
                                         CELL WIDTH
                                                        FACTOR
 dir
        nC
                 min max
                                        min max
                                                          max
  Х
        48
                -662.16 662.16
                                        25.00 37.01
        32
                -857.96
                              857.96
                                        50.00
                                                  63.34
                                                          1.03
  V
        32
                              540.80
                -540.80
                                                  44.32
                                                          1.05
  Z
```

Next we define a very simple fullspace model with $\rho_x=1.5\,\Omega$ m, $\rho_y=1.8\,\Omega$ m, and $\rho_z=3.3\,\Omega$ m. The source is an x-directed dipole at the origin, with a 10 Hz signal of 1 A.

```
>>> model = emg3d.models.Model(grid, res_x=1.5, res_y=1.8, res_z=3.3)
>>> sfield = emg3d.fields.get_source_field(
>>> grid, src=[0, 0, 0, 0, 0], freq=10.0)
```

Now we can compute the electric field with emg3d:

(continues on next page)

(continued from previous page)

```
Coarsest grid :
                                       => 12 cells
  Coarsest level :
                           4 ;
   [hh:mm:ss] rel. error
                                         [abs. error, last/prev]
      h_
     2h_ \
     4h_
     8h_
    16h_
   [11:18:17]
             2.623e-02 after
                                 1 F-cycles
                                              [1.464e-06, 0.026]
   [11:18:17]
               2.253e-03 after
                                 2 F-cycles
                                              [1.258e-07, 0.086]
                                              [1.704e-08, 0.135]
               3.051e-04 after
                                 3 F-cycles
   [11:18:17]
               5.500e-05 after
                                              [3.071e-09, 0.180]
                                 4 F-cycles
   [11:18:17]
               1.170e-05 after
                                5 F-cycles
                                              [6.531e-10, 0.213]
                                                                   0 0
   [11:18:18]
               2.745e-06 after
                                              [1.532e-10, 0.235]
                                6 F-cycles
                                                                   0 0
   [11:18:18]
                                              [3.837e-11, 0.250]
               6.873e-07 after
                                7 F-cycles
   [11:18:18]
                                                                   0 0
  > CONVERGED
  > MG cycles
  > Final rel. error : 6.873e-07
:: emg3d END :: 15:24:42 :: runtime = 0:00:02
```

So the computation required seven multigrid F-cycles and took just a bit more than 2 seconds. It was able to coarsen in each dimension four times, where the input grid had 49,152 cells, and the coarsest grid had 12 cells.

5.1.3 Related ecosystem

To create advanced meshes it is recommended to use discretize from the SimPEG framework. It also comes with some neat plotting functionalities to plot model parameters and resulting fields. Furthermore, it can serve as a link to use PyVista to create nice 3D plots even within a notebook.

Projects which can be used to compare or validate the results are, e.g., empymod for layered models or SimPEG for 3D models. It is also possible to create a geological model with GemPy and, again via discretize, move it to emg3d to compute CSEM responses for it.

Have a look at the gallery for many examples of how to use emg3d together with the mentioned projects and more!

5.1.4 Tipps and Tricks

The function <code>emg3d.solver.solve()</code> is the main entry point, and it takes care whether multigrid is used as a solver or as a preconditioner (or not at all), while the actual multigrid solver is <code>emg3d.solver.multigrid()</code>. Most input parameters for <code>emg3d.solver.solve()</code> are sufficiently described in its docstring. Here a few additional information.

• You can input any three-dimensional grid into emg3d. However, the implemented multigrid technique works with the existing nodes, meaning there are no new nodes created as coarsening is done by combining adjacent cells. The more times the grid dimension can be divided by two the better it is suited for MG. Ideally, the dimension of the coarsest grid should be a low prime number p, for which good sizes can then be computed with $p2^n$. Good grid sizes (in each direction) up to 1024 are

```
- 22<sup>0,1,...,9</sup>: 2, 4, 8, 16, 32, 64, 128, 256, 512, 1024,

- 32<sup>0,1,...,8</sup>: 3, 6, 12, 24, 48, 96, 192, 384, 768,
```

- 52^{0,1,...,7}: 5, 10, 20, 40, 80, 160, 320, 640,

 $-72^{0,1,\dots,7}$: 7, 14, 28, 56, 112, 224, 448, 896,

and preference decreases from top to bottom row. Good grid sizes in sequential order: 2, 3, 4, 5, 6, 7, 8, 10, 12, 14, 16, 20, 24, 28, 32, 40, 48, 56, 64, 80, 96, 112, 128, 160, 192, 224, 256, 320, 384, 448, 512, 640, 768, 896, 1024.

- The multigrid method can be used as a solver or as a preconditioner, for instance for BiCGSTAB. Using multigrid as a preconditioner for BiCGSTAB together with semicoarsening and line relaxation is the most stable version, but expensive, and therefore only recommended on highly stretched grids. Which combination of solver is best (fastest) depends to a large extent on the grid stretching. As a rule of thumb:
 - No stretching: Multigrid (MG);
 - Moderate stretching (< 1.04): BiCGSTAB with MG as pre-conditioner;
 - Strong stretching (> 1.04): BicGSTAB with MG as preconditioner and line relaxation/semicoarsening.

5.1.5 Contributing and Roadmap

New contributions, bug reports, or any kind of feedback is always welcomed! Have a look at the Roadmap-project to get an idea of things that could be implemented. The GitHub issues and PR's are also a good starting point. The best way for interaction is at https://github.com/empymod or by joining the Slack channel «em-x-d» of SimPEG. If you prefer to get in touch outside of GitHub/Slack use the contact form on https://werthmuller.org.

To install emg3d from source, you can download the latest version from GitHub and install it in your python distribution via:

```
python setup.py install
```

Please make sure your code follows the pep8-guidelines by using, for instance, the python module flake8, and also that your code is covered with appropriate tests. Just get in touch if you have any doubts.

The structure of emg3d is:

- solver: These are the main routines, the flow of the multigrid method;
- n jited: The expensive parts (computation, memory) are here in jitted functions; and
- utils: Some helper routines.

5.1.6 Tests and benchmarks

The modeller comes with a test suite using pytest. If you want to run the tests, just install pytest and run it within the emg3d-top-directory.

```
> pytest --cov=emg3d --flake8
```

It should run all tests successfully. Please let us know if not!

Note that installations of em3gd via conda or pip do not have the test-suite included. To run the test-suite you must download emg3d from GitHub.

There is also a benchmark suite using *airspeed velocity*, located in the empymod/emg3d-asv-repository. The results of my machine can be found in the empymod/emg3d-bench, its rendered version at empymod.github.io/emg3d-asv.

5.1.7 License

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5.2 Multi-what?

If you have never heard of the multigrid method before you might ask yourself "*multi-what*?" The following is an intent to describe the multigrid method without the maths; just some keywords and some figures. **It is a heavily simplified intro, using a 2D grid for simplicity.** Have a look at the *Theory*-section for more details. A good, fourpage intro with some maths is given by [Muld11]. More in-depth information can be found, e.g., in [BrHM00], [Hack85], and [Wess91].

The multigrid method ([Fedo64])

- is an iterative solver;
- scales almost linearly (CPU & RAM);
- can serve as a pre-conditioner or as a solver on its own.

The main driving motivation to use multigrid is the part about linear scaling.

5.2.1 Matrix-free solver

The implemented multigrid method is a matrix free solver, it never constructs the full matrix. This is how it achieves its relatively low memory consumption. To solve the system, it solves for all fields adjacent to one node, moves then to the next node, and so on until it reaches the last node, see Figure 5.1, where the red lines indicate the fields which are solved simultaneously per step (the fields on the boundaries are never computed, as they are assumed to be 0).

Figure 5.1:: The multigrid solver solves by default on a node-by-node basis.

Normally, you would have to do this over and over again to achieve a good approximate solution. multigrid typically does it only a few times per grid, typically 2 times (one forward, one backward). This is why it is called **smoother**, as it only smoothes the error, it does not solve it. The implemented method for this is the *Gauss-Seidel* method.

Iterative solver which work in this matrix-free manner are typically **very fast at solving for the local problem**, hence at reducing the **high frequency error**, but **very slow at solving the global problem**, hence at reducing the **low frequency error**. High and low frequency errors are meant relatively to cell-size here.

5.2.2 Moving between different grids

The main thinking behind multigrid is now that we move to coarser grids. This has two advantages:

- Fewer cells means faster computation and less memory.
- Coarser grid size transforms lower frequency error to higher frequency error, relatively to cell size, which means faster convergence.

The implemented multigrid method simply joins two adjacent cells to get from finer to coarser grids, see Figure 5.2 for an example coarsening starting with a 16 cells by 16 cells grid.

Figure 5.2:: Example of the implemented coarsening scheme.

There are different approaches how to cycle through different grid sizes, see Figures 5.7 to 5.9. The downsampling from a finer grid to a coarser grid is often termed **restriction**, whereas the interpolation from a coarser grid to a finer grid is termed **prolongation**.

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5.2.3 Specialities

The convergence rate of the multigrid method suffers on severely stretched grids or by models with strong anisotropy. Two techniques are implemented, **semicoarsening** (Figure 5.3) and **line relaxation** (Figure 5.4). Both require more CPU and higher RAM per grid than the standard multigrid, but they can improve the convergence rate, which then in turn improves the overall CPU time.

Figure 5.3:: Example of semicoarsening: The cell size is kept constant in one direction. The direction can be alternated between iterations.

Figure 5.4:: Example of line relaxation: The system is solved for all fields adjacent to a whole line of nodes simultaneously in some direction. The direction can be alternated between iterations.

5.3 Theory

The following provides an introduction to the theoretical foundation of the solver *emg3d*. More specific theory is covered in the docstrings of many functions, have a look at the *Code*-section or follow the links to the corresponding functions here within the theory. If you just want to use the solver, but do not care much about the internal functionality, then the function emg3d.solver.solve() is the only function you will ever need. It is the main entry point, and it takes care whether multigrid is used as a solver or as a preconditioner (or not at all), while the actual multigrid solver is emg3d.solver.multigrid().

Note: This section is not an independent piece of work. Most things are taken from one of the following sources:

- [Muld06], pages 634-639:
 - The Maxwell's equations and Discretisation sections correspond with some adjustemens and additions to pages 634-636.
 - The start of *The Multigrid Method* corresponds roughly to page 637.
 - Pages 638 and 639 are in parts reproduced in the code-docstrings of the corresponding functions.
- [BrHM00]: This book is an excellent introduction to multigrid methods. Particularly the *Iterative Solvers* section is taken to a big extent from the book.

Please consult these original resources for more details, and refer to them for citation purposes and not to this manual. More in-depth information can also be found in, e.g., [Hack85] and [Wess91].

5.3.1 Maxwell's equations

Maxwell's equations in the presence of a current source J_s are

$$\partial_t \mathbf{B}(\mathbf{x}, t) + \nabla \times \mathbf{E}(\mathbf{x}, t) = 0,
\nabla \times \mathbf{H}(\mathbf{x}, t) - \partial_t \mathbf{D}(\mathbf{x}, t) = \mathbf{J}_c(\mathbf{x}, t) + \mathbf{J}_s(\mathbf{x}, t),$$
(5.1)

where the conduction current $J_{\rm c}$ obeys Ohm's law,

$$\mathbf{J}_{c}(\mathbf{x},t) = \sigma(\mathbf{x})\mathbf{E}(\mathbf{x},t). \tag{5.2}$$

Here, $\sigma(\mathbf{x})$ is the conductivity. $\mathbf{E}(\mathbf{x},t)$ is the electric field and $\mathbf{H}(\mathbf{x},t)$ is the magnetic field. The electric displacement $\mathbf{D}(\mathbf{x},t) = \varepsilon(\mathbf{x})\mathbf{E}(\mathbf{x},t)$ and the magnetic induction $\mathbf{B}(\mathbf{x},t) = \mu(\mathbf{x})\mathbf{H}(\mathbf{x},t)$. The dielectric constant or permittivity ε can be expressed as $\varepsilon = \varepsilon_r \varepsilon_0$, where ε_r is the relative permittivity and ε_0 is the vacuum value. Similarly, the magnetic permeability μ can be written as $\mu = \mu_r \mu_0$, where μ_r is the relative permeability and μ_0 is the vacuum value.

The magnetic field can be eliminated from Equation (5.1), yielding the second-order parabolic system of equations,

$$\varepsilon \partial_{tt} \mathbf{E} + \sigma \partial_{t} \mathbf{E} + \nabla \times \mu^{-1} \nabla \times \mathbf{E} = -\partial_{t} \mathbf{J}_{s}. \tag{5.3}$$

To transform from the time domain to the frequency domain, we substitute

$$\mathbf{E}(\mathbf{x},t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathbf{\hat{E}}(\mathbf{x},\omega) e^{-i\omega t} d\omega, \tag{5.4}$$

and use a similar representation for $\mathbf{H}(\mathbf{x},t)$. The resulting system of equations is

$$-s\mu_0(\sigma + s\varepsilon)\hat{\mathbf{E}} - \nabla \times \mu_r^{-1}\nabla \times \hat{\mathbf{E}} = s\mu_0\hat{\mathbf{J}}_s, \tag{5.5}$$

where $s=-\mathrm{i}\omega$. The multigrid method converges in the case of the diffusive approximation (with its smoothing and approximation properties), but not in the high-frequency range (at least not in the implemented form of the multigrid method in emg3d). The code emg3d assumes therefore the diffusive approximation, hence only low frequencies are considered that obey $|\omega\varepsilon| \ll \sigma$. In this case we can set $\varepsilon=0$, and Equation (5.5) simplifies to

$$-s\mu_0\sigma\hat{\mathbf{E}} - \nabla \times \mu_r^{-1}\nabla \times \hat{\mathbf{E}} = s\mu_0\hat{\mathbf{J}}_s,\tag{5.6}$$

From here on, the hats are omitted. We use the perfectly electrically conducting boundary

$$\mathbf{n} \times \mathbf{E} = 0 \quad \text{and} \quad \mathbf{n} \cdot \mathbf{H} = 0,$$
 (5.7)

where ${\bf n}$ is the outward normal on the boundary of the domain.

The Maxwell's equations and Ohm's law are solved in the **frequency domain**. The **time-domain** solution can be obtained by taking the inverse Fourier transform.

Note: [Muld06] uses the time convention $e^{-i\omega t}$, see Equation (5.4), with $s=-i\omega$. However, the code emg3d uses the convention $e^{i\omega t}$, hence $s=i\omega$. This is the same convention as used in empymod, and commonly in CSEM.

Laplace domain

It is also possible to solve the problem in the **Laplace domain**, by using a real value for s in Equation (5.6), instead of the complex value $-i\omega$. This simplifies the problem from complex numbers to real numbers, which accelerates the computation. It also improves the convergence rate, as the solution is a smoother function. The solver emg3d. solver.solve() is agnostic to the data type of the provided source field, and can solve for real and complex problems, hence frequency and Laplace domain. See the documentation of the functions $emg3d.fields.get_source_field()$ and emg3d.models.Model() to see how you can use emg3d for Laplace-domain computations.

5.3.2 Discretisation

Equation (5.6) can be discretised by the finite-integration technique ([Weil77], [ClWe01]). This scheme can be viewed as a finite-volume generalization of [Yee66]'s scheme for tensor-product Cartesian grids with variable grid spacings. An error analysis for the constant-coefficient case ([MoSu94]) showed that both the electric and magnetic field components have second-order accuracy.

Consider a tensor-product Cartesian grid with nodes at positions (x_k, y_l, z_m) , where $k = 0, \dots, N_x, l = 0, \dots, N_y$ and $m = 0, \dots, N_z$. There are $N_x \times N_y \times N_z$ cells having these nodes as vertices. The cell centres are located at

$$x_{k+1/2} = \frac{1}{2} (x_k + x_{k+1}),$$

$$y_{l+1/2} = \frac{1}{2} (y_l + y_{l+1}),$$

$$z_{m+1/2} = \frac{1}{2} (z_m + z_{m+1}).$$
(5.8)

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The material properties, σ and μ_r , are assumed to be given as cell-averaged values. The electric field components are positioned at the edges of the cells, as shown in Figure 5.5, in a manner similar to Yee's scheme. The first component of the electric field $E_{1,k+1/2,l,m}$ should approximate the average of $E_1(x,y_l,z_m)$ over the edge from x_k to x_{k+1} at given y_l and z_m . Here, the average is defined as the line integral divided by the length of the integration interval. The other components, $E_{2,k,l+1/2,m}$ and $E_{3,k,l,m+1/2}$, are defined in a similar way. Note that these averages may also be interpreted as point values at the midpoint of edges:

$$E_{1,k+1/2,l,m} \simeq E_1 \left(x_{k+1/2}, y_l, z_m \right),$$

$$E_{2,k,l+1/2,m} \simeq E_2 \left(x_k, y_{l+1/2}, z_m \right),$$

$$E_{3,k,l,m+1/2} \simeq E_3 \left(x_k, y_l, z_{m+1/2} \right).$$
(5.9)

The averages and point-values are the same within second-order accuracy.

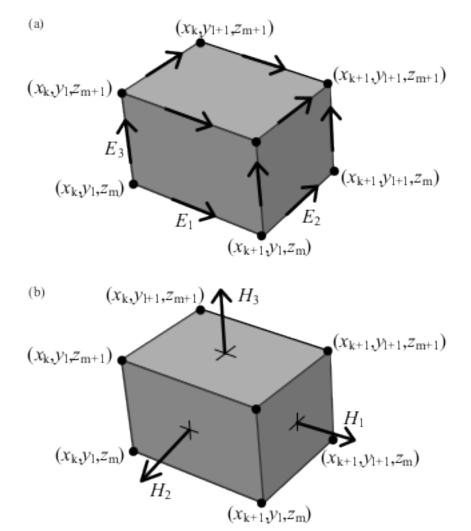


Figure 5.5:: (a) A grid cell with grid nodes and edge-averaged components of the electric field. (b) The face-averaged magnetic field components that are obtained by taking the curl of the electric field.

For the discretisation of the term $-s\mu_0\sigma\mathbf{E}$ related to Ohm's law, dual volumes related to edges are introduced. For a given edge, the dual volume is a quarter of the total volume of the four adjacent cells. An example for E_1 is shown in Figure 5.6(b). The vertices of the dual cell are located at the midpoints of the cell faces.

The volume of a normal cell is defined as

$$V_{k+1/2,l+1/2,m+1/2} = h_{k+1/2}^x h_{l+1/2}^y h_{m+1/2}^z, (5.10)$$

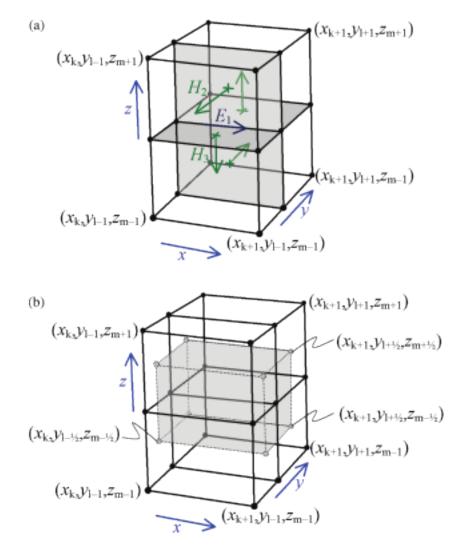


Figure 5.6:: The first electric field component $E_{1,k,l,m}$ is located at the intersection of the four cells shown in (a). Four faces of its dual volume are sketched in (b). The first component of the curl of the magnetic field should coincide with the edge on which E_1 is located. The four vectors that contribute to this curl are shown in (a). They are defined as normals to the four faces in (a). Before computing their curl, these vectors are interpreted as tangential components at the faces of the dual volume shown in (b). The curl is evaluated by taking the path integral over a rectangle of the dual volume that is obtained for constant x and by averaging over the interval $[x_k, x_{k+1}]$.

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where

$$h_{k+1/2}^{x} = x_{k+1} - x_{k},$$

$$h_{l+1/2}^{y} = y_{l+1} - y_{l},$$

$$h_{m+1/2}^{z} = z_{m+1} - z_{m}.$$
(5.11)

For an edge parallel to the x-axis on which $E_{1,k+1/2,l,m}$ is located, the dual volume is

$$V_{k+1/2,l,m} = \frac{1}{4} h_{k+1/2}^x \sum_{m_2=0}^1 \sum_{m_2=0}^1 h_{l-1/2+m_2}^y h_{m-1/2+m_3}^z.$$
 (5.12)

With the definitions,

$$d_k^x = x_{k+1/2} - x_{k-1/2},$$

$$d_l^y = y_{l+1/2} - y_{l-1/2},$$

$$d_m^z = z_{m+1/2} - z_{m-1/2},$$
(5.13)

we obtain

$$\begin{aligned} V_{k+1/2,l,m} &= h_{k+1/2}^x d_l^y d_m^z, \\ V_{k,l+1/2,m} &= d_k^x h_{l+1/2}^y d_m^z, \\ V_{k,l,m+1/2} &= d_k^x d_l^y h_{m+1/2}^z. \end{aligned} \tag{5.14}$$

Note that Equation (5.13) does not define d_k^x , etc., at the boundaries. We may simply take $d_0^x = h_{1/2}^x$ at k = 0, $d_{N_x}^x = h_{N_x - 1/2}^x$ at $k = N_x$ and so on, or use half of these values as was done by [MoSu94].

The discrete form of the term $-s\mu_0\sigma\mathbf{E}$ in Equation (5.6), with each component multiplied by the corresponding dual volume, becomes $\mathcal{S}_{k+1/2,l,m}$ $E_{1,k+1/2,l,m}$, $\mathcal{S}_{k,l+1/2,m}$ $E_{2,k,l+1/2,m}$ and $\mathcal{S}_{k,l,m+1/2}$ for the first, second and third components, respectively. Here $\mathcal{S} = -s\mu_0\sigma V$ is defined in terms of cell-averages. At the edges parallel to the x-axis, an averaging procedure similar to (5.12) gives

$$S_{k+1/2,l,m} = \frac{1}{4} \left(S_{k+1/2,l-1/2,m-1/2} + S_{k+1/2,l+1/2,m-1/2} + S_{k+1/2,l-1/2,m+1/2} + S_{k+1/2,l-1/2,m+1/2} + S_{k+1/2,l+1/2,m+1/2} \right).$$
(5.15)

 $\mathcal{S}_{k,l+1/2,m}$ and $\mathcal{S}_{k,l,m+1/2}$ are defined in a similar way.

The curl of ${\bf E}$ follows from path integrals around the edges that bound a face of a cell, drawn in Figure 5.5(a). After division by the area of the faces, the result is a face-averaged value that can be positioned at the centre of the face, as sketched in Figure 5.5(b). If this result is divided by ${\rm i}\omega\mu$, the component of the magnetic field that is normal to the face is obtained. In order to find the curl of the magnetic field, the magnetic field components that are normal to faces are interpreted as tangential components at the faces of the dual volumes. For E_1 , this is shown in Figure 5.6. For the first component of Equation (5.6) on the edge (k+1/2,l,m) connecting (x_k,y_l,z_m) and (x_{k+1},y_l,z_m) , the corresponding dual volume comprises the set $[x_k,x_{k+1}]\times[y_{l-1/2},y_{l+1/2}]\times[z_{m-1/2},z_{m+1/2}]$ having volume $V_{k+1/2,l,m}$.

The scaling by μ_r^{-1} at the face requires another averaging step because the material properties are assumed to be given as cell-averaged values. We define $\mathcal{M}=V\mu_r^{-1}$, so

$$\mathcal{M}_{k+1/2,l+1/2,m+1/2} = h_{k+1/2}^x h_{l+1/2}^y h_{m+1/2}^z \mu_{r,k+1/2,l+1/2,m+1/2}^{-1}$$
(5.16)

for a given cell (k+1/2, l+1/2, m+1/2). An averaging step in, for instance, the z-direction gives

$$\mathcal{M}_{k+1/2,l+1/2,m} = \frac{1}{2} \left(\mathcal{M}_{k+1/2,l+1/2,m-1/2} + \mathcal{M}_{k+1/2,l+1/2,m+1/2} \right)$$
 (5.17)

at the face (k+1/2, l+1/2, m) between the cells (k+1/2, l+1/2, m-1/2) and (k+1/2, l+1/2, m+1/2).

Starting with $\mathbf{v} = \nabla \times \mathbf{E}$, we have

$$v_{1,k,l+1/2,m+1/2} = e_{l+1/2}^{y} \left(E_{3,k,l+1,m+1/2} - E_{3,k,l,m+1/2} \right)$$

$$- e_{m+1/2}^{z} \left(E_{2,k,l+1/2,m+1} - E_{2,k,l+1/2,m} \right),$$

$$v_{2,k+1/2,l,m+1/2} = e_{m+1/2}^{z} \left(E_{1,k+1/2,l,m+1} - E_{1,k+1/2,l,m} \right)$$

$$- e_{k+1/2}^{x} \left(E_{3,k+1,l,m+1/2} - E_{3,k,l,m+1/2} \right),$$

$$v_{3,k+1/2,l+1/2,m} = e_{k+1/2}^{x} \left(E_{2,k+1/2,l+1,m} - E_{1,k+1/2,l,m} \right)$$

$$- e_{l+1/2}^{y} \left(E_{1,k+1/2,l+1,m} - E_{1,k+1/2,l,m} \right).$$

$$(5.18)$$

Here,

$$e_{k+1/2}^x = 1/h_{k+1/2}^x, \quad e_{l+1/2}^y = 1/h_{l+1/2}^y, \quad e_{m+1/2}^z = 1/h_{m+1/2}^z.$$
 (5.19)

Next, we let

$$u_{1,k,l+1/2,m+1/2} = \mathcal{M}_{k,l+1/2,m+1/2} v_{1,k,l+1/2,m+1/2},$$

$$u_{2,k+1/2,l,m+1/2} = \mathcal{M}_{k+1/2,l,m+1/2} v_{2,k+1/2,l+1/2,m},$$

$$u_{3,k+1/2,l+1/2,m} = \mathcal{M}_{k+1/2,l+1/2,m} v_{3,k+1/2,l+1/2,m}.$$
(5.20)

Note that these components are related to the magnetic field components by

$$u_{1,k,l+1/2,m+1/2} = i\omega\mu_0 V_{k,l+1/2,m+1/2} H_{1,k+1/2,l,m+1/2},$$

$$u_{2,k+1/2,l,m+1/2} = i\omega\mu_0 V_{k+1/2,l,m+1/2} H_{2,k+1/2,l,m+1/2},$$

$$u_{3,k+1/2,l+1/2,m} = i\omega\mu_0 V_{k+1/2,l+1/2,m} H_{3,k+1/2,l+1/2,m},$$
(5.21)

where

$$\begin{split} V_{k,l+1/2,m+1/2} &= d_k^x h_{l+1/2}^y h_{m+1/2}^z, \\ V_{k+1/2,l,m+1/2} &= h_{k+1/2}^x d_l^y h_{m+1/2}^z, \\ V_{k+1/2,l+1/2,m} &= h_{k+1/2}^x h_{l+1/2}^y d_m^z. \end{split} \tag{5.22}$$

The discrete representation of the source term $i\omega\mu_0 \mathbf{J}_s$, multiplied by the appropriate dual volume, is

$$\begin{split} s_{1,k+1/2,l,m} &= \mathrm{i}\omega \mu_0 V_{k+1/2,l,m} J_{1,k+1/2,l,m}, \\ s_{2,k,l+1/2,m} &= \mathrm{i}\omega \mu_0 V_{k,l+1/2,m} J_{2,k,l+1/2,m}, \\ s_{3,k,l,m+1/2} &= \mathrm{i}\omega \mu_0 V_{k,l,m+1/2} J_{3,k,l,m+1/2}. \end{split} \tag{5.23}$$

Let the residual for an arbitrary electric field that is not necessarily a solution to the problem be defined as

$$\mathbf{r} = V \left(i\omega \mu_0 \mathbf{J}_s + -s\mu_0 \sigma \mathbf{E} - \nabla \times \mu_r^{-1} \nabla \times \mathbf{E} \right). \tag{5.24}$$

Its discretisation is

$$r_{1,k+1/2,l,m} = s_{1,k+1/2,l,m} + \mathcal{S}_{k+1/2,l,m} E_{1,k+1/2,l,m} \\ - \left[e_{l+1/2}^{y} u_{3,k+1/2,l+1/2,m} - e_{l-1/2}^{y} u_{3,k+1/2,l-1/2,m} \right] \\ + \left[e_{m+1/2}^{z} u_{2,k+1/2,l,m+1/2} - e_{m-1/2}^{z} u_{2,k+1/2,l,m-1/2} \right], \\ r_{2,k,l+1/2,m} = s_{2,k,l+1/2,m} + \mathcal{S}_{k,l+1/2,m} E_{2,k,l+1/2,m} \\ - \left[e_{m+1/2}^{z} u_{1,k,l+1/2,m+1/2} - e_{m-1/2}^{z} u_{1,k,l+1/2,m-1/2} \right] \\ + \left[e_{k+1/2}^{x} u_{3,k+1/2,l+1/2,m} - e_{k-1/2}^{x} u_{3,k-1/2,l+1/2,m} \right], \\ r_{3,k,l,m+1/2} = s_{3,k,l,m+1/2} + \mathcal{S}_{k,l,m+1/2} E_{3,k,l,m+1/2} \\ - \left[e_{k+1/2}^{x} u_{2,k+1/2,l,m+1/2} - e_{k-1/2}^{x} u_{2,k-1/2,m+1/2} \right] \\ + \left[e_{l+1/2}^{y} u_{1,k,l+1/2,m+1/2} - e_{l-1/2}^{y} u_{1,k,l-1/2,m+1/2} \right].$$

The weighting of the differences in u_1 , etc., may appear strange. The reason is that the differences have been multiplied by the local dual volume. As already mentioned, the dual volume for $E_{1,k,l,m}$ is shown in Figure 5.6(b).

For further details of the discretisation see [Muld06] or [Yee66]. The actual meshing is done using discretize (part of the SimPEG-framework). The coordinate system of discretize uses a coordinate system were positive z is upwards.

The method is implemented in a matrix-free manner: the large sparse linear matrix that describes the discretised problem is never explicitly formed, only its action is evaluated on the latest estimate of the solution, thereby reducing storage requirements.

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5.3.3 Iterative Solvers

The multigrid method is an iterative (or relaxation) method and shares as such the underlying idea of iterative solvers. We want to solve the linear equation system

$$A\mathbf{x} = \mathbf{b},\tag{5.26}$$

where A is the $n \times n$ system matrix and x the unknown. If v is an approximation to x, then we can define two important measures. One is the error e

$$\mathbf{e} = \mathbf{x} - \mathbf{v},\tag{5.27}$$

which magnitude can be measured by any standard vector norm, for instance the maximum norm and the Euclidean or 2-norm defined respectively, by

$$\|\mathbf{e}\|_{\infty} = \max_{1 \le j \le n} |e_j|$$
 and $\|\mathbf{e}\|_2 = \sqrt{\sum_{j=1}^n e_j^2}$.

However, as the solution is not known the error cannot be computed either. The second important measure, however, is a computable measure, the residual r (computed in emg3d.solver.residual())

$$\mathbf{r} = \mathbf{b} - A\mathbf{v}.\tag{5.28}$$

Using Equation (5.27) we can rewrite Equation (5.26) as

$$A\mathbf{e} = \mathbf{b} - A\mathbf{v}$$
,

from which we obtain with Equation (5.28) the Residual Equation

$$A\mathbf{e} = \mathbf{r}.\tag{5.29}$$

The Residual Correction is given by

$$\mathbf{x} = \mathbf{v} + \mathbf{e}.\tag{5.30}$$

5.3.4 The Multigrid Method

Note: If you have never heard of multigrid methods before you might want to read through the *Multi-what?*-section.

Multigrid is a numerical technique for solving large, often sparse, systems of equations, using several grids at the same time. An elementary introduction can be found in [BrHM00]. The motivation for this approach follows from the observation that it is fairly easy to determine the local, short-range behaviour of the solution, but more difficult to find its global, long-range components. The local behaviour is characterized by oscillatory or rough components of the solution. The slowly varying smooth components can be accurately represented on a coarser grid with fewer points. On coarser grids, some of the smooth components become oscillatory and again can be easily determined.

The following constituents are required to carry out multigrid. First, a sequence of grids is needed. If the finest grid on which the solution is to be found has a constant grid spacing h, then it is natural to define coarser grids with spacings of 2h, 4h, etc. Let the problem on the finest grid be defined by $A^h \mathbf{x}^h = \mathbf{b}^h$. The residual is $\mathbf{r}^h = \mathbf{b}^h - A^h \mathbf{x}^h$ (see the corresponding function emg3d.solver.residual (), and for more details also the function $emg3d.core.amat_x$ ()). To find the oscillatory components for this problem, a smoother or relaxation scheme is applied. Such a scheme is usually based on an approximation of A^h that is easy to invert. After one or more smoothing steps (see the corresponding function emg3d.solver.smoothing()), say ν_1 in total, convergence will slow down because it is generally difficult to find the smooth, long-range components of the solution. At this point, the problem is mapped to a coarser grid, using a restriction operator \hat{I}_h^{2h} (see

the corresponding function emg3d.solver.restriction(), and for more details, the functions $emg3d.core.restrict_weights()$ and emg3d.core.restrict(). On the coarse-grid, $\mathbf{b}^{2h} = \tilde{I}_h^{2h}\mathbf{r}^h$. The problem $\mathbf{r}^{2h} = \mathbf{b}^{2h} - A^{2h}\mathbf{x}^{2h} = 0$ is now solved for \mathbf{x}^{2h} , either by a direct method if the number of points is sufficiently small or by recursively applying multigrid. The resulting approximate solution needs to be interpolated back to the fine grid and added to the solution. An interpolation operator I_{2h}^h , usually called prolongation in the context of multigrid, is used to update $\mathbf{x}^h := \mathbf{x}^h + I_{2h}^h\mathbf{x}^{2h}$ (see the corresponding function emg3d.solver.prolongation()). Here $I_{2h}^h\mathbf{x}^{2h}$ is called the coarse-grid correction. After prolongation, ν_2 additional smoothing steps can be applied. This constitutes one multigrid iteration.

So far, we have not specified the coarse-grid operator A^{2h} . It can be formed by using the same discretisation scheme as that applied on the fine grid. Another popular choice, $A^{2h} = \tilde{I}_h^{2h} A^h I_{2h}^h$, has not been considered here. Note that the tilde is used to distinguish restriction of the residual from operations on the solution, because these act on elements of different function spaces.

If multigrid is applied recursively, a strategy is required for moving through the various grids. The simplest approach is the V-cycle shown in Figure 5.7 for the case of four grids. Here, the same number of pre- and post-smoothing steps is used on each grid, except perhaps on the coarsest. In many cases, the V-cycle does not solve the coarse-grid equations sufficiently well. The W-cycle, shown in Figure 5.8, will perform better in that case. In a W-cycle, the number of coarse-grid corrections is doubled on subsequent coarser grids, starting with one coarse-grid correction on the finest grid. Because of its cost, it is often replaced by the F-cycle (Figure 5.9). In the F-cycle, the number of coarse-grid corrections increases by one on each subsequent coarser grid.

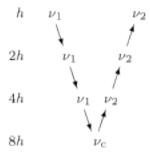


Figure 5.7:: V-cycle with ν_1 pre-smoothing steps and ν_2 post-smoothing steps. On the coarsest grid, ν_c smoothing steps are applied or an exact solver is used. The finest grid has a grid spacing h and the coarsest 8h. A single coarse-grid correction is computed for all grids but the coarsest.

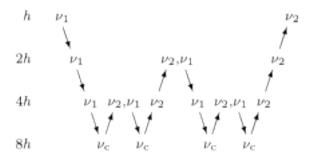


Figure 5.8:: W-cycle with ν_1 pre-smoothing steps and ν_2 post-smoothing steps. On each grid except the coarsest, the number of coarse-grid corrections is twice that of the underlying finer grid.

One reason why multigrid methods may fail to reach convergence is strong anisotropy in the coefficients of the governing partial differential equation or severely stretched grids (which has the same effect as anisotropy). In that case, more sophisticated smoothers or coarsening strategies may be required. Two strategies are currently implemented, *semicoarsening* and *line relaxation*, which can be used on their own or combined. Semicoarsening is when the grid is only coarsened in some directions. Line relaxation is when in some directions the whole gridlines of values are found simultaneously. If slow convergence is caused by just a few components of the solution, a Krylov subspace method can be used to remove them. In this way, multigrid is accelerated by a Krylov method. Alternatively, multigrid might be viewed as a preconditioner for a Krylov method.

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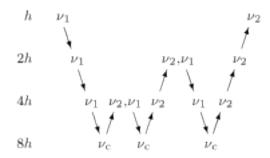


Figure 5.9:: F-cycle with ν_1 pre-smoothing steps and ν_2 post-smoothing steps. On each grid except the coarsest, the number of coarse-grid corrections increases by one compared to the underlying finer grid.

Gauss-Seidel

The smoother implemented in emg3d is a Gauss-Seidel smoother. The Gauss-Seidel method solves the linear equation system $A\mathbf{x} = \mathbf{b}$ iteratively using the following method:

$$\mathbf{x}^{(k+1)} = L_*^{-1} \left(\mathbf{b} - U \mathbf{x}^{(k)} \right) , \qquad (5.31)$$

where L_* is the lower triangular component, and U the strictly upper triangular component, $A = L_* + U$. On the coarsest grid it acts as direct solver, whereas on the finer grid it acts as a smoother with only few iterations.

See the function emg3d.solver.smoothing(), and for more details, the functions emg3d.core.gauss_seidel(), emg3d.core.gauss_seidel_x(), emg3d.core.gauss_seidel_y(), emg3d.core.gauss_seidel_z(), and also emg3d.core.blocks_to_amat().

Choleski factorisation

The actual solver of the system $A\mathbf{x} = \mathbf{b}$ is a non-standard Cholesky factorisation without pivoting for a symmetric, complex matrix A tailored to the problem of the multigrid solver, using only the main diagonal and five lower off-diagonals of the banded matrix A. The result is the same as simply using, e.g., numpy.linalg.solve(), but faster for the particular use-case of this code.

See emg3d.core.solve() for more details.

5.4 CPU & RAM

The multigrid method is attractive because it shows optimal scaling for both runtime and memory consumption. In the following are a few notes regarding memory and runtime requirements. It also contains information about what has been tried and what still could be tried in order to improve the current code.

5.4.1 Runtime

The gallery contains a script to do some testing with regards to runtime, see the Tools Section. An example output of that script is shown in Figure 5.10.

Figure 5.10:: Runtime as a function of cell size, which shows nicely the linear scaling of multigrid solvers (using a single thread).

The costliest functions (for big models) are:

- >90 %: emg3d.solver.smoothing() (emg3d.core.gauss_seidel())
- <5 % each, in decreasing importance:

- emg3d.solver.prolongation() (emg3d.solver.RegularGridProlongator)
- emg3d.solver.residual()(emg3d.core.amat_x())
- emg3d.solver.restriction()

Example with 262,144 / 2,097,152 cells (nu_{i,1,c,2}=0,2,1,2; sslsolver=False; semicoarsening=True; linerelaxation=True):

- 93.7/95.8 % smoothing
- 3.6/2.0% prolongation
- 1.9/1.9% residual
- 0.6/0.4% restriction

The rest can be ignored. For small models, the percentage of smoothing goes down and of prolongation and restriction go up. But then the modeller is fast anyway.

 $emg3d.core.gauss_seidel()$ and $emg3d.core.amat_x()$ are written in numba; jitting emg3d.solver.RegularGridProlongator turned out to not improve things, and many functions used in the restriction are jitted too. The costliest functions (RAM- and CPU-wise) are therefore already written in numba.

Any serious attempt to improve the speed will have to tackle the smoothing itself.

Things which could be tried

- Not much has been tested with the numba-options parallel; prange; and nogil.
- There might be an additional gain by making emg3d.meshes.TensorMesh, emg3d.models. Model, and emg3d.fields.Field instances jitted classes.

Things which have been tried

- One important aspect of the smoothing part is the memory layout. <code>emg3d.core.gauss_seidel()</code> and <code>emg3d.core.gauss_seidel_x()</code> are ideal for F-arrays (loop z-y-x, hence slowest to fastest axis). <code>emg3d.core.gauss_seidel_y()</code> and <code>emg3d.core.gauss_seidel_z()</code>, however, would be optimal for C-arrays. But copying the arrays to C-order and afterwards back is costlier in most cases for both CPU and RAM. The one possible and therefore implemented solution was to swap the loop-order in <code>emg3d.core.gauss_seidel_y()</code>.
- Restriction and prolongation information could be saved in a dictionary instead of recomputing it every time. Turns out to be not worth the trouble.
- Rewrite emg3d.RegularGridInterpolator as jitted function, but the iterator approach seems to be better for large grids.

5.4.2 Memory

Most of the memory requirement comes from storing the data itself, mainly the fields (source field, electric field, and residual field) and the model parameters (resistivity, eta, mu). For a big model, they some up; e.g., almost 3 GB for an isotropic model with 256x256x256 cells.

The gallery contains a script to do some testing with regards to the RAM usage, see the Tools Section. An example output of that script is shown in Figure 5.11.

Figure 5.11:: RAM usage, showing the optimal behaviour of multigrid methods. "Data RAM" is the memory required by the fields (source field, electric field, residual field) and by the model parameters (resistivity; and eta, mu). "MG Base" is for solving one Gauss-Seidel iteration on the original grid. "MG full RAM" is for solving one multigrid F-Cycle.

The theory of multigrid says that in an ideal scenario, multigrid requires 8/7 (a bit over 1.14) the memory requirement of carrying out one Gauss-Seidel step on the finest grid. As can be seen in the figure, for models up to 2 million cells that holds pretty much, afterwards it becomes a bit worse.

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However, for this estimation one has to run the model first. Another way to estimate the requirement is by starting from the RAM used to store the fields and parameters. As can be seen in the figure, for big models one is on the save side estimating the required RAM as 1.35 times the storage required for the fields and model parameters.

The figure also shows nicely the linear behaviour of multigrid; for twice the number of cells twice the memory is required (from a certain size onwards).

Attempts at improving memory usage should focus on the difference between the red line (actual usage) and the dashed black line (1.14 x base usage).

5.5 Gallery

The gallery with many examples can be found at empymod.github.io/emg3d-gallery.

5.6 References

5.7 Credits

This project was started by **Dieter Werthmüller**. Every contributor will be listed here and is considered to be part of «The emg3d Developers»:

• Dieter Werthmüller

Various bits got improved through discussions on Slack at SWUNG and at SimPEG, thanks to both communities. Special thanks to @jokva (general), @banesullivan (visualization), @joferkington (interpolation), and @jcapriot (volume averaging).

5.7.1 Historical credits

The core of *emg3d* is a complete rewrite and redesign of the multigrid code by **Wim A. Mulder** ([Muld06], [Muld07], [Muld08], [MuWS08]), developed at Shell and at TU Delft. Various authors contributed to the original code, amongst others, **Tom Jönsthövel** ([JoOM06]; improved solver for strongly stretched grids), **Marwan Wirianto** ([WiMS10], [WiMS11]; computation of time-domain data), and **Evert C. Slob** ([SIHM10]; analytical solutions). The original code was written in Matlab, where the most time- and memory-consuming parts were sped up through mex-files (written in C). It included multigrid with or without BiCGSTAB, VTI resistivity, semi-coarsening, and line relaxation; the number of cells had to be powers of two, and coarsening was done only until the first dimension was at two cells. As such it corresponded roughly to *emg3d v0.3.0*.

See the References in the manual for the full citations and a more extensive list.

Note: This software was initially (till 05/2021) developed at *Delft University of Technology* (https://www.tudelft. nl) within the **Gitaro.JIM** project funded through MarTERA as part of Horizon 2020, a funding scheme of the European Research Area (ERA-NET Cofund, https://www.martera.eu).

5.8 Changelog

5.8.1 recent versions

v0.12.0 : Survey & Simulation

2020-07-25

This is a big release with many new features, and unfortunately not completely backwards compatible. The main new features are the new **Survey** and **Simulation** classes, as well as some initial work for **optimization** (misfit, gradient). Also, a **Model** can now be a resistivity model, a conductivity model, or the logarithm (natural or base 10) therefore. Receivers can now be arbitrarily rotated, just as the sources. In addition to the existing **soft-dependencies** *empymod*, *discretize*, and *h5py* there are the new soft-dependencies *xarray* and *tqm*; *discretize* is now much tighter integrated. For the new survey and simulation classes *xarray* is a required dependency. However, the only hard dependency remain *scipy* and *numba*, if you use *emg3d* purely as a solver. Data reading and writing has new a JSON-backend, in addition to the existing HDF5 and NumPy-backends.

In more detail:

- Modules:
 - surveys (**new**; requires xarray):
 - * Class surveys. Survey, which combines sources, receivers, and data.
 - * Class surveys. Dipole, which defines electric or magnetic point dipoles and finite length dipoles.
 - *simulations* (**new**; requires *xarray*; soft-dependency *tqdm*):
 - * Class *simulations.Simulation*, which combines a survey with a model. A simulation computes the e-field (and h-field) asynchronously using *concurrent.futures*. This class will include automatic, source- and frequency-dependent gridding in the future. If *tqdm* is installed it displays a progress bar for the asynchronous computation. Note that the simulation class has still some limitations, consult the class documentation.

- models:

- * Model instances take new the parameters *property_{x,y;z}* instead of *res_{x,y;z}*. The properties can be either resistivity, conductivity, or log_{e;10} thereof. What is actually provided has to be defined with the parameter *mapping*. By default, it remains resistivity, as it was until now. The keywords *res_{x,y;z}* are **deprecated**, but still accepted at the moment. The attributes *model.res_{x,y;z}* are still available too, but equally **deprecated**. However, it is **no longer possible to assign values to these attributes**, which is a **backwards incompatible** change.
- * A model knows now how to interpolate itself from its grid to another grid (interpolate2grid).

- maps:

- * **New** mappings for *models.Model* instances: The mappings take care of how to transform the investigation variable to conductivity and back, and how it affects its derivative.
- * New interpolation routine edges2cellaverages.

- fields:

- * Function get_receiver_response (new), which returns the response for arbitrarily rotated receivers.
- * Improvements to Field and SourceField:
 - · sval and smu0 not stored any longer, derived from freq.
 - · SourceField is now using the copy() and from_dict() from its parents class Field.

- *io*:

- * File-format *json* (**new**), writes to a hierarchical, plain json file.
- * **Deprecated** the use of *backend*, it uses the file extension of *fname* instead.
- * This means .npz (instead of numpy), .h5 (instead of h5py), and new .json.
- * New parameter *collect_classes*, which can be used to switch-on collection of the main classes in root-level dictionaries. By default, they are no longer collected (**changed**).

- meshes:

* meshes. Tensor Mesh new inherits from discretize if installed.

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- * Added <u>eq</u> to *models.TensorMesh* to compare meshes.
- optimize (new)
 - * Functionalities related to inversion (data misfit, gradient, data weighting, and depth weighting). This module is in an early stage, and the API will likely change in the future. Current functions are *misfit*, *gradient* (using the adjoint-state method), and *data_weighting*. These functionalities are best accessed through the *Simulation* class.

· Dependencies:

- *empymod* is now a soft dependency (no longer a hard dependency), only required for *utils.Fourier* (time-domain modelling).
- Existing soft dependency discretize is now baked straight into meshes.
- New soft dependency xarray for the Survey class (and therefore also for the Simulation class and the optimize module).
- New soft dependency *tqdm* for nice progress bars in asynchronous computation.

• **Deprecations** and removals:

- Removed deprecated functions *data_write* and *data_read*.
- Removed all deprecated functions from utils.

• Miscellaneous:

- Re-organise API-docs.
- Much bookkeeping (improve error raising and checking; chaining errors, numpy types, etc).

v0.11.0 : Refactor

2020-05-05

Grand refactor with new internal layout. Mainly splitting-up *utils* into smaller bits. Most functionalities (old names) are currently retained in *utils* and it should be mostly backwards compatible for now, but they are deprecated and will eventually be removed. Some previously deprecated functions were removed, however.

- Removed deprecated functions:
 - emg3d.solver.solver (use emg3d.solver.solve instead).
 - Aliases of emg3d.io.data_write and emg3d.io.data_read in emg3d.utils.

• Changes:

- SourceField has now the same signature as Field (this might break your code if you called SourceField directly, with positional arguments, and not through get_source_field).
- More functions and classes in the top namespace.
- Replaced *core.l2norm* with *scipy.linalg.norm*, as SciPy 1.4 got the following PR: https://github.com/scipy/scipy/pull/10397 (reason to raise minimum SciPy to 1.4).
- Increased minimum required versions of dependencies to
 - * scipy >= 1.4.0 (raised from 1.1, see note above)
 - * *empymod*>=2.0.0 (no min requirement before)
 - * numba > = 0.45.0 (raised from 0.40)

• New layout

- njitted -> core.
- utils split in fields, meshes, models, maps, and utils.
- Bugfixes:

- Fixed to_dict, from_dict, and copy for the SourceField.
- Fixed *io* for *SourceField*, that was not implemented properly.

5.8.2 v0.8.0 - v0.10.x

v0.10.1 : Zero Source

2020-04-29

- Bug fixes:
 - Checks now if provided source-field is zero, and exists gracefully if so, returning a zero electric field.
 Until now it failed with a division-by-zero error.
- Improvements:
 - Warnings: If verb=1 it prints a warning in case it did not converge (it finished silently until now).
 - Improvements to docs (figures-scaling; intersphinx).
 - Adjust Fields.pha and Fields.amp in accordance with empymod v2: .pha and .amp are now methods; uses directly empymod.utils.EMArray.
 - Adjust tests for empymod v2 (Fields, Fourier).

v0.10.0 : Data persistence

2020-03-25

- New:
 - New functions emg3d.save and emg3d.load to save and load all sort of emg3d instances. The
 currently implemented backends are h5py for .h5-files (default, but requires h5py to be installed)
 and numpy for .npz-files.
 - Classes emg3d.utils.Field, emg3d.utils.Model, and emg3d.utils.TensorMesh have new methods.copy(),.to_dict(), and .from_dict().
 - emg3d.utils.Model: Possible to create new models by adding or subtracting existing models, and comparing two models (+, -, == and !=). New attributes shape and size.
 - emg3d.utils.Model does not store the volume any longer (just vnC).
- Deprecations:
 - Deprecated data_write and data_read.
- Internal and bug fixes:
 - All I/O-related stuff moved to its own file io.py.
 - Change from NUMBA_DISABLE_JIT to use py_func for testing and coverage.
 - Bugfix: emg3d.njitted.restrict did not store the $\{x;y;z\}$ -field if sc_dir was $\{4;5;6\}$, respectively.

v0.9.3 : Sphinx gallery

2020-02-11

 Rename solver.solver to solver.solve; load solve also into the main namespace as emg3d. solve.

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- Adjustment to termination criterion for *STAGNATION*: The current error is now compared to the last error of the same cycle type. Together with this the workaround for sslsolver when called with an initial efield introduced in v0.8.0 was removed.
- Adjustment to utils.get_hx_h0 (this might change your boundaries): The computation domain is now computed so that the distance for the signal travelling from the source to the boundary and back to the most remote receiver is at least two wavelengths away. If this is within the provided domain, then now extra buffer is added around the domain. Additionally, the function has a new parameter max_domain, which is the maximum distance from the center to the boundary; defaults to 100 km.
- New parameter log for utils.grid2grid; if True, then the interpolation is carried out on a log10-scale
- Change from the notebook-based emg3d-examples-repo to the sphinx-based emg3d-gallery-repo.

v0.9.2 : Complex sources

2019-12-26

- Strength input for get_source_field can now be complex; it also stores now the source location and its strength and moment.
- get_receiver can now take entire Field instances, and returns in that case (fx, fy, fz) at receiver locations.
- Krylov subspace solvers:
 - Solver now finishes in the middle of preconditioning cycles if tolerance is reached.
 - Solver now aborts if solution diverges or stagnates also for the SSL solvers; it fails and returns a zero field.
 - Removed gmres and lgmres from the supported SSL solvers; they do not work nice for this problem. Supported remain bicgstab (default), cgs, and gcrotmk.
- Various small things:
 - New attribute Field.is_electric, so the field knows if it is electric or magnetic.
 - New verb-possibility: verb=−1 is a continuously updated one-liner, ideal to monitor large sets of computations or in inversions.
 - The returned info dictionary contains new keys:
 - * runtime_at_cycle: accumulated total runtime at each cycle;
 - * error_at_cycle: absolute error at each cycle.
 - Simple __repr__ for TensorMesh, Model, Fourier, Time.
- Bugfixes:
 - Related to get_hx_h0, data_write, printing in Fourier.

v0.9.1: VolumeModel

2019-11-13

- New class VolumeModel; changes in Model:
 - Model now only contains resistivity, magnetic permeability, and electric permittivity.
 - VolumeModel contains the volume-averaged values eta and zeta; called from within emg3d. solver.solver.
 - Full wave equation is enabled again, via epsilon_r; by default it is set to None, hence diffusive approximation.

- Model parameters are now internally stored as 1D arrays.
- An {isotropic, VTI, HTI} initiated model can be changed by providing the missing resistivities.
- Bugfix: Up and till version 0.8.1 there was a bug. If resistivity was set with slices, e.g., model.res[:, :, :5]=1e10, it DID NOT update the corresponding eta. This bug was unintentionally fixed in 0.9.0, but only realised now.

• Various:

- The log now lists the version of emg3d.
- PEP8: internal imports now use absolute paths instead of relative ones.
- Move from conda-channel prisae to conda-forge.
- Automatic deploy for PyPi and conda-forge.

v0.9.0 : Fourier

2019-11-07

- New routine:
 - emg3d.utils.Fourier, a class to handle Fourier-transform related stuff for time-domain modelling. See the example notebooks for its usage.

• Utilities:

- Fields and returned receiver-arrays (EMArray) both have amplitude (.amp) and phase (.pha) attributes.
- Fields have attributes containing frequency-information (freq, smu0).
- New class SourceField; a subclass of Field, adding vector and v{x,y,z} attributes for the
 real valued source vectors.
- The Model is not frequency-dependent any longer and does NOT take a freq-parameter any more (currently it still takes it, but it is deprecated and will be removed in the future).
- data_write automatically removes _vol from TensorMesh instances and _eta_{x,y,z}, _zeta from Model instances. This makes the archives smaller, and they are not required, as they are simply reconstructed if needed.

• Internal changes:

- The multigrid method, as implemented, only works for the diffusive approximation. Nevertheless, we always used \sigma-i\omega\epsilon, hence a complex number. This is now changed and \epsilon set to 0, leaving only \sigma.
- Change time convention from exp(-iwt) to exp(iwt), as used in empymod and commonly in CSEM. Removed the parameter conjugate from the solver, to simplify.
- Change own private class variables from ___ to _.
- res and mu_r are now checked to ensure they are >0; freq is checked to ensure !=0.
- New dependencies and maintenance:
 - empymod is a new dependency.
 - Travis now checks all the url's in the documentation, so there should be no broken links down the road. (Check is allowed to fail, it is visual QC.)

• Bugfixes:

- Fixes to the setuptools_scm-implementation (MANIFEST.in).

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v0.8.1: setuptools scm

2019-10-22

• Implement setuptools_scm for versioning (adds git hashes for dev-versions).

v0.8.0 : Laplace

2019-10-04

- Laplace-domain computation: By providing a negative freq-value to utils.get_source_field and utils.Model, the computation is carried out in the real Laplace domain s = freq instead of the complex frequency domain s = 2i*pi*freq.
- New meshing helper routines (particularly useful for transient modelling where frequency-dependent/adaptive meshes are inevitable):
 - utils.get_hx_h0 to get cell widths and origin for given parameters including a few fixed interfaces (center plus two, e.g. top anomaly, sea-floor, and sea-surface).
 - utils.get_cell_numbers to get good values of number of cells for given primes.
- Speed-up njitted.volume_average significantly thanks to @jcapriot.
- Bugfixes and other minor things:
 - Abort if 12-norm is NaN (only works for MG).
 - Workaround for the case where a sslsolver is used together with a provided initial efield.
 - Changed parameter rho to res for consistency reasons in utils.get_domain.
 - Changed parameter h_min to min_width for consistency reasons in utils. get_stretched_h.

5.8.3 v0.1.0 - v0.7.x

v0.7.1: JOSS article

2019-07-17

- Version of the JOSS article, https://doi.org/10.21105/joss.01463.
- New function utils.grid2grid to move from one grid to another. Both functions (utils.get_receiver and utils.grid2grid) can be used for fields and model parameters (with or without extrapolation). They are very similar, the former taking coordinates (x, y, z) as new points, the latter one another TensorMesh instance.
- New jitted function njitted.volume_average for interpolation using the volume-average technique.
- New parameter conjugate in solver.solver to permit both Fourier transform conventions.
- Added exit_status and exit_message to info_dict.
- Add section Related ecosystem to documentation.

v0.7.0 : H-field

2019-07-05

- New routines:
 - utils.get_h_field: Small routine to compute the magnetic field from the electric field using Faraday's law.

- utils.get_receiver: Small wrapper to interpolate a field at receiver positions. Added 3D spline interpolation; is the new default.
- Re-implemented the possibility to define isotropic magnetic permeabilities in utils.Model. Magnetic permeability is not tri-axially included in the solver currently; however, it would not be too difficult to include if there is a need.
- CPU-graph added on top of RAM-graph.
- Expand utils.Field to work with pickle/shelve.
- Jit np.linalg.norm (njitted.12norm).
- Use scooby (soft dependency) for versioning, rename Version to Report (backwards incompatible).
- Bug fixes:
 - Small bugfix introduced in ebd2c9d5: sc_cycle and lr_cycle was not updated any longer at the end of a cycle (only affected sslsolver=True.
 - Small bugfix in utils.get_hx.

v0.6.2: CPU & RAM

2019-06-03

Further speed and memory improvements:

- Add CPU & RAM-page to documentation.
- Change loop-order from x-z-y to z-x-y in Gauss-Seidel smoothing with line relaxation in y-direction. Hence reversed lexicographical order. This results in a significant speed-up, as x is the fastest changing axis.
- Move total residual computation from solver.residual into njitted.amat_x.
- Simplifications in utils:
 - Simplify utils.get_source_field.
 - Simplify utils. Model.
 - Removed unused timing-stuff from early development.

v0.6.1: Memory

2019-05-28

Memory and speed improvements:

- Only compute residual and 12-norm when absolutely necessary.
- Inplace computations for np.conjugate in solver.solver and np.subtract in solver. residual.

v0.6.0 : RegularGridInterpolator

2019-05-26

- Replace scipy.interpolate.RegularGridInterpolator with a custom tailored version of it (solver.RegularGridProlongator); results in twice as fast prolongation.
- Simplify the fine-grid computation in prolongation without using gridE*; memory friendlier.
- Submission to JOSS.
- Add *Multi-what?*-page to documentation.
- Some major refactoring, particularly in solver.

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- Removed discretize as hard dependency.
- Rename rdir and ldir (and related p*dir; *cycle) to the more descriptive sc_dir and lr_dir.

v0.5.0: Accept any grid size

2019-05-01

- First open-source version.
- Include RTD, Travis, Coveralls, Codacy, and Zenodo. No benchmarks yet.
- Accepts now any grid size (warns if a bad grid size for MG is provided).
- Coarsens now to the lowest level of each dimension, not only to the coarsest level of the smallest dimension.
- Combined restrict_rx, restrict_ry, and restrict_rz to restrict.
- Improve speed by passing pre-allocated arrays to jitted functions.
- Store res_y, res_z and corresponding eta_y, eta_z only if res_y, res_z were provided in initial call to utils.model.
- Change zeta to v_mu_r.
- Include rudimentary TensorMesh-class in utils; removes hard dependency on discretize.
- Bugfix: Take a provided efield into account; don't return if provided.

v0.4.0 : Cholesky

2019-03-29

- Use solve_chol for everything, remove solve_zlin.
- Moved mesh.py and some functionalities from solver.py into utils.py.
- New mesh-tools. Should move to discretize eventually.
- Improved source generation tool. Might also move to discretize.
- printversion is now included in utils.
- · Many bug fixes.
- Lots of improvements to tests.
- Lots of improvements to documentation. Amongst other, moved docs from __init__.py into the docs rst.

v0.3.0 : Semicoarsening

2019-01-18

- Semicoarsening option.
- Number of cells must still be 2ⁿ, but n can be different in the x-, y-, and z-directions.
- Many other iterative solvers from scipy.sparse.linalg can be used. It seems to work fine with the following methods:
 - scipy.sparse.linalg.bicgstab(): BIConjugate Gradient STABilize;
 - scipy.sparse.linalg.cgs(): Conjugate Gradient Squared;
 - scipy.sparse.linalg.gmres(): Generalized Minimal RESidual;
 - scipy.sparse.linalg.lgmres(): Improvement of GMRES using alternating residual vectors;

- scipy.sparse.linalg.gcrotmk(): GCROT: Generalized Conjugate Residual with inner Orthogonalization and Outer Truncation.
- The SciPy-solver or MG can be used all in combination or on its own, hence only MG, SciPy-solver with MG preconditioning, only SciPy-solver.

v0.2.0: Line relaxation

2019-01-14

• Line relaxation option.

v0.1.0 : Initial

2018-12-28

- Standard multigrid with or without BiCGSTAB.
- Tri-axial anisotropy.
- Number of cells must be 2ⁿ, and n has to be the same in the x-, y-, and z-directions.

5.9 Maintainers Guide

5.9.1 Making a release

- 1. Update CHANGELOG.rst.
- 2. Push it to GitHub, create a release tagging it.
- 3. Tagging it on GitHub will automatically deploy it to PyPi, which in turn will create a PR for the conda-forge feedstock. Merge that PR.
- 4. Check that:
- PyPi deployed;
- conda-forge deployed;
- Zenodo minted a DOI;
- emg3d.rtfd.io created a tagged version.

5.9.2 Useful things

• If there were changes to README, check it with:

```
python setup.py --long-description | rst2html.py --no-raw > index.html
```

• If unsure, test it first on testpypi (requires ~/.pypirc):

```
\sim/anaconda3/bin/twine upload dist/* -r testpypi
```

• If unsure, test the test-pypi for conda if the skeleton builds:

```
conda skeleton pypi --pypi-url https://test.pypi.io/pypi/ emg3d
```

• If it fails, you might have to install python3-setuptools:

```
sudo apt install python3-setuptools
```

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5.9.3 CI

Automatic bits

- Testing on Travis, includes:
 - Tests using pytest
 - Linting / code style with pytest-flake8
 - Ensure all http(s)-links work (sphinx linkcheck)
- Line-coverage with pytest-cov on Coveralls
- Code-quality on Codacy
- Manual on ReadTheDocs
- DOI minting on Zenodo

Manual things

- Benchmarks with Airspeed Velocity (asv)
- Gallery in emg3d-gallery (sphinx-gallery)

Automatically deploys if tagged

- PyPi
- conda -c conda-forge

5.10 Main solver routine

```
emg3d.solver.solve(grid, model, sfield, efield=None, cycle='F', sslsolver=False, semicoarsen-
ing=False, linerelaxation=False, verb=2, **kwargs)
Solver for 3D CSEM data with tri-axial electrical anisotropy.
```

The principal solver of emg3d is using the multigrid method as presented in [Muld06]. Multigrid can be used as a standalone solver, or as a preconditioner for an iterative solver from the <code>scipy.sparse.linalg-library</code>, e.g., <code>scipy.sparse.linalg.bicgstab()</code>. Alternatively, these Krylov subspace solvers can also be used without multigrid at all. See the cycle and sslsolver parameters.

Implemented are the F-, V-, and W-cycle schemes for multigrid (cycle parameter), and the amount of smoothing steps (initial smoothing, pre-smoothing, coarsest-grid smoothing, and post-smoothing) can be set individually (nu_init , nu_pre , nu_coarse , and nu_post , respectively). The maximum level of coarsening can be restricted with the clevel parameter.

Semicoarsening and line relaxation, as presented in [Muld07], are implemented, see the *semicoarsening* and *linerelaxation* parameters. Using the BiCGSTAB solver together with multigrid preconditioning with semicoarsening and line relaxation is slow but generally the most robust. Not using BiCGSTAB nor semicoarsening nor line relaxation is fast but may fail on stretched grids.

Parameters

```
grid [emg3d.meshes.TensorMesh] The grid. See emg3d.meshes.TensorMesh.
model [emg3d.models.Model] The model. See emg3d.models.Model.
sfield [emg3d.fields.SourceField] The source field. See emg3d.fields.
    get_source_field().
```

efield [emg3d.fields.Field, optional] Initial electric field. It is initiated with zeroes if not provided. A provided efield MUST have frequency information (initiated with emg3d.fields.Field(..., freq)).

If an initial efield is provided nothing is returned, but the final efield is directly put into the provided efield.

If an initial field is provided and a sslsolver is used, then it first carries out one multigrid cycle without semicoarsening nor line relaxation. The sslsolver is at times unstable with an initial guess, carrying out one MG cycle helps to stabilize it.

cycle [str; optional.] Type of multigrid cycle. Default is 'F'.

- 'V': V-cycle, simplest version;
- 'W': W-cycle, most expensive version;
- 'F': F-cycle, sort of a compromise between 'V' and 'W';
- None: Does not use multigrid, only sslsolver.

If None, *sslsolver* must be provided, and the *sslsolver* will be used without multigrid pre-conditioning.

Comparison of V (left), F (middle), and W (right) cycles for the case of four grids (three relaxation and prolongation steps):



sslsolver [str, optional] A scipy.sparse.linalg-solver, to use with MG as preconditioner or on its own (if cycle=None). Default is False.

Current possibilities:

- True or 'bicgstab': BIConjugate Gradient STABilized scipy.sparse.linalg.bicgstab();
- 'cgs': Conjugate Gradient Squared scipy.sparse.linalg.cgs();
- 'gcrotmk': GCROT: Generalized Conjugate Residual with inner Orthogonalization and Outer Truncation scipy.sparse.linalg.gcrotmk().

It does currently not work with 'cg', 'bicg', 'qmr', and 'minres' for various reasons (e.g., some require *rmatvec* in addition to *matvec*).

semicoarsening [int; optional] Semicoarsening. Default is False.

- True: Cycling over 1, 2, 3.
- 0 or False: No semicoarsening.
- 1: Semicoarsening in x direction.
- 2: Semicoarsening in y direction.
- 3: Semicoarsening in z direction.
- Multi-digit number containing digits from 0 to 3. Multigrid will cycle over these values, e.g., semicoarsening=1213 will cycle over [1, 2, 1, 3].

linerelaxation [int; optional] Line relaxation. Default is False.

This parameter is not respected on the coarsest grid, except if it is set to 0. If it is bigger than zero line relaxation on the coarsest grid is carried out along all dimensions which have more than 2 cells.

• True: Cycling over [4, 5, 6].

- 0 or False: No line relaxation.
- 1: line relaxation in x direction.
- 2: line relaxation in y direction.
- 3: line relaxation in z direction.
- 4: line relaxation in y and z directions.
- 5: line relaxation in x and z directions.
- 6: line relaxation in x and y directions.
- 7: line relaxation in x, y, and z directions.
- Multi-digit number containing digits from 0 to 7. Multigrid will cycle over these values, e.g., linerelaxation=1213 will cycle over [1, 2, 1, 3].

Note: Smoothing is generally done in lexicographical order, except for line relaxation in y direction; the reason is speed (memory access).

verb [int; optional] Level of verbosity (the higher the more verbose). Default is 2.

- 0: Print nothing.
- 1: Print warnings.
- 2: Print runtime and information about the method.
- 3: Print additional information for each MG-cycle.
- 4: Print everything (slower due to additional error computations).
- -1: Print one-liner (dynamically updated).

**kwargs [Optional solver options:]

• tol: float

Convergence tolerance. Default is 1e-6.

Iterations stop as soon as the norm of the residual has decreased by this factor, relative to the residual norm obtained for a zero electric field.

• maxit: int

Maximum number of multigrid iterations. Default is 50.

If sslsolver is used, this applies to the sslsolver.

In the case that multigrid is used as a pre-conditioner for the *sslsolver*, the maximum iteration for multigrid is defined by the maximum length of the *linerelaxation* and *semicoarsening*-cycles.

• nu_init : int

Number of initial smoothing steps, before MG cycle. Default is 0.

• nu pre: int

Number of pre-smoothing steps. Default is 2.

• nu_coarse : int

Number of smoothing steps on coarsest grid. Default is 1.

• nu_post: int

Number of post-smoothing steps. Default is 2.

• clevel: int

The maximum coarsening level can be different for each dimension and is, by default, automatically determined (clevel=-1). The parameter *clevel* can be used to restrict the maximum coarsening level in any direction by its value. Default is -1.

• return_info: bool

If True, a dictionary is returned with runtime info (final norm and number of iterations of MG and the sslsolver).

Returns

efield [emg3d.fields.Field] Resulting electric field. Is not returned but replaced inplace if an initial efield was provided.

info_dict [dict] Dictionary with runtime info; only if return_info=True.

Keys:

- exit: Exit status, 0=Success, 1=Failure;
- exit_message: Exit message, check this if exit=1;
- abs error: Absolute error;
- rel error: Relative error;
- ref_error: Reference error [norm(sfield)];
- *tol*: Tolerance (abs_error<ref_error*tol);
- *it_mg*: Number of multigrid iterations;
- it ssl: Number of SSL iterations;
- time: Runtime (s).
- runtime_at_cycle: Runtime after each cycle (s).
- *error_at_cycle*: Absolute error after each cycle.

Examples

```
>>> import emg3d
>>> import numpy as np
>>> # Create a simple grid, 8 cells of length 1 in each direction,
>>> # starting at the origin.
>>> grid = emg3d.meshes.TensorMesh(
>>>
          [np.ones(8), np.ones(8), np.ones(8)],
           x0=np.array([0, 0, 0]))
>>>
>>> # The model is a fullspace with tri-axial anisotropy.
>>> model = emg3d.models.Model(grid, res_x=1.5, res_y=1.8, res_z=3.3)
>>> # The source is a x-directed, horizontal dipole at (4, 4, 4)
>>> # with a frequency of 10 Hz.
>>> sfield = emg3d.fields.get_source_field(
          grid, src=[4, 4, 4, 0, 0], freq=10)
>>> # Compute the electric signal.
>>> efield = emg3d.solve(grid, model, sfield, verb=3)
>>> # Get the corresponding magnetic signal.
>>> hfield = emg3d.fields.get_h_field(grid, model, efield)
:: emg3d START :: 10:27:25 :: v0.9.1
                : 'F'
                                       sslsolver : False
  MG-cvcle
  semicoarsening : False [0]
                                       tol : 1e-06
   linerelaxation : False [0]
                                       maxit
                                                 : 50
```

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```
nu_{1,1,c,2} : 0, 2, 1, 2
                                   verb
  Original grid : 8 x 8 x 8
                                  => 512 cells
  Coarsest grid : 2 x 2 x 2
                                   => 8 cells
  Coarsest level: 2; 2; 2
                                     [abs. error, last/prev] l s
  [hh:mm:ss] rel. error
     h_
     2h_ \
     4h_ \/\/
  [10:27:25] 2.284e-02 after 1 F-cycles [1.275e-06, 0.023]
                                         [8.739e-08, 0.069]
  [10:27:25]
             1.565e-03 after
                               2 F-cycles
             1.295e-04 after
                                          [7.232e-09, 0.083]
                               3 F-cycles
  [10:27:25]
                                                             0 0
                                         [6.685e-10, 0.092]
            1.197e-05 after 4 F-cycles
                                                            0 0
  [10:27:25]
                                         [6.886e-11, 0.103]
                                                            0 0
            1.233e-06 after 5 F-cycles
  [10:27:25]
  [10:27:25] 1.415e-07 after 6 F-cycles [7.899e-12, 0.115] 0 0
  > CONVERGED
  > MG cycles
                  : 6
  > Final rel. error : 1.415e-07
:: emg3d END :: 10:27:25 :: runtime = 0:00:00
```

5.11 Code

Electromagnetic modeller in the diffusive limit (low frequencies) for 3D media with tri-axial electrical anisotropy. The matrix-free multigrid solver can be used as main solver or as preconditioner for one of the Krylov subspace methods implemented in <code>scipy.sparse.linalg</code>, and the governing equations are discretized on a staggered Yee grid. The code is written completely in Python using the <code>numpy/scipy-stack</code>, where the most time-consuming parts are sped-up through jitted <code>numba-functions</code>.

5.11.1 emg3d.meshes Module

meshes - Discretization

Everything related to meshes appropriate for the multigrid solver.

Functions

<pre>get_hx_h0(freq, res, domain[, fixed,])</pre>	Return cell widths and origin for given parameters.	
<pre>get_cell_numbers(max_nr[, max_prime,</pre>	Returns 'good' cell numbers for the multigrid method.	
min_div])		
<pre>get_stretched_h(min_width, domain, nx[, x0,</pre>	Return cell widths for a stretched grid within the do-	
7)		
])	main.	
get_domain([x0, freq, res, limits,])	Main. Get domain extent and minimum cell width as a func-	

get_hx_h0

```
emg3d.meshes.get_hx_h0 (freq, res, domain, fixed=0.0, possible_nx=None, min_width=None, pps=3, alpha=None, max_domain=100000.0, raise_error=True, verb=1, return\_info=False)
```

Return cell widths and origin for given parameters.

Returns cell widths for the provided frequency, resistivity, domain extent, and other parameters using a flexible amount of cells. See input parameters for more details. A maximum of three hard/fixed boundaries can be provided (one of which is the grid center).

The minimum cell width is computed through δ/pps , where the skin depth is given by $\delta=503.3\sqrt{\rho/f}$, and the parameter pps stands for 'points-per-skindepth'. The minimum cell width can be restricted with the parameter min_width .

The actual computation domain adds a buffer zone around the (survey) domain. The thickness of the buffer is six times the skin depth. The field is basically zero after two wavelengths. A wavelength is $2\pi\delta$, hence roughly 6 times the skin depth. Taking a factor 6 gives therefore almost two wavelengths, as the field travels to the boundary and back. The actual buffer thickness can be steered with the *res* parameter.

One has to take into account that the air is very resistive, which has to be considered not just in the vertical direction, but also in the horizontal directions, as the airwave will bounce back from the sides otherwise. In the marine case this issue reduces with increasing water depth.

Parameters

- freq [float] Frequency (Hz) to compute the skin depth. The skin depth is a concept defined in the frequency domain. If a negative frequency is provided, it is assumed that the computation is carried out in the Laplace domain. To compute the skin depth, the value of *freq* is then multiplied by -2π , to simulate the closest frequency-equivalent.
- **res** [float or list] Resistivity (Ohm m) to compute the skin depth. The skin depth is used to compute the minimum cell width and the boundary thicknesses. Up to three resistivities can be provided:
 - float: Same resistivity for everything;
 - [min_width, boundaries];
 - [min_width, left boundary, right boundary].
- **domain** [list] Contains the survey-domain limits [min, max]. The actual computation domain consists of this domain plus a buffer zone around it, which depends on frequency and resistivity.
- **fixed** [list, optional] Fixed boundaries, one, two, or maximum three values. The grid is centered around the first value. Hence it is the center location with the smallest cell. Two more fixed boundaries can be added, at most one on each side of the first one. Default is 0.
- possible_nx [list, optional] List of possible numbers of cells. See
 get_cell_numbers(). Default is get_cell_numbers(500, 5, 3),
 which corresponds to [16, 24, 32, 40, 48, 64, 80, 96, 128, 160, 192, 256, 320, 384].

min_width [float, list or None, optional] Minimum cell width restriction:

- None : No restriction;
- float: Fixed to this value, ignoring skin depth and pps.
- list [min, max]: Lower and upper bounds.

Default is None.

pps [int, optional] Points per skindepth; minimum cell width is computed via *dmin* = *skindepth/pps*. Default = 3.

alpha [list, optional] Maximum alpha and step size to find a good alpha. The first value is the maximum alpha of the survey domain, the second value is the maximum alpha for the buffer zone, and the third value is the step size. Default = [1, 1.5, .01], hence no stretching within the survey domain and a maximum stretching of 1.5 in the buffer zone; step size is 0.01.

max_domain [float, optional] Maximum computation domain from fixed[0] (usually source position). Default is 100,000.

raise_error [bool, optional] If True, an error is raised if no suitable grid is found. Otherwise it just prints a message and returns None's. Default is True.

verb [int, optional] Verbosity, 0 or 1. Default = 1.

return_info [bool] If True, a dictionary is returned with some grid info (min and max cell width and alpha).

Returns

hx [ndarray] Cell widths of mesh.

x0 [float] Origin of the mesh.

info [dict] Dictionary with mesh info; only if return_info=True.

Keys:

- *dmin*: Minimum cell width;
- dmax: Maximum cell width:
- amin: Minimum alpha;
- amax: Maximum alpha.

See also:

get_stretched_h Get hx for a fixed number nx and within a fixed domain.

get_cell_numbers

```
emg3d.meshes.get_cell_numbers(max_nr, max_prime=5, min_div=3)
```

Returns 'good' cell numbers for the multigrid method.

'Good' cell numbers are numbers which can be divided by 2 as many times as possible. At the end there will be a low prime number.

The function adds all numbers $p2^n \le M$ for $p=2,3,...,p_{\text{max}}$ and $n=n_{\text{min}},n_{\text{min}}+1,...,\infty;M,p_{\text{max}},n_{\text{min}}$ correspond to max_nr, max_prime , and min_div , respectively.

Parameters

max_nr [int] Maximum number of cells.

max_prime [int] Highest permitted prime number p for p*2^n. {2, 3, 5, 7} are good upper limits in order to avoid too big lowest grids in the multigrid method. Default is 5.

min_div [int] Minimum times the number can be divided by two. Default is 3.

Returns

numbers [array] Array containing all possible cell numbers from lowest to highest.

get stretched h

emg3d.meshes.get_stretched_h (min_width , domain, nx, x0=0, x1=None, $resp_domain=False$) Return cell widths for a stretched grid within the domain.

Returns nx cell widths within *domain*, where the minimum cell width is min_width . The cells are not stretched within x0 and x1, and outside uses a power-law stretching. The actual stretching factor and the number of cells left and right of x0 and x1 are find in a minimization process.

The domain is not completely respected. The starting point of the domain is, but the endpoint of the domain might slightly shift (this is more likely the case for small nx, for big nx the shift should be small). The new endpoint can be obtained with domain [0]+np.sum(hx). If you want the domain to be respected absolutely, set resp_domain=True. However, be aware that this will introduce one stretch-factor which is different from the other stretch factors, to accommodate the restriction. This one-off factor is between the left- and right-side of x0, or, if x1 is provided, just after x1.

Parameters

min_width [float] Minimum cell width. If x1 is provided, the actual minimum cell width might be smaller than min_width.

domain [list] [start, end] of model domain.

nx [int] Number of cells.

x0 [float] Center of the grid. *x0* is restricted to *domain*. Default is 0.

x1 [float] If provided, then no stretching is applied between x0 and x1. The non-stretched part starts at x0 and stops at the first possible location at or after x1. x1 is restricted to domain. This will min_width so that an integer number of cells fit within x0 and x1.

resp_domain [bool] If False (default), then the domain-end might shift slightly to assure that the same stretching factor is applied throughout. If set to True, however, the domain is respected absolutely. This will introduce one stretch-factor which is different from the other stretch factors, to accommodate the restriction. This one-off factor is between the left- and right-side of x0, or, if x1 is provided, just after x1.

Returns

hx [ndarray] Cell widths of mesh.

See also:

get_hx_x0 Get hx and x0 for a flexible number of nx with given bounds.

get_domain

emg3d.meshes.get_domain(x0=0, freq=1, res=0.3, limits=None, min_width=None, fact_min=0.2, fact_neg=5, fact_pos=None)

Get domain extent and minimum cell width as a function of skin depth.

Returns the extent of the computation domain and the minimum cell width as a multiple of the skin depth, with possible user restrictions on minimum computation domain and range of possible minimum cell widths.

$$\begin{split} \delta &= 503.3 \sqrt{\frac{\rho}{f}}, \\ x_{\text{start}} &= x_0 - k_{\text{neg}} \delta, \\ x_{\text{end}} &= x_0 + k_{\text{pos}} \delta, \\ h_{\text{min}} &= k_{\text{min}} \delta. \end{split}$$

Parameters

x0 [float] Center of the computation domain. Normally the source location. Default is 0.

freq [float] Frequency (Hz) to compute the skin depth. The skin depth is a concept defined in the frequency domain. If a negative frequency is provided, it is assumed that the computation is carried out in the Laplace domain. To compute the skin depth, the value of *freq* is then multiplied by -2π , to simulate the closest frequency-equivalent.

Default is 1 Hz.

res [float, optional] Resistivity (Ohm m) to compute skin depth. Default is 0.3 Ohm m (sea water).

limits [None or list] [start, end] of model domain. This extent represents the minimum extent of the domain. The domain is therefore only adjusted if it has to reach outside of [start, end]. Default is None.

min_width [None, float, or list of two floats] Minimum cell width is computed as a function of skin depth: fact_min*sd. If *min_width* is a float, this is used. If a list of two values [min, max] are provided, they are used to restrain min_width. Default is None.

fact_min, fact_neg, fact_pos [floats] The skin depth is multiplied with these factors to estimate:

- Minimum cell width (fact_min, default 0.2)
- Domain-start (fact_neg, default 5), and
- Domain-end (fact_pos, defaults to fact_neg).

Returns

h_min [float] Minimum cell width.

domain [list] Start- and end-points of computation domain.

get_hx

emg3d.meshes.get_hx(alpha, domain, nx, x0, resp_domain=True)

Return cell widths for given input.

Find the number of cells left and right of x0, nl and nr respectively, for the provided alpha. For this, we solve

$$\frac{x_{\max} - x_0}{x_0 - x_{\min}} = \frac{a^{nr} - 1}{a^{nl} - 1}$$

where $a = 1 + \alpha$.

Parameters

alpha [float] Stretching factor a is given by a=1+alpha.

domain [list] [start, end] of model domain.

nx [int] Number of cells.

x0 [float] Center of the grid. *x0* is restricted to *domain*.

resp_domain [bool] If False (default), then the domain-end might shift slightly to assure that the same stretching factor is applied throughout. If set to True, however, the domain is respected absolutely. This will introduce one stretch-factor which is different from the other stretch factors, to accommodate the restriction. This one-off factor is between the left- and right-side of x0, or, if x1 is provided, just after x1.

Returns

hx [ndarray] Cell widths of mesh.

Classes

TensorMesh(h, x0)	A slightly modified discretize. TensorMesh.
-------------------	---

TensorMesh

```
class emg3d.meshes.TensorMesh (h, x0)
```

Bases: discretize. TensorMesh. TensorMesh, emg3d.meshes._TensorMesh

A slightly modified discretize. TensorMesh.

Adds a few attributes ($_eq_$, copy, to_dict , and $from_dict$) to the discretize. TensorMesh.

Falls back to a minimal TensorMesh if *discretize* is not installed. Nothing fancy is possible with the minimal TensorMesh, particularly NO plotting nor nice repr-functions.

Parameters

h [list of three ndarrays]

Cell widths in [x, y, z] directions.

x0 [ndarray of dimension (3,)] Origin (x, y, z).

Required Properties:

- * **axis_u (Vector3): Vector orientation of u-direction. For more details see the docs for the rotation_n
- * **axis_v (Vector3): Vector orientation of v-direction. For more details see the docs for the rotation_m
- * **axis_w (Vector3): Vector orientation of w-direction. For more details see the docs for the rotation_
- * **h (a list of Array): h is a list containing the cell widths of the tensor mesh in each dimension., a list (each
- * **reference_system (String): The type of coordinate reference frame. Can take on the values cartesian,
- * **x0 (Array): origin of the mesh (dim,), a list or numpy array of <class 'float'>, <class 'int'> with shape

Methods Summary

copy()	Return a copy of the TensorMesh.
from_dict(inp)	Convert dictionary into TensorMesh instance.
to_dict([copy])	Store the necessary information of the TensorMesh
	in a dict.

Methods Documentation

copy()

Return a copy of the TensorMesh.

classmethod from_dict(inp)

Convert dictionary into TensorMesh instance.

Parameters

inp [dict] Dictionary as obtained from *TensorMesh.to_dict()*. The dictionary needs the keys *hx*, *hy*, *hz*, and *x0*.

Returns

obj [TensorMesh instance]

to_dict (copy=False)

Store the necessary information of the TensorMesh in a dict.

5.11.2 emg3d.models Module

models - Earth properties

Everything to create model-properties for the multigrid solver.

Classes

<pre>Model(grid[, property_x, property_y,])</pre>	Create a model instance.
VolumeModel(grid, model, sfield)	Return a volume-averaged version of provided model.

Model

Bases: object

Create a model instance.

Class to provide model parameters (x-, y-, and z-directed properties [resistivity or conductivity; linear or on log_10/log_e-scale], electric permittivity and magnetic permeability) to the solver. Relative magnetic permeability $\mu_{\rm r}$ is by default set to one and electric permittivity $\varepsilon_{\rm r}$ is by default set to zero, but they can also be provided (isotropically). Keep in mind that the multigrid method as implemented in emg3d only works for the diffusive approximation. As soon as the displacement-part in the Maxwell's equations becomes too dominant it will fail (high frequencies or very high electric permittivity).

Parameters

grid [TensorMesh] Grid on which to apply model.

property_{x;y;z} [float or ndarray; default to 1.] Material property in x-, y-, and z-directions. If ndarray, they must have the shape of grid.vnC (F-ordered) or grid.nC.

By default, property refers to electrical resistivity. However, this can be changed with an appropriate map. For more info, see the description of the parameter mapping. The internals of emg3d work, irrelevant of the map, with electrical conductivities.

Resistivities and conductivities have to be bigger than zero and smaller than infinity (if provided on a linear scale; not on logarithmic scales).

- mu_r [None, float, or ndarray] Relative magnetic permeability (isotropic). If ndarray it must have the shape of grid.vnC (F-ordered) or grid.nC. Default is None, which corresponds to 1., but avoids the computation of zeta. Magnetic permeability has to be bigger than zero and smaller than infinity.
- **epsilon_r** [None, float, or ndarray] Relative electric permittivity (isotropic). If ndarray it must have the shape of grid.vnC (F-ordered) or grid.nC. The displacement part is completely neglected (diffusive approximation) if set to None, which is the default. Electric permittivity has to be bigger than zero and smaller than infinity.
- **mapping** [str] Defines what type the input *property_{x;y;z}*-values correspond to. By default, they represent resistivities (Ohm.m). The implemented types are:

- 'Conductivity'; σ (S/m),
- 'LgConductivity'; $\log_{10}(\sigma)$,
- 'LnConductivity'; $\log_e(\sigma)$,
- 'Resistivity'; ρ (Ohm.m); Default,
- 'LgResistivity'; $\log_{10}(\rho)$,
- 'LnResistivity'; $\log_e(\rho)$.

Attributes Summary

epsilon_r	Electric permittivity.
mu_r	Magnetic permeability.
property_x	Property in x-direction.
property_y	Property in y-direction.
property_z	Property in z-direction.
res_x	
res_y	
res_z	

Methods Summary

copy()	Return a copy of the Model.
from_dict(inp)	Convert the dictionary into a Model instance.
<pre>interpolate2grid(grid, new_grid,)</pre>	Interpolate <i>Model</i> located on <i>grid</i> to <i>new_grid</i> .
to_dict([copy])	Store the necessary information of the Model in a
	dict.

Attributes Documentation

epsilon_r

Electric permittivity.

mu_r

Magnetic permeability.

property_x

Property in x-direction.

property_y

Property in y-direction.

property_z

Property in z-direction.

res_x

res_y

res_z

Methods Documentation

copy()

Return a copy of the Model.

classmethod from_dict(inp)

Convert the dictionary into a Model instance.

Parameters

inp [dict] Dictionary as obtained from Model.to_dict(). The dictionary needs the keys property_x, property_y, property_z, mu_r, epsilon_r, vnC, and mapping.

Returns

obj [Model instance]

interpolate2grid(grid, new_grid, **grid2grid_opts)

Interpolate *Model* located on *grid* to *new_grid*.

Parameters

grid, **new_grid** [TensorMesh] Input and output model grids; emg3d.meshes.

TensorMesh instances.

grid2grid_opts [dict] Passed through to maps.grid2grid(). Defaults are method='volume', log=True, and extrapolate=True.

Returns

NewModel [Model] New Model instance on new_grid.

to_dict (copy=False)

Store the necessary information of the Model in a dict.

VolumeModel

class emg3d.models.VolumeModel (grid, model, sfield)

Bases: object

Return a volume-averaged version of provided model.

Takes a Model instance and returns the volume averaged values. This is used by the solver internally.

$$\eta_{\{x,y,z\}} = -Vi\omega\mu_0 \left(\rho_{\{x,y,z\}}^{-1} + i\omega\varepsilon \right)$$
$$\zeta = V\mu_r^{-1}$$

Parameters

grid [TensorMesh] Grid on which to apply model.

model [Model] Model to transform to volume-averaged values.

sfield [SourceField] A VolumeModel is frequency-dependent. The frequency-information is taken from the provided source filed.

Attributes Summary

eta_x	eta in x-direction.
eta_y	eta in y-direction.
eta_z	eta in z-direction.
zeta	zeta.

Methods Summary

calculate_eta(name, grid, model, field)	eta: volume multiplied with conductivity.
calculate_zeta(name, grid, model)	zeta: volume divided by mu_r.

Attributes Documentation

```
eta_x
eta in x-direction.

eta_y
eta in y-direction.

eta_z
eta in z-direction.

zeta
```

zeta.

Methods Documentation

```
static calculate_eta (name, grid, model, field)
    eta: volume multiplied with conductivity.
static calculate_zeta (name, grid, model)
    zeta: volume divided by mu r.
```

5.11.3 emg3d.fields Module

fields - Electric and magnetic fields

Everything related to the multigrid solver that is a field: source field, electric and magnetic fields, and fields at receivers.

Functions

<pre>get_source_field(grid, src, freq[, strength])</pre>	Return the source field.
<pre>get_receiver(grid, values, coordinates[,])</pre>	Return values corresponding to grid at coordinates.
<pre>get_receiver_response(grid, field, rec)</pre>	Return the field (response) at receiver coordinates.
<pre>get_h_field(grid, model, field)</pre>	Return magnetic field corresponding to provided elec-
	tric field.

get_source_field

```
emg3d.fields.get_source_field(grid, src, freq, strength=0)
Return the source field.
```

The source field is given in Equation 2 in [Muld06],

 $s\mu_0 \mathbf{J}_{\mathrm{s}},$

where $s = i\omega$. Either finite length dipoles or infinitesimal small point dipoles can be defined, whereas the return source field corresponds to a normalized (1 Am) source distributed within the cell(s) it resides (can be changed with the *strength*-parameter).

The adjoint of the trilinear interpolation is used to distribute the point(s) to the grid edges, which corresponds to the discretization of a Dirac ([PIDM07]).

Parameters

```
grid [TensorMesh] Model grid; a emg3d.meshes.TensorMesh instance.
src [list of floats] Source coordinates (m). There are two formats:
```

• Finite length dipole: [x0, x1, y0, y1, z0, z1].

• Point dipole: [x, y, z, azimuth, dip].

freq [float] Source frequency (Hz), used to compute the Laplace parameter *s*. Either positive or negative:

- freq > 0: Frequency domain, hence $s = -i\omega = -2i\pi f$ (complex);
- freq < 0: Laplace domain, hence s = f (real).

strength [float or complex, optional] Source strength (A):

- If 0, output is normalized to a source of 1 m length, and source strength of 1 A.
- If != 0, output is returned for given source length and strength.

Default is 0.

Returns

sfield [SourceField() instance] Source field, normalized to 1 A m.

get_receiver

emg3d.fields.get_receiver(grid, values, coordinates, method='cubic', extrapolate=False)
Return values corresponding to grid at coordinates.

Works for electric fields as well as magnetic fields obtained with $get_h_field()$, and for model parameters.

Parameters

```
grid [emg3d.meshes.TensorMesh] The model grid.
```

values [ndarray] Field instance, or a particular field (e.g. field.fx); Model parameters.

coordinates [tuple (x, y, z)] Coordinates (x, y, z) where to interpolate *values*; e.g. receiver locations.

method [str, optional] The method of interpolation to perform, 'linear' or 'cubic'. Default is 'cubic' (forced to 'linear' if there are less than 3 points in any direction).

extrapolate [bool] If True, points on *new_grid* which are outside of *grid* are filled by the nearest value (if method='cubic') or by extrapolation (if method='linear'). If False, points outside are set to zero.

Default is False.

Returns

new_values [ndarray or utils.EMArray] Values at coordinates.

If input was a field it returns an EMArray, which is a subclassed ndarray with . pha and . amp attributes.

If input was an entire Field instance, output is a tuple (fx, fy, fz).

See also:

grid2grid Interpolation of model parameters or fields to a new grid.

get_receiver_response Get response for arbitrarily rotated receivers.

get_receiver_response

```
emg3d.fields.get_receiver_response(grid, field, rec)
```

Return the field (response) at receiver coordinates.

Parameters

```
grid [emg3d.meshes.TensorMesh] The model grid.
```

field [Field] The electric or magnetic field.

rec [tuple (x, y, z, azimuth, dip)] Receiver coordinates and angles (m, $^{\circ}$).

All values can either be a scalar or having the same length as number of receivers.

Angles:

- azimuth (°): horizontal deviation from x-axis, anti-clockwise.
- dip (°): vertical deviation from xy-plane up-wards.

Returns

```
responses [utils.EMArray] Responses at receiver.
```

Note: Currently only implemented for point receivers, not for finite length dipoles.

See also:

get_receiver Get values at coordinates (fields and models).

get_h_field

```
emg3d.fields.get_h_field(grid, model, field)
```

Return magnetic field corresponding to provided electric field.

Retrieve the magnetic field H from the electric field E using Farady's law, given by

$$\nabla \times \mathbf{E} = i\omega \mu \mathbf{H}.$$

Note that the magnetic field in x-direction is defined in the center of the face defined by the electric field in y- and z-directions, and similar for the other field directions. This means that the provided electric field and the returned magnetic field have different dimensions:

```
E-field: x: [grid.vectorCCx, grid.vectorNy, grid.vectorNz]
    y: [ grid.vectorNx, grid.vectorCCy, grid.vectorNz]
    z: [ grid.vectorNx, grid.vectorNy, grid.vectorCCz]

H-field: x: [ grid.vectorNx, grid.vectorCCy, grid.vectorCCz]
    y: [grid.vectorCCx, grid.vectorNy, grid.vectorCCz]
    z: [grid.vectorCCx, grid.vectorCCy, grid.vectorNz]
```

Parameters

```
grid [TensorMesh] Model grid; TensorMesh instance.
```

model [Model] Model; Model instance.

field [Field] Electric field; Field instance.

Returns

hfield [Field] Magnetic field; Field instance.

Classes

Field	Create a Field instance with x-, y-, and z-views of the
	field.

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SourceField	Create a Source-Field instance with x-, y-, and z-
	views of the field.

Field

class emg3d.fields.Field

Bases: numpy.ndarray

Create a Field instance with x-, y-, and z-views of the field.

A *Field* is an *ndarray* with additional views of the x-, y-, and z-directed fields as attributes, stored as fx, fy, and fz. The default array contains the whole field, which can be the electric field, the source field, or the residual field, in a 1D array. A *Field* instance has additionally the property *ensure_pec* which, if called, ensures Perfect Electric Conductor (PEC) boundary condition. It also has the two attributes *amp* and *pha* for the amplitude and phase, as common in frequency-domain CSEM.

A *Field* can be initiated in three ways:

- 1. Field (grid, dtype=np.complex128): Calling it with a *emg3d.meshes.TensorMesh* instance returns a *Field* instance of correct dimensions initiated with zeroes of data type *dtype*.
- 2. Field (grid, field): Calling it with a *emg3d.meshes.TensorMesh* instance and an *ndar-ray* returns a *Field* instance of the provided *ndarray*, of same data type.
- 3. Field (fx, fy, fz): Calling it with three *ndarray*'s which represent the field in x-, y-, and z-direction returns a *Field* instance with these views, of same data type.

Sort-order is 'F'.

Parameters

- **fx_or_grid** [emg3d.meshes.TensorMesh or ndarray] Either a TensorMesh instance or an ndarray of shape grid.nEx or grid.vnEx. See explanations above. Only mandatory parameter; if the only one provided, it will initiate a zero-field of *dtype*.
- **fy_or_field** [Field or ndarray, optional] Either a Field instance or an ndarray of shape grid.nEy or grid.vnEy. See explanations above.
- fz [ndarray, optional] An ndarray of shape grid.nEz or grid.vnEz. See explanations above.
- **dtype** [dtype, optional] Only used if fy_or_field=None and fz=None; the initiated zero-field for the provided TensorMesh has data type *dtype*. Default: complex.
- **freq** [float, optional] Source frequency (Hz), used to compute the Laplace parameter *s*. Either positive or negative:
 - freq > 0: Frequency domain, hence $s = -i\omega = -2i\pi f$ (complex);
 - freq < 0: Laplace domain, hence s = f (real).

Just added as info if provided.

Attributes Summary

ensure_pec	Set Perfect Electric Conductor (PEC) boundary
	condition.
field	Entire field, 1D [fx, fy, fz].
freq	Return frequency.
fx	View of the x-directed field in the x-direction (nCx,
	nNy, nNz).
fy	View of the field in the y-direction (nNx, nCy,
	nNz).
	Continued on port page

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Table 5.11 – continued from previous page

	1 1 5
fz	View of the field in the z-direction (nNx, nNy,
	nCz).
is_electric	Returns True if Field is electric, False if it is mag-
	netic.
smu0	Return s*mu_0; mu_0 = Magn.
sval	Return s; s=iw in frequency domain; s=freq in
	Laplace domain.

Methods Summary

amp()	Amplitude of the electromagnetic field.
copy()	Return a copy of the Field.
<pre>from_dict(inp)</pre>	Convert dictionary into Field instance.
pha([deg, unwrap, lag])	Phase of the electromagnetic field.
to_dict([copy])	Store the necessary information of the Field in a
	dict.

Attributes Documentation

ensure_pec

Set Perfect Electric Conductor (PEC) boundary condition.

field

Entire field, 1D [fx, fy, fz].

freq

Return frequency.

fx

View of the x-directed field in the x-direction (nCx, nNy, nNz).

fy

View of the field in the y-direction (nNx, nCy, nNz).

fz

View of the field in the z-direction (nNx, nNy, nCz).

is_electric

Returns True if Field is electric, False if it is magnetic.

smu0

Return $s*mu_0$; $mu_0 = Magn$. permeability of free space [H/m].

sval

Return s; s=iw in frequency domain; s=freq in Laplace domain.

Methods Documentation

amp()

Amplitude of the electromagnetic field.

copy()

Return a copy of the Field.

classmethod from_dict(inp)

Convert dictionary into Field instance.

Parameters

inp [dict] Dictionary as obtained from Field.to_dict(). The dictionary needs the keys field, freq, vnEx, vnEy, and vnEz.

Returns

obj [Field instance]

pha (deg=False, unwrap=True, lag=True)

Phase of the electromagnetic field.

Parameters

deg [bool] If True the returned phase is in degrees, else in radians. Default is False (radians).

unwrap [bool] If True the returned phase is unwrapped. Default is True (unwrapped).

lag [bool] If True the returned phase is lag, else lead defined. Default is True (lag defined).

to_dict (copy=False)

Store the necessary information of the Field in a dict.

SourceField

class emg3d.fields.SourceField

Bases: emg3d.fields.Field

Create a Source-Field instance with x-, y-, and z-views of the field.

A subclass of Field. Additional properties are the real-valued source vector (vector, vx, vy, vz), which sum is always one. For a SourceField frequency is a mandatory parameter, unlike for a Field (recommended also for Field though),

Parameters

- **fx_or_grid** [emg3d.meshes.TensorMesh or ndarray] Either a TensorMesh instance or an ndarray of shape grid.nEx or grid.vnEx. See explanations above. Only mandatory parameter; if the only one provided, it will initiate a zero-field of *dtype*.
- **fy_or_field** [Field or ndarray, optional] Either a Field instance or an ndarray of shape grid.nEy or grid.vnEy. See explanations above.
- fz [ndarray, optional] An ndarray of shape grid.nEz or grid.vnEz. See explanations above.
- **dtype** [dtype, optional] Only used if fy_or_field=None and fz=None; the initiated zero-field for the provided TensorMesh has data type *dtype*. Default: complex.
- **freq** [float] Source frequency (Hz), used to compute the Laplace parameter *s*. Either positive or negative:
 - freq > 0: Frequency domain, hence $s = -i\omega = -2i\pi f$ (complex);
 - freq < 0: Laplace domain, hence s = f (real).

In difference to *Field*, the frequency has to be provided for a *SourceField*.

Attributes Summary

vector	Entire vector, 1D [vx, vy, vz].
VX	View of the x-directed vector in the x-direction
	(nCx, nNy, nNz).
vy	View of the vector in the y-direction (nNx, nCy,
	nNz).
VZ	View of the vector in the z-direction (nNx, nNy,
	nCz).

Attributes Documentation

vector

Entire vector, 1D [vx, vy, vz].

vx

View of the x-directed vector in the x-direction (nCx, nNy, nNz).

vу

View of the vector in the y-direction (nNx, nCy, nNz).

νz

View of the vector in the z-direction (nNx, nNy, nCz).

5.11.4 emg3d.io Module

io - I/O utilities

Utility functions for writing and reading data.

Functions

save(fname[, backend, compression])	Save surveys, meshes, models, fields, and more to
	disk.
load(fname, **kwargs)	Load meshes, models, fields, and other data from disk.

save

```
emg3d.io.save (fname, backend=None, compression='gzip', **kwargs)
Save surveys, meshes, models, fields, and more to disk.
```

Serialize and save data to disk in different formats (see parameter description of *fname* for the supported file formats). The main emg3d-classes (type *emg3d.io.KNOWN_CLASSES* to get a list) can be collected in corresponding root-folders by setting *collect_classes=True*.

Any other (non-emg3d) object can be added too, as long as it knows how to serialize itself.

The serialized instances will be de-serialized if loaded with load().

Parameters

fname [str] File name inclusive ending, which defines the used data format. Implemented are currently:

- .h5 (default): Uses h5py to store inputs to a hierarchical, compressed binary hdf5 file. Recommended file format, but requires the module h5py. Default format if ending is not provided or not recognized.
- .npz: Uses numpy to store inputs to a flat, compressed binary file. Default format if h5py is not installed.
- .json: Uses json to store inputs to a hierarchical, plain text file.

backend [deprecated] Set the appropriate file-ending in *fname* instead.

compression [int or str, optional] Passed through to h5py, default is 'gzip'.

json_indent [int or None] Passed through to json, default is 2.

collect_classes [bool] If True, input data is collected in folders for the principal emg3d-classes (type *emg3d.io.KNOWN_CLASSES* to get a list) and everything else collected in a *Data*-folder. Defaults to False.

verb [int] If 1 (default) verbose, if 0 silent.

kwargs [Keyword arguments, optional] Data to save using its key as name. The following instances will be properly serialized: emg3d.meshes.TensorMesh, emg3d.fields.Field, and emg3d.models.Model and serialized again if loaded with load(). These instances are collected in their own group if h5py is used.

Note that the provided data cannot contain the before described parameters as keys.

load

```
emg3d.io.load(fname, **kwargs)
```

Load meshes, models, fields, and other data from disk.

Load and de-serialize emg3d.meshes.TensorMesh, emg3d.fields.Field, and emg3d.models.Model instances and add arbitrary other data that were saved with save().

Parameters

fname [str] File name including extension. Used backend depends on the file extensions:

- '.npz': numpy-binary
- '.h5': h5py-binary (needs h5py)
- '.json': json

verb [int] If 1 (default) verbose, if 0 silent.

Returns

out [dict] A dictionary containing the data stored in fname; emg3d.meshes. TensorMesh, emg3d.fields.Field, and emg3d.models.Model instances are de-serialized and returned as instances.

5.11.5 emg3d.surveys Module

survey - Surveys

A survey stores a set of sources, receivers, and the measured data.

Classes

Survey(name, sources, receivers, frequencies)	Create a survey with sources, receivers, and data.
Dipole(name, coordinates[, electric])	Finite length dipole or point dipole.
PointDipole(name, xco, yco, zco, azm, dip,)	Infinitesimal small electric or magnetic point dipole.

Survey

class emg3d.surveys.Survey (name, sources, receivers, frequencies, data=None, fixed=0)
Bases: object

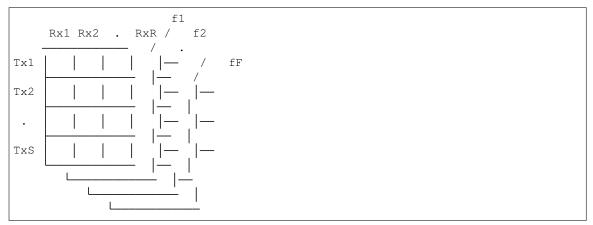
Create a survey with sources, receivers, and data.

A survey contains all the sources with their frequencies, receivers, and corresponding data.

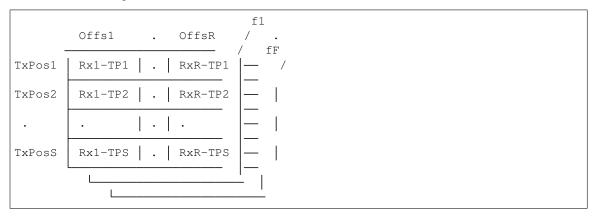
Underlying the survey-class is an xarray, which is basically a regular ndarray with axis labels and more. The module *xarray* is a soft dependency, and has to be installed manually to use the *Survey* functionality.

This class was developed with a node-based, marine CSEM survey layout in mind. It is therefore optimised for and mostly tested with that setup. This means for a number of receivers which measure for all source

positions. The general layout of the data for such a survey is (S, R, F), where S is the number of sources, R the number of receivers, and F the number of frequencies:



However, the class can also be used for a CSEM streamer-style survey layout (by setting fixed=True), where there is a moving source with one or several receivers at a fixed offset. The layout of the data is then also (S, R, F), but here S is the number of locations of the only source, R is the number of receiver-offsets, and F is the number of frequencies:



This means that even though there is only one source, there are actually *S* source dipoles, as each position is treated as a different dipole. The number of receiver dipoles in this case is *SxR*. This setup can also be used for airborne EM.

Parameters

name [str] Name of the survey

sources, receivers [tuple, list, or dict] Sources and receivers.

- Tuples: Coordinates in one of the two following formats:
 - (x, y, z, azimuth, dip) [m, m, m, °, °];
 - (x0, x1, y0, y1, z0, z1) [m, m, m, m, m, m].

Dimensions will be expanded (hence, if n dipoles, each parameter must have length 1 or n). These dipoles will be named sequential with Tx### and Rx####.

The tuple can additionally contain an additional element at the end (after dip or z1), electric, a boolean of length 1 or n, that indicates if the dipoles are electric or magnetic.

- List: A list of <code>Dipole</code>-instances. The names of all dipoles in the list must be unique.
- Dictionary: A dict of de-serialized Dipole-instances; mainly used for loading from file.

frequencies [ndarray] Source frequencies (Hz).

data [ndarray or None] The observed data (dtype=np.complex128); must have shape (nsrc, nrec, nfreq) or, if *fixed=True*, (nsrc, noff, nfreq). If None, it will be initiated with NaN's.

fixed [bool] Node-based CSEM survey (*fixed=False*; default) or streamer-type CSEM survey (*fixed=True*). In the streamer-type survey, the number of *receivers* supplied must be a multiple of the source positions. In this case, the receivers are grouped into offsets.

Attributes Summary

data	Data, a xarray.DataSet instance.
frequencies	Frequency array.
rec_coords	Return receiver coordinates.
receivers	Receiver dict containing all receiver dipoles.
shape	Return nsrc x nrec x nfreq.
size	Return actual data size (does NOT equal nsrc x
	nrec x nfreq).
sources	Source dict containing all source dipoles.
src_coords	Return source coordinates.

Methods Summary

copy()	Return a copy of the Survey.
from_dict(inp)	Convert dictionary into Survey instance.
<pre>from_file(fname[, verb])</pre>	Load Survey from a file.
to_dict([copy])	Store the necessary information of the Survey in a
	dict.
to_file(fname[, compression, json_indent,	Store Survey to a file.
verb])	

Attributes Documentation

data

 $Data,\, a\, \verb|xarray.DataSet| instance.$

Contains the xarray. DataArray element .observed, but other data can be added. E.g., emg3d. simulations. Simulation adds the synthetic array.

frequencies

Frequency array.

rec_coords

Return receiver coordinates.

The returned format is (x, y, z, azm, dip), a tuple of 5 tuples. If fixed=True it returns a dict with the offsets as keys, and for each offset it returns the corresponding receiver coordinates as just outlined.

receivers

Receiver dict containing all receiver dipoles.

shape

Return nsrc x nrec x nfreq.

Note that not all source-receiver-frequency pairs do actually have data. Check *size* to see how many data points there are.

size

Return actual data size (does NOT equal nsrc x nrec x nfreq).

sources

Source dict containing all source dipoles.

src_coords

Return source coordinates.

The returned format is (x, y, z, azm, dip), a tuple of 5 tuples.

Methods Documentation

```
copy()
```

Return a copy of the Survey.

classmethod from_dict(inp)

Convert dictionary into Survey instance.

Parameters

inp [dict] Dictionary as obtained from Survey.to_dict(). The dictionary needs the keys name, sources, receivers frequencies, observed, and fixed.

Returns

obj [Survey instance]

classmethod from_file (fname, verb=1)

Load Survey from a file.

Parameters

fname [str] File name including extension. Used backend depends on the file extensions:

- '.npz': numpy-binary
- '.h5': h5py-binary (needs h5py)
- '.json': json

verb [int] Silent if 0, verbose if 1.

Returns

survey [Survey] The survey that was stored in the file.

to dict(copy=False)

Store the necessary information of the Survey in a dict.

```
to_file (fname, compression='gzip', json_indent=2, verb=1)
Store Survey to a file.
```

Parameters

fname [str] File name inclusive ending, which defines the used data format. Implemented are currently:

- .h5 (default): Uses h5py to store inputs to a hierarchical, compressed binary hdf5 file. Recommended file format, but requires the module h5py. Default format if ending is not provided or not recognized.
- .npz: Uses numpy to store inputs to a flat, compressed binary file. Default format if h5py is not installed.
- .json: Uses json to store inputs to a hierarchical, plain text file.

compression [int or str, optional] Passed through to h5py, default is 'gzip'.

json_indent [int or None] Passed through to json, default is 2.

verb [int] Silent if 0, verbose if 1.

Dipole

class emg3d.surveys.Dipole (name, coordinates, electric=True, **kwargs)
Bases: emg3d.surveys.PointDipole

Finite length dipole or point dipole.

Expansion of the basic PointDipole to allow for finite length dipoles, and to provide coordinate inputs in the form of (x, y, z, azimuth, dip) or (x0, x1, y0, y1, z0, z1).

Adds attributes is_finite, electrode1, electrode2, length, and coordinates to the class.

For *point dipoles*, this gives it a length of unity (1 m), takes its coordinates as center, and computes the two electrode positions.

For finite length dipoles it sets the coordinates to its center and computes its length, azimuth, and dip.

Finite length dipoles and point dipoles have therefore the exactly same signature, and can only be distinguished by the attribute *is_finite*.

Parameters

name [str] Dipole name.

coordinates [tuple of floats] Source coordinates, one of the following:

- (x0, x1, y0, y1, z0, z1): finite length dipole,
- (x, y, z, azimuth, dip): point dipole.

The coordinates x, y, and z are in meters (m), the azimuth and dip in degree (°).

Angles (coordinate system is right-handed with positive z up; East-North-Depth):

- azimuth (°): horizontal deviation from x-axis, anti-clockwise.
- +/-dip (°): vertical deviation from xy-plane down/up-wards.

electric [bool] Electric dipole if True, magnetic dipole otherwise. Default is True.

Attributes Summary

azm	
dip	
electric	
name	
XCO	
усо	
ZCO	

Attributes Documentation

azm

dip

electric

name

xco

yco

zco

PointDipole

Bases: object

Infinitesimal small electric or magnetic point dipole.

Defined by its coordinates (xco, yco, zco), its azimuth (azm), its dip, and its type (electric).

Not meant to be used directly. Use Dipole instead.

Parameters

```
name [str] Dipole name.
```

xco, yco, zco [float] x-, y-, and z-coordinates (m).

azm, dip [float] Angles (in degrees $^{\circ}$); coordinate system is right-handed with positive z up; East-North-Depth:

- azimuth (°): horizontal deviation from x-axis, anti-clockwise.
- +/-dip (°): vertical deviation from xy-plane down/up-wards.

electric [bool] Electric dipole if True, magnetic dipole otherwise. Default is True.

Attributes Summary

azm			
dip			
electric			
name			
XCO			
усо			
ZCO			

Attributes Documentation

azm

dip

electric

name

xco

усо

zco

5.11.6 emg3d.simulations Module

simulation - Model a survey

A simulation is the computation (modelling) of electromagnetic responses of a resistivity (conductivity) model for a given survey.

In its heart, *emg3d* is a multigrid solver for 3D electromagnetic diffusion with tri-axial electrical anisotropy. However, it contains most functionalities to also act as a modeller. The simulation module combines all these things by combining surveys with computational meshes and fields and providing high-level, specialised modelling routines.

Classes

Simulation(name, survey, grid, model[, ...]) Create a simulation for a given survey on a given model.

Simulation

Bases: object

Create a simulation for a given survey on a given model.

The computational grid(s) can be either the same as the provided model grid, or automatic gridding can be used.

Note: The Simulation-class has currently a few limitations:

- gridding must be 'same';
- survey.fixed: must be False;
- sources and receivers must be electric;
- sources strength is always normalized to 1 Am.
- Anything related to optimization is considered experimental/alpha, and might change in the future.

Parameters

survey [emg3d.surveys.Survey] The survey layout, containing sources, receivers, frequencies, and optionally the measured data.

The survey-data will be modified in place. Provide survey.copy() if you want to avoid this.

grid [meshes.TensorMesh] The grid. See meshes.TensorMesh.

model [emg3d.models.Model] The model. See emg3d.models.Model.

max_workers [int] The maximum number of processes that can be used to execute the given calls. Default is 4.

gridding [str, TensorMesh, or dict] Method how the computational grids are computed. The default is currently 'same', the only supported string-method so far (automatic gridding will be implemented in the future).

- 'same': Same grid as for the input model.
- TensorMesh: The provided TensorMesh is used for all sources and frequencies.
- dict: The dict must have the form *dict[source][frequency]*, containing a TensorMesh for each source-frequency pair.

solver_opts [dict, optional] Passed through to <code>emg3d.solver.solve()</code>. The dict can contain any parameter that is accepted by the <code>emg3d.solver.solve()</code> except for <code>grid, model, sfield, and efield.</code> If not provided the following defaults are used:

- *sslsolver* = *True*;
- *semicoarsening* = *True*;
- *linerelaxation* = *True*;
- verb = 0 (yet warnings are capture and shown).

Note that these defaults are different from the defaults in <code>emg3d.solver.solve()</code>. The defaults chosen here will be slower in many cases, but they are the most robust combination at which you can throw most things.

- *gamma_d* : float <0.5>; Offset weighting exponent.
- *beta_d* : float <1.0>; Data weighting exponent.
- *beta_f* : float <0.25>; Frequency weighting exponent.
- noise_floor: float <1e-15>; Data with amplitudes below the noise floor are switched off.
- min_off: float <1000>; Receiver closer to the source than min_offest are switched off.
- reference: str <'reference'>; Name of the data to use for normalization. By default the data from the reference model; if not found, the observed data are used.

Attributes Summary

data	Shortcut to survey.data.
gradient	Return the gradient of the misfit function.
misfit	Return the misfit function.

Methods Summary

clean([what])	Clean part of the data base.
compute([observed, reference])	Compute efields asynchronously for all sources
	and frequencies.
copy([what])	Return a copy of the Simulation.
<pre>from_dict(inp)</pre>	Convert dictionary into Simulation instance.
<pre>from_file(fname[, verb])</pre>	Load Simulation from a file.
<pre>get_efield(source, frequency, **kwargs)</pre>	Return electric field for given source and fre-
	quency.
<pre>get_efield_info(source, frequency)</pre>	Return the solver information of the corresponding
	computation.
<pre>get_grid(source, frequency)</pre>	Return computational grid of the given source and
	frequency.
<pre>get_hfield(source, frequency, **kwargs)</pre>	Return magnetic field for given source and fre-
	quency.
<pre>get_model(source, frequency)</pre>	Return model on the grid of the given source and
	frequency.
<pre>get_sfield(source, frequency)</pre>	Return source field for given source and frequency.
to_dict([what, copy])	Store the necessary information of the Simulation
	in a dict.
to_file(fname[, what, compression,])	Store Simulation to a file.

Attributes Documentation

data

Shortcut to survey.data.

gradient

Return the gradient of the misfit function.

```
See emg3d.optimize.gradient().
```

misfit

Return the misfit function.

```
See emg3d.optimize.misfit().
```

Methods Documentation

```
clean (what='computed')
```

Clean part of the data base.

Parameters

what [str] What to clean. Currently implemented:

- 'computed' (default): Removes all computed properties: electric and magnetic fields and responses at receiver locations.
- 'keepresults': Removes everything except for the responses at receiver locations.
- 'all': Removes everything (leaves it plain as initiated).

```
compute (observed=False, reference=False)
```

Compute efields asynchronously for all sources and frequencies.

Parameters

observed [bool] By default, the data at receiver locations is stored in the *Survey* as *synthetic*. If *observed=True*, however, it is stored in *observed*.

reference [bool] If True, it stores the current result also as reference model, which is used by the data weighting functions. This is usually done for the initial model in an inversion.

```
copy (what='computed')
```

Return a copy of the Simulation.

See to_file for more information regarding what.

classmethod from_dict(inp)

Convert dictionary into Simulation instance.

Parameters

```
inp [dict] Dictionary as obtained from Simulation.to_dict().
```

Returns

```
obj [Simulation instance]
```

$\verb|classmethod from_file| (fname, verb=1)$

Load Simulation from a file.

Parameters

fname [str] File name including extension. Used backend depends on the file extensions:

- '.npz': numpy-binary
- '.h5': h5py-binary (needs *h5py*)
- · '.json': json

verb [int] Silent if 0, verbose if 1.

Returns

simulation [Simulation] The simulation that was stored in the file.

```
get_efield(source, frequency, **kwargs)
```

Return electric field for given source and frequency.

get_efield_info (source, frequency)

Return the solver information of the corresponding computation.

get_grid (source, frequency)

Return computational grid of the given source and frequency.

get_hfield(source, frequency, **kwargs)

Return magnetic field for given source and frequency.

get_model (source, frequency)

Return model on the grid of the given source and frequency.

get_sfield(source, frequency)

Return source field for given source and frequency.

to_dict (what='computed', copy=False)

Store the necessary information of the Simulation in a dict.

See *to_file* for more information regarding *what*.

 $\verb"to_file" (fname, what='computed', compression='gzip', json_indent=2, verb=1)$

Store Simulation to a file.

Parameters

fname [str] File name inclusive ending, which defines the used data format. Implemented are currently:

- .h5 (default): Uses h5py to store inputs to a hierarchical, compressed binary hdf5 file. Recommended file format, but requires the module h5py. Default format if ending is not provided or not recognized.
- .npz: Uses numpy to store inputs to a flat, compressed binary file. Default format if h5py is not installed.
- .json: Uses json to store inputs to a hierarchical, plain text file.

what [str] What to store. Currently implemented:

- 'computed' (default): Stores all computed properties: electric fields and responses at receiver locations.
- 'results': Stores only the response at receiver locations.
- 'all': Stores everything.
- 'plain': Only stores the plain Simulation (as initiated).

compression [int or str, optional] Passed through to h5py, default is 'gzip'.

json_indent [int or None] Passed through to json, default is 2.

verb [int] Silent if 0, verbose if 1.

5.11.7 emg3d.maps Module

maps - Interpolation routines

Interpolation routines mapping grids to grids, grids to fields, and fields to grids.

Functions

grid2grid(grid, values, new_grid[, method,])	Interpolate values located on grid to new_grid.
<pre>interp3d(points, values, new_points, method,)</pre>	Interpolate values in 3D either linearly or with a cubic
	spline.
edges2cellaverages(ex, ey, ez, vol, out_x,)	Interpolate fields defined on edges to volume-
	averaged cell values.

grid2grid

emg3d.maps.grid2grid(grid, values, new_grid, method='linear', extrapolate=True, log=False)
Interpolate values located on grid to new_grid.

Note 1: The default method is 'linear', because it works with fields and model parameters. However, recommended are 'volume' for model parameters and 'cubic' for fields.

Note 2: For model parameters with *method='volume'* the result is quite different if you provide resistivity, conductivity, or the logarithm of any of the two. The recommended way is to provide the logarithm of resistivity or conductivity, in which case the output of one is indeed the inverse of the output of the other.

Parameters

grid, new_grid [TensorMesh] Input and output model grids; TensorMesh instances.

values [ndarray] Model parameters; emg3d.fields.Field instance, or a particular field (e.g. field.fx). For fields the method cannot be 'volume'.

method [{<'linear'>, 'volume', 'cubic'}, optional] The method of interpolation to perform. The volume averaging method ensures that the total sum of the property stays constant.

Volume averaging is only implemented for model parameters, not for fields. The method 'cubic' requires at least three points in any direction, otherwise it will fall back to 'linear'.

Default is 'linear', because it works with fields and model parameters. However, recommended are 'volume' for model parameters and 'cubic' for fields.

extrapolate [bool] If True, points on new_grid which are outside of grid are filled by the
 nearest value (if method='cubic') or by extrapolation (if method='linear').
 If False, points outside are set to zero.

For method='volume' it always uses the nearest value for points outside of grid.

Default is True.

log [bool] If True, the interpolation is carried out on a log10-scale; hence the same as 10**grid2grid(grid, np.log10(values), ...). Default is False.

Returns

new values [ndarray] Values corresponding to new grid.

See also:

get_receiver Interpolation of model parameters or fields to (x, y, z).

interp3d

emg3d.maps.interp3d (points, values, new_points, method, fill_value, mode)
Interpolate values in 3D either linearly or with a cubic spline.

Return values corresponding to a regular 3D grid defined by points on new_points.

This is a modified version of scipy.interpolate.interpn(), using scipy.interpolate. RegularGridInterpolator if method='linear' and a custom-wrapped version of scipy. ndimage.map_coordinates() if method='cubic'. If speed is important then choose 'linear', as it can be significantly faster.

Parameters

points [tuple of ndarray of float, with shapes ((nx,), (ny,) (nz,))] The points defining the regular grid in three dimensions.

values [array_like, shape (nx, ny, nz)] The data on the regular grid in three dimensions.

new_points [tuple (rec_x, rec_y, rec_z)] Coordinates (x, y, z) of new points.

method [{'cubic', 'linear'}, optional] The method of interpolation to perform, 'linear' or 'cubic'. Default is 'cubic' (forced to 'linear' if there are less than 3 points in any direction).

fill_value [float or None] Passed to scipy.interpolate. RegularGridInterpolator if method='linear': The value to use for points outside of the interpolation domain. If None, values outside the domain are extrapolated.

mode [{'constant', 'nearest', 'mirror', 'reflect', 'wrap'}] Passed to scipy.ndimage.
 map_coordinates() if method='cubic': Determines how the input array is
 extended beyond its boundaries.

Returns

new_values [ndarray] Values corresponding to *new_points*.

edges2cellaverages

emg3d.maps.edges2cellaverages (ex, ey, ez, vol, out_x, out_y, out_z)
Interpolate fields defined on edges to volume-averaged cell values.

Parameters

ex, ey, ez [ndarray] Electric fields in x-, y-, and z-directions, as obtained from emg3d. fields.Field.

vol [ndarray] Volumes of the grid, as obtained from emg3d.meshes.TensorMesh.

out_x, out_y, out_z [ndarray] Arrays where the results are placed (per direction).

Classes

MapConductivity()	Maps σ to computational variable σ (conductivity).
MapLgConductivity()	Maps $log_10(\sigma)$ to computational variable σ (conduc-
	tivity).
MapLnConductivity()	Maps $log_e(\sigma)$ to computational variable σ (conduc-
	tivity).
MapResistivity()	Maps ρ to computational variable σ (conductivity).
MapLgResistivity()	Maps $log_10(\rho)$ to computational variable σ (conduc-
	tivity).
MapLnResistivity()	Maps $log_e(\rho)$ to computational variable σ (conduc-
	tivity).

MapConductivity

class emg3d.maps.MapConductivity

Bases: emg3d.maps._Map

Maps σ to computational variable σ (conductivity).

forward: x = σ
backward: σ = x

Methods Summary

backward(mapped)	Mapping to conductivity.
derivative(gradient, conductivity)	Map derivative from conductivity back to mapping
	space.
forward(conductivity)	Conductivity to mapping.

Methods Documentation

backward(mapped)

Mapping to conductivity.

derivative (gradient, conductivity)

Map derivative from conductivity back to mapping space.

forward(conductivity)

Conductivity to mapping.

MapLgConductivity

class emg3d.maps.MapLgConductivity

Bases: emg3d.maps._Map

Maps $log_10(\sigma)$ to computational variable σ (conductivity).

• forward: $x = log_10(\sigma)$

• backward: $\sigma = 10^x$

Methods Summary

backward(mapped)	Mapping to conductivity.
derivative(gradient, conductivity)	Map derivative from conductivity back to mapping
	space.
forward(conductivity)	Conductivity to mapping.

Methods Documentation

backward(mapped)

Mapping to conductivity.

derivative (gradient, conductivity)

Map derivative from conductivity back to mapping space.

forward(conductivity)

Conductivity to mapping.

MapLnConductivity

class emg3d.maps.MapLnConductivity

Bases: emg3d.maps._Map

Maps $log_e(\sigma)$ to computational variable σ (conductivity).

forward: x = log_e(σ)
backward: σ = exp(x)

Methods Summary

backward(mapped)	Mapping to conductivity.
derivative(gradient, conductivity)	Map derivative from conductivity back to mapping
	space.
forward(conductivity)	Conductivity to mapping.

Methods Documentation

backward(mapped)

Mapping to conductivity.

derivative (gradient, conductivity)

Map derivative from conductivity back to mapping space.

forward(conductivity)

Conductivity to mapping.

MapResistivity

class emg3d.maps.MapResistivity

Bases: emg3d.maps._Map

Maps ρ to computational variable σ (conductivity).

• forward: $x = \rho = \sigma^{-1}$

• backward: $\sigma = \rho^{-1} = x^{-1}$

Methods Summary

backward(mapped)	Mapping to conductivity.
derivative(gradient, conductivity)	Map derivative from conductivity back to mapping
	space.
forward(conductivity)	Conductivity to mapping.

Methods Documentation

backward(mapped)

Mapping to conductivity.

derivative (gradient, conductivity)

Map derivative from conductivity back to mapping space.

forward(conductivity)

Conductivity to mapping.

MapLgResistivity

class emg3d.maps.MapLgResistivity

Bases: emg3d.maps._Map

Maps $log_10(\rho)$ to computational variable σ (conductivity).

- forward: $x = \log_{10}(\rho) = \log_{10}(\sigma^{-1})$
- backward: $\sigma = \rho^{-1} = 10^{-x}$

Methods Summary

backward(mapped)	Mapping to conductivity.
derivative(gradient, conductivity)	Map derivative from conductivity back to mapping
	space.
forward(conductivity)	Conductivity to mapping.

Methods Documentation

backward(mapped)

Mapping to conductivity.

derivative (gradient, conductivity)

Map derivative from conductivity back to mapping space.

forward(conductivity)

Conductivity to mapping.

MapLnResistivity

class emg3d.maps.MapLnResistivity

Bases: emg3d.maps._Map

Maps $log_e(\rho)$ to computational variable σ (conductivity).

- forward: $x = \log_e(\rho) = \log_e(\sigma^{-1})$
- backward: $\sigma = \rho^{-1} = \exp(x^{-1})$

Methods Summary

backward(mapped)	Mapping to conductivity.
derivative(gradient, conductivity)	Map derivative from conductivity back to mapping
	space.
forward(conductivity)	Conductivity to mapping.

Methods Documentation

backward(mapped)

Mapping to conductivity.

derivative (gradient, conductivity)

Map derivative from conductivity back to mapping space.

forward(conductivity)

Conductivity to mapping.

5.11.8 emg3d.optimize Module

optimize - Inversion

Functionalities related to optimization (inversion), e.g., misfit function, gradient of the misfit function, or dataand depth-weighting.

Currently it follows the implementation of [PlMu08], using the adjoint-state technique for the gradient.

Functions

gradient(simulation)	Compute the discrete gradient using the adjoint-state
	method.
misfit(simulation)	Return the misfit function.
data_weighting(simulation)	Return weighted residual.

gradient

emg3d.optimize.gradient(simulation)

Compute the discrete gradient using the adjoint-state method.

The discrete gradient for a single source at a single frequency is given by Equation (10) in [PlMu08],

$$\nabla_p J(\mathbf{p}) = -\sum_{k,l,m} \bar{\lambda}_x^E \frac{\partial S}{\partial \mathbf{p}} \mathbf{E}_x - \sum_{k,l,m} \bar{\lambda}_y^E \frac{\partial S}{\partial \mathbf{p}} \mathbf{E}_y - \sum_{k,l,m} \bar{\lambda}_z^E \frac{\partial S}{\partial \mathbf{p}} \mathbf{E}_z ,$$

where the grid notation ($\{k, l, m\}$ and its $\{+1/2\}$ equivalents) have been omitted for brevity (except for the sum symbols).

Note: The gradient has currently additional limitations to the one in the *Simulation* class:

- Only x-directed, electric receivers (E_x) .
- · Only isotropic models.

Parameters

simulation [emg3d.simulations.Simulation] The simulation.

Returns

grad [ndarray] Adjoint-state gradient (same shape as simulation.model).

misfit

emg3d.optimize.misfit(simulation)

Return the misfit function.

The weighted least-squares functional, often called objective function or misfit function, as implemented in *emg3d*, is given by Equation 1 in [PlMu08],

$$J(\mathbf{p}) = \frac{1}{2} \sum_{s} \sum_{s} \sum_{r} \left\{ \left\| W_{s,r,f}^{e} \Delta^{e} \right\|^{2} + \left\| W_{s,r,f}^{h} \Delta^{h} \right\|^{2} \right\} + R(\mathbf{p}),$$
 (5.32)

where $\Delta^{\{e;h\}}$ are the residuals between the observed and synthetic data,

$$\Delta^e = \mathbf{e}_{s,r,f}[\sigma(\mathbf{p})] - \mathbf{e}_{s,r,f}^{\text{obs}} , \qquad (5.33)$$

and

$$\Delta^{h} = \mathbf{h}_{s,r,f}[\sigma(\mathbf{p})] - \mathbf{h}_{s,r,f}^{\text{obs}}. \tag{5.34}$$

Here, f, s, r stand for frequency, source, and receiver, respectively; $W^{\{e;h\}}$ are the weighting functions for the electric and magnetic data residual, $\{\mathbf{e};\mathbf{h}\}^{\mathrm{obs}}$ are the observed electric and magnetic data, and $\{\mathbf{e};\mathbf{h}\}$ are the synthetic electric and magnetic data, computed for a given conductivity σ , which depends on the model parameters \mathbf{p} . Finally, $R(\mathbf{p})$ is a regularization term.

Note: This is an early implementation of the misfit function. Currently not yet implemented are:

- · Magnetic data;
- · Regularization term.

Parameters

simulation [emg3d.simulations.Simulation] The simulation.

Returns

misfit [float] Value of the misfit function.

data_weighting

emg3d.optimize.data_weighting(simulation)

Return weighted residual.

Returns the weighted residual as given in Equation 18 of [PlMu08],

$$W(\mathbf{x}_s, \mathbf{x}_r, \omega) = \frac{\|\mathbf{x}_s - \mathbf{x}_r\|^{\gamma_d}}{\omega^{\beta_f} \|E^{\text{ref}}(\mathbf{x}_s, \mathbf{x}_r, \omega)\|^{\beta_d}}.$$
 (5.35)

Parameters

simulation [emg3d.simulations.Simulation] The simulation. The parameters for data weighting are set in the call to Simulation through the parameter data_weight_opts.

Returns

wresidual [DataArray] The weighted residual $(W^e \Delta^e)$.

5.11.9 emg3d.utils Module

utils - Utilities

Utility functions for the multigrid solver.

Classes

Fourier(time, fmin, fmax[, signal, ft, ftarg])	Time-domain CSEM computation.
Time()	Class for timing (now; runtime).
Report([add_pckg, ncol, text_width, sort])	Print date, time, and version information.
EMArray	Create an EM-ndarray: add amplitude <amp> and</amp>
	phase <pha> methods.</pha>

Fourier

```
class emg3d.utils.Fourier(time, fmin, fmax, signal=0, ft='dlf', ftarg=None, **kwargs)
Bases: object
```

Time-domain CSEM computation.

Class to carry out time-domain modelling with the frequency-domain code *emg3d*. Instances of the class take care of computing the required frequencies, the interpolation from coarse, limited-band frequencies to the required frequencies, and carrying out the actual transform.

Everything related to the Fourier transform is done by utilising the capabilities of the 1D modeller empymod. The input parameters *time*, *signal*, *ft*, and *ftarg* are passed to the function empymod.utils.check_time() to obtain the required frequencies. The actual transform is subsequently carried out by calling empymod.model.tem(). See these functions for more details about the exact implementations of the Fourier transforms and its parameters. Note that also the *verb*-argument follows the definition in *empymod*.

The mapping from computed frequencies to the frequencies required for the Fourier transform is done in three steps:

- Data for $f > f_{\text{max}}$ is set to 0+0j.
- Data for $f < f_{\min}$ is interpolated by adding an additional data point at a frequency of 1e-100 Hz. The data for this point is data.real[0]+0j, hence the real part of the lowest computed frequency and zero imaginary part. Interpolation is carried out using PCHIP scipy.interpolate. pchip_interpolate().
- Data for $f_{\min} \leq f \leq f_{\max}$ is computed with cubic spline interpolation (on a log-scale) scipy. interpolate.InterpolatedUnivariateSpline.

Note that fmin and fmax should be chosen wide enough such that the mapping for $f > f_{max}$ $f < f_{min}$ does not matter that much.

Parameters

time [ndarray] Desired times (s).

fmin, fmax [float] Minimum and maximum frequencies (Hz) to compute:

- Data for freq > fmax is set to 0+0j.
- Data for freq < fmin is interpolated, using an extra data-point at f = 1e-100 Hz, with value data.real[0]+0j. (Hence zero imaginary part, and the lowest computed real value.)

```
signal [\{0, 1, -1\}, optional]
```

Source signal, default is 0:

- None: Frequency-domain response
- -1 : Switch-off time-domain response
- 0 : Impulse time-domain response
- +1 : Switch-on time-domain response
- ft [{'sin', 'cos', 'fftlog'}, optional] Flag to choose either the Digital Linear Filter method (Sine- or Cosine-Filter) or the FFTLog for the Fourier transform. Defaults to 'sin'.

ftarg [dict, optional] Depends on the value for ft:

- If *ft='dlf'*:
 - dlf: string of filter name in empymod.filters or the filter method itself. (Default: empymod.filters.key_201_CosSin_2012())
 - pts_per_dec: points per decade; (default: -1)

- * If 0: Standard DLF.
- * If < 0: Lagged Convolution DLF.
- * If > 0: Splined DLF
- If *ft='fftlog'*:
 - pts_per_dec: sampels per decade (default: 10)
 - add_dec: additional decades [left, right] (default: [-2, 1])
 - q: exponent of power law bias (default: 0); -1 <= q <= 1

freq_inp [array] Frequencies to use for computation. Mutually exclusive with *every_x_freq*.

every_x_freq [int] Every *every_x_freq*-th frequency of the required frequency-range is used for computation. Mutually exclusive with *freq_calc*.

Attributes Summary

every_x_freq	If set, freq_coarse is every_x_freq-frequency of
	freq_req.
fmax	Maximum frequency (Hz) to compute.
fmin	Minimum frequency (Hz) to compute.
freq_calc	Frequencies at which the model has to be com-
	puted.
freq_calc_i	Indices of <i>freq_coarse</i> which have to be computed.
freq_coarse	Coarse frequency range, can be different from
	freq_req.
freq_extrapolate	These are the frequencies to extrapolate.
freq_extrapolate_i	Indices of the frequencies to extrapolate.
freq_inp	If set, freq_coarse is set to freq_inp.
freq_interpolate	These are the frequencies to interpolate.
freq_interpolate_i	Indices of the frequencies to interpolate.
freq_req	Frequencies required to carry out the Fourier trans-
	form.
ft	Type of Fourier transform.
ftarg	Fourier transform arguments.
signal	Signal in time domain {0, 1, -1}.
time	Desired times (s).

Methods Summary

fourier_arguments(ft, ftarg)	Set Fourier type and its arguments.
freq2time(fdata, off)	Compute corresponding time-domain signal.
interpolate(fdata)	Interpolate from computed data to required data.

Attributes Documentation

every_x_freq

If set, freq_coarse is every_x_freq-frequency of freq_req.

fmax

Maximum frequency (Hz) to compute.

fmin

Minimum frequency (Hz) to compute.

freq_calc

Frequencies at which the model has to be computed.

freq calc i

Indices of *freq_coarse* which have to be computed.

freq_coarse

Coarse frequency range, can be different from freq_req.

freq_extrapolate

These are the frequencies to extrapolate.

In fact, it is dow via interpolation, using an extra data-point at f = 1e-100 Hz, with value data.real[0]+0j. (Hence zero imaginary part, and the lowest computed real value.)

freq_extrapolate_i

Indices of the frequencies to extrapolate.

freq_inp

If set, freq_coarse is set to freq_inp.

freq_interpolate

These are the frequencies to interpolate.

If freq_req is equal freq_coarse, then this is eual to freq_calc.

freq_interpolate_i

Indices of the frequencies to interpolate.

If freq_req is equal freq_coarse, then this is eual to freq_calc_i.

freq_req

Frequencies required to carry out the Fourier transform.

ft

Type of Fourier transform. Set via fourier_arguments(ft, ftarg).

ftarg

Fourier transform arguments. Set via fourier_arguments (ft, ftarg).

signal

Signal in time domain $\{0, 1, -1\}$.

time

Desired times (s).

Methods Documentation

fourier_arguments (ft, ftarg)

Set Fourier type and its arguments.

freq2time (fdata, off)

Compute corresponding time-domain signal.

Carry out the actual Fourier transform.

Parameters

fdata [ndarray] Frequency-domain data corresponding to *freq_calc*.

off [float] Corresponding offset (m).

Returns

tdata [ndarray] Time-domain data corresponding to Fourier.time.

interpolate(fdata)

Interpolate from computed data to required data.

Parameters

fdata [ndarray] Frequency-domain data corresponding to *freq_calc*.

Returns

full_data [ndarray] Frequency-domain data corresponding to freq_req.

Time

```
class emg3d.utils.Time
```

Bases: object

Class for timing (now; runtime).

Attributes Summary

elapsed	Return runtime in seconds since time zero.
now	Return string of current time.
runtime	Return string of runtime since time zero.
t0	Return time zero of this class instance.

Attributes Documentation

elapsed

Return runtime in seconds since time zero.

now

Return string of current time.

runtime

Return string of runtime since time zero.

t0

Return time zero of this class instance.

Report

```
class emg3d.utils.Report(add_pckg=None, ncol=3, text_width=80, sort=False)
    Bases: scooby.report.Report
```

Print date, time, and version information.

Use *scooby* to print date, time, and package version information in any environment (Jupyter notebook, IPython console, Python console, QT console), either as html-table (notebook) or as plain text (anywhere).

Always shown are the OS, number of CPU(s), numpy, scipy, emg3d, numba, sys.version, and time/date.

Additionally shown are, if they can be imported, *IPython* and *matplotlib*. It also shows MKL information, if available.

All modules provided in *add_pckg* are also shown.

Note: The package *scooby* has to be installed in order to use *Report*: pip install scooby.

Parameters

add_pckg [packages, optional] Package or list of packages to add to output information (must be imported beforehand).

ncol [int, optional] Number of package-columns in html table (no effect in text-version); Defaults to 3.

text_width [int, optional] The text width for non-HTML display modes
sort [bool, optional] Sort the packages when the report is shown

Examples

EMArray

```
class emg3d.utils.EMArray
    Bases: numpy.ndarray
```

Create an EM-ndarray: add *amplitude* <amp> and *phase* <pha> methods.

Parameters

data [array] Data to which to add .amp and .pha attributes.

Examples

Methods Summary

amp()	Amplitude of the electromagnetic field.
pha([deg, unwrap, lag])	Phase of the electromagnetic field.

Methods Documentation

$\mathtt{amp}\left(\right)$

Amplitude of the electromagnetic field.

pha (*deg=False*, *unwrap=True*, *lag=True*) Phase of the electromagnetic field.

Parameters

deg [bool] If True the returned phase is in degrees, else in radians. Default is False (radians).

unwrap [bool] If True the returned phase is unwrapped. Default is True (unwrapped).

lag [bool] If True the returned phase is lag, else lead defined. Default is True (lag defined).

5.11.10 emg3d.solver Module

solver - Multigrid solver

The actual solver routines. The most computationally intensive parts, however, are in the <code>emg3d.core</code> as numbajitted functions.

Functions

multigrid(grid, model, sfield, efield, var,)	Multigrid solver for 3D controlled-source electromagnetic (CSEM) data.
smoothing(grid, model, sfield, efield, nu,)	Reducing high-frequency error by smoothing.
restriction(grid, model, sfield, residual,)	Downsampling of grid, model, and fields to a coarser
	grid.
prolongation(grid, efield, cgrid, cefield,)	Interpolating the electric field from coarse grid to fine
	grid.
residual(grid, model, sfield, efield[, norm])	Computing the residual.
krylov(grid, model, sfield, efield, var)	Krylov Subspace iterative solver for 3D CSEM data.

multigrid

emg3d.solver.multigrid(grid, model, sfield, efield, var, **kwargs)

Multigrid solver for 3D controlled-source electromagnetic (CSEM) data.

Multigrid solver as presented in [Muld06], including semicoarsening and line relaxation as presented in and [Muld07].

- The electric field is stored in-place in *efield*.
- The number of multigrid cycles is stored in var.it.
- The current error (l2-norm) is stored in *var.l2*.
- The reference error (12-norm of sfield) is stored in *var.l2_refe*.

This function is called by solve().

Parameters

```
grid [emg3d.meshes.TensorMesh] The grid. See emg3d.meshes.
    TensorMesh.

model [emg3d.models.VolumeModel] The Model. See emg3d.models.
    VolumeModel.

sfield [emg3d.fields.SourceField] The source field. See emg3d.fields.
    get_source_field().

efield [emg3d.fields.Field] The electric field. See emg3d.fields.Field.

var [MGParameters instance] As returned by multigrid().
```

**kwargs [Recursion parameters.] Do not use; only used internally by recursion; *level* (current coarsening level) and *new_cycmax* (new maximum of MG cycles, takes care of V/W/F-cycling).

smoothing

```
emg3d.solver.smoothing (grid, model, sfield, efield, nu, lr_dir) Reducing high-frequency error by smoothing.
```

Solves the linear equation system Ax = b iteratively using the Gauss-Seidel method. This acts as smoother or, on the coarsest grid, as a direct solver.

This is a simple wrapper for the jitted computation in $emg3d.core.gauss_seidel()$, $emg3d.core.gauss_seidel_x()$, $emg3d.core.gauss_seidel_y()$, and $emg3d.core.gauss_seidel_y()$, and $emg3d.core.gauss_seidel_z()$ (@njit can not [yet] access class attributes). See these functions for more details and corresponding theory.

The electric fields are updated in-place.

This function is called by multigrid().

Parameters

```
grid [emg3d.meshes.TensorMesh] Input grid.
model [emg3d.models.VolumeModel] Input model.
sfield [emg3d.fields.SourceField] Input source field.
efield [emg3d.fields.Field] Input electric field.
nu [int] Number of Gauss-Seidel steps; odd numbers are forward, even numbers are reversed. E.g., nu=2 is one symmetric Gauss-Seidel iteration, with a forward and a backward step.
```

lr_dir [int] Direction of line relaxation $\{0, 1, 2, 3, 4, 5, 6, 7\}$.

restriction

```
emg3d.solver.restriction (grid, model, sfield, residual, sc_dir)

Downsampling of grid, model, and fields to a coarser grid.
```

The restriction of the residual is used as source term for the coarse grid.

Corresponds to Equations 8 and 9 in [Muld06] and surrounding text. In the case of the restriction of the residual, this function is a wrapper for the jitted functions <code>emg3d.core.restrict_weights()</code> and <code>emg3d.core.restrict()</code> (@njit can not [yet] access class attributes). See these functions for more details and corresponding theory.

This function is called by multigrid().

Parameters

```
grid [emg3d.meshes.TensorMesh] Input grid.
model [emg3d.models.VolumeModel] Input model.
sfield [emg3d.fields.SourceField] Input source field.
sc_dir [int] Direction of semicoarsening (0, 1, 2, or 3).
```

Returns

```
cgrid [emg3d.meshes.TensorMesh] Coarse grid.
cmodel [emg3d.models.VolumeModel] Coarse model.
csfield [emg3d.fields.SourceField] Coarse source field. Corresponds to restriction of fine-grid residual.
cefield [emg3d.fields.Field] Coarse electric field, complex zeroes.
```

prolongation

```
emg3d.solver.prolongation(grid, efield, cgrid, cefield, sc_dir)
```

Interpolating the electric field from coarse grid to fine grid.

The prolongation from a coarser to a finer grid is the inverse process of the restriction (restriction ()) from a finer to a coarser grid. The interpolated values of the coarse grid electric field are added to the fine grid electric field, in-place. Piecewise constant interpolation is used in the direction of the field, and bilinear interpolation in the other two directions.

See Equation 10 in [Muld06] and surrounding text.

This function is called by multigrid().

Parameters

```
grid, cgrid [emg3d.meshes.TensorMesh] Fine and coarse grids.
efield, cefield [emg3d.fields.Field] Fine and coarse grid electric fields.
sc dir [int] Direction of semicoarsening (0, 1, 2, or 3).
```

residual

```
emg3d.solver.residual(grid, model, sfield, efield, norm=False)
     Computing the residual.
```

Returns the complete residual as given in [Muld06], page 636, middle of the right column:

$$\mathbf{r} = V \left(i\omega \mu_0 \mathbf{J_s} + i\omega \mu_0 \tilde{\sigma} \mathbf{E} - \nabla \times \mu_r^{-1} \nabla \times \mathbf{E} \right).$$

This is a simple wrapper for the jitted computation in emg3d.core.amat_x() (@njit can not [yet] access class attributes). See emg3d.core.amat_x() for more details and corresponding theory.

This function is called by multigrid().

Parameters

```
grid [emg3d.meshes.TensorMesh] Input grid.
model [emg3d.models.VolumeModel] Input model.
sfield [emg3d.fields.SourceField] Input source field.
efield [emg3d.fields.Field] Input electric field.
norm [bool] If True, the error (12-norm) of the residual is returned, not the residual.
```

Returns

```
residual [Field] Returned if norm=False. The residual field; emg3d.fields.
    Field instance.
norm [float] Returned if norm=True. The error (12-norm) of the residual
```

krylov

```
emg3d.solver.krylov(grid, model, sfield, efield, var)
     Krylov Subspace iterative solver for 3D CSEM data.
```

Using a Krylov subspace iterative solver (defined in var.sslsolver) implemented in SciPy with or without multigrid as a pre-conditioner ([Muld06]).

- The electric field is stored in-place in *efield*.
- The current error (12-norm) is stored in *var.l2*.

• The reference error (12-norm of sfield) is stored in var.l2_refe.

This function is called by solve().

Parameters

```
grid [emg3d.meshes.TensorMesh] The grid. See emg3d.meshes.
    TensorMesh.

model [emg3d.models.VolumeModel] The Model. See emg3d.models.
    VolumeModel.

sfield [emg3d.fields.SourceField] The source field. See emg3d.fields.
    get_source_field().

efield [emg3d.fields.Field] The electric field. See emg3d.fields.Field.

var [MGParameters instance] As returned by multigrid().
```

Classes

MGParameters(verb, cycle, sslsolver,)	Collect multigrid solver settings.
RegularGridProlongator(x, y, cxy)	Prolongate field from coarse to fine grid.

MGParameters

```
class emg3d.solver.MGParameters (verb: int, cycle: str, sslsolver: str, linerelaxation: int, semi-
coarsening: int, vnC: tuple, tol: float = 1e-06, maxit: int
= 50, nu_init: int = 0, nu_pre: int = 2, nu_coarse: int =
1, nu_post: int = 2, clevel: int = -1, return_info: bool =
False)
```

Bases: object

Collect multigrid solver settings.

This dataclass is used by the main solve()-routine. See solve() for a description of the mandatory and optional input parameters and more information.

Returns

var [class:MGParameters] As required by multigrid().

Attributes Summary

clevel	
max_level	Sets dimension-dependent level variable <i>clevel</i> .
maxit	
nu_coarse	
nu_init	
nu_post	
nu_pre	
return_info	
tol	

Methods Summary

cprint(info, verbosity, **kwargs)	Conditional printing.
one_liner(l2_last[, last])	Print continuously updated one-liner.

Attributes Documentation

```
clevel = -1
max level
     Sets dimension-dependent level variable clevel.
     Requires at least two cells in each direction (for nCx, nCy, and nCz).
maxit = 50
nu_coarse = 1
nu init = 0
nu_post = 2
nu_pre = 2
return info = False
tol = 1e-06
Methods Documentation
cprint (info, verbosity, **kwargs)
     Conditional printing.
     Prints info if self.verb > verbosity.
          Parameters
               info [str] String to be printed.
               verbosity [int] Verbosity of info.
               kwargs [optional] Arguments passed to print.
one_liner(l2_last, last=False)
     Print continuously updated one-liner.
          Parameters
               12_last [float] Current error.
```

RegularGridProlongator

```
class emg3d.solver.RegularGridProlongator(x, y, cxy)
    Bases: object
    Prolongate field from coarse to fine grid.
    This is a heavily modified and adapted version of scipy.interpolate.
    RegularGridInterpolator.
```

last [bool] If True, adds exit_message and finishes line.

The main difference (besides the pre-sets) is that this version allows to initiate an instance with the coarse and fine grids. This initialize will compute the required weights, and it has therefore only to be done once.

After this, interpolating values from the coarse to the fine grid can be carried out much faster.

Simplifications in comparison to scipy.interpolate.RegularGridInterpolator:

- No sanity checks what-so-ever.
- · Only 2D data;
- method='linear';

- bounds_error=False;
- fill_value=None.

It results in a speed-up factor of about 2, independent of grid size, for this particular case. The prolongation is the second-most expensive part of multigrid after the smoothing. Trying to improve this further might therefore be useful.

Parameters

x, y [ndarray] The x/y-coordinates defining the coarse grid.

cxy [ndarray of shape (..., 2)] The ([[x], [y]]).T-coordinates defining the fine grid.

Methods Summary

call(values) Return values of coarse grid on fine grid locations.

Methods Documentation

__call__(values)

Return values of coarse grid on fine grid locations.

Parameters

values [ndarray] Values corresponding to x/y-coordinates.

Returns

result [ndarray] Values corresponding to cxy-coordinates.

5.11.11 emg3d.core Module

core - Number crunching

The core functionalities, the most computationally demanding parts, of the <code>emg3d.solver</code> as just-in-time (jit) compiled functions using numba.

Functions

$amat_x(rx, ry, rz, ex, ey, ez, eta_x, eta_y,)$	Residual without or with source term.
blocks_to_amat(amat, bvec, middle, left,)	Insert middle, left, and rhs into main arrays amat and
	bvec.
gauss_seidel(ex, ey, ez, sx, sy, sz, eta_x,)	Gauss-Seidel method.
gauss_seidel_x(ex, ey, ez, sx, sy, sz,)	Gauss-Seidel method with line relaxation in x-
	direction.
gauss_seidel_y(ex, ey, ez, sx, sy, sz,)	Gauss-Seidel method with line relaxation in y-
	direction.
gauss_seidel_z(ex, ey, ez, sx, sy, sz,)	Gauss-Seidel method with line relaxation in z-
	direction.
restrict(crx, cry, crz, rx, ry, rz, wx, wy,)	Restriction of residual from fine to coarse grid.
restrict_weights(vectorN, vectorCC, h,)	Restriction weights for the coarse-grid correction op-
	erator.
solve(amat, bvec)	Solve A $x = b$ using a non-standard Cholesky factori-
	sation.

amat x

emg3d.core.amat_x (*rx*, *ry*, *rz*, *ex*, *ey*, *ez*, *eta_x*, *eta_y*, *eta_z*, *zeta*, *hx*, *hy*, *hz*) Residual without or with source term.

Compute the residual as given in [Muld06] in middle of the right column on page 636, but without the source term:

$$\mathbf{r} = V \left(i\omega \mu_0 \tilde{\sigma} \mathbf{E} - \nabla \times \mu_r^{-1} \nabla \times \mathbf{E} \right).$$

The computation is carried out in a matrix-free manner; on said page 636 (or in the *Theory* of the manual) are the various steps laid out to discretise the different parts, for instance involved curls. This can also be understood as the left-hand-side of Ax = b, as given in Equation 2 in [Muld06] (here without the cell volumes V),

$$i\omega\mu_0\tilde{\sigma}E - \nabla\times\zeta^{-1}\nabla\times E = -i\omega\mu_0J_s$$
.

It can therefore be used as matvec to create a LinearOperator, which can be passed to a solver.

It is assumed that ex, ey, and ez have PEC boundaries; otherwise the output will not have PEC boundaries.

The residuals are subtracted in-place from rx, ry, and rz. That means that if rx, ry, and rz contain the source field, they will contain the total residual afterwards; if they are empty fields, they will contain the negative partial residual afterwards.

Parameters

rx, ry, rz [ndarray] Source field or pre-allocated zero residual field in x-, y-, and z-directions.

ex, ey, ez [ndarray] Electric fields in x-, y-, and z-directions, as obtained from *emg3d*. *fields*. *Field*.

eta_x, eta_y, eta_z, zeta [ndarray] VolumeModel parameters (multiplied by volumes) as obtained from emg3d.models.VolumeModel().

hx, hy, hz [ndarray] Cell widths in x-, y-, and z-directions.

blocks_to_amat

emg3d.core.blocks_to_amat(amat, bvec, middle, left, rhs, im, nC)

Insert middle, left, and rhs into main arrays amat and bvec.

The banded matrix amat contains the main diagonal and the first five lower off-diagonals. They are stored one column after the other, in a 6*n ndarray.

The complete main matrix amat and the middle and left blocks are given by:

Both, *middle* and *left*, are 5x5 matrices. The corresponding right-hand-side *rhs* is filled into *bvec*. The matrices *left* and *middle* provided in a single call are horizontally aligned (not vertically). The sorting of amat (banded matrix) and bvec are given by:

amat (66,) example: n	= 11 bvec (11,)	
01	FIRST CALL 01 Only `middle` and `rhs` 02 are used, not `left`. 03 04 05	
0 11 16 21 26 31	SUBSEQUENT CALLS 06 (normal case) 07 Complete `left`, 08 `middle` and `rhs` 09	
0 0 0 0	LAST CALL 11 Only top row of `left` and the first elements of `middle` and `rhs` are used.	
Single zeros (0) show elements in amat which are 0, hence not used. Their location in amat can be deduced from their neighbours.		

Parameters

amat [ndarray] Main banded matrix (stored as array) of length 6*n.

bvec [ndarray] Main right-hand-side of length n.

middle [ndarray] Middle block of size 5x5, as ndarray of length 25. Only the diagonal and the lower triangular part are used.

left [ndarray] Left block of size 5x5, as ndarray of length 25. Only the diagonal and the first row are used.

rhs [ndarray] Corresponding right-hand-side of length 5.

im [int] Current minus-index of direction of line relaxation, {ixm, iym, izm}.

nC [int] Total number of cells in direction of line relaxation, {nCx, nCy, nCz}.

gauss seidel

emg3d.core.gauss_seidel (ex, ey, ez, sx, sy, sz, eta_x, eta_y, eta_z, zeta, hx, hy, hz, nu) Gauss-Seidel method.

Solves the linear equation system Ax = b iteratively using the following method:

$$\mathbf{x}^{(k+1)} = L_*^{-1} \left(\mathbf{b} - U \mathbf{x}^{(k)} \right) ,$$

where L_* is the lower triangular component, and U the strictly upper triangular component, $A = L_* + U$:

$$L_* = \begin{bmatrix} a_{11} & 0 & \cdots & 0 \\ a_{21} & a_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}, \quad U = \begin{bmatrix} 0 & a_{12} & \cdots & a_{1n} \\ 0 & 0 & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}.$$

On the coarsest grid it acts as direct solver, whereas on the fine grid it acts as a smoother with only few iterations, defined by ν (nu). Odd numbers of nu use forward ordering, even numbers use backwards ordering. nu=2 is therefore one symmetric Gauss-Seidel iteration, one forward ordered iteration followed by one backward ordered iteration.

From [Muld06]: The method proposed by [ArFW00] is chosen as a smoother. It selects one node of the grid and simultaneously solves for the six degrees of freedom on the six edges attached to the node. If node (x_k, y_l, z_m) is selected, the six equations, $r_{x;k\pm 1/2,l,m}=0$, $r_{y;k,l\pm 1/2,m}=0$ and $r_{z;k,l,m\pm 1/2}=0$, are solved for $e_{x;k\pm 1/2,l,m}$, $e_{y;k,l\pm 1/2,m}$ and $e_{z;k,l,m\pm 1/2}$. Here, this smoother is applied in a symmetric Gauss-Seidel fashion, following the lexicographical ordering of the nodes (x_k, y_l, z_m) , with fastest index $k=1,\ldots,N_x-1$, intermediate index $l=1,\ldots,N_y-1$, and slowest index $m=1,\ldots,N_z-1$.

To actually solve the system of six equations a non-standard Cholesky factorisation is used, solve().

Tangential components at the boundaries are assumed to be zero (PEC boundaries).

The result is stored in the provided electric fields ex, ey, and ez.

Parameters

```
ex, ey, ez [ndarray] Electric fields in x-, y-, and z-directions, as obtained from emg3d. fields.Field.
```

```
sx, sy, sz: Source fields in x-, y-, and z-directions, as obtained from emg3d.fields. Field.
```

```
eta_x, eta_y, eta_z, zeta: VolumeModel parameters (multiplied by volumes) as obtained from emg3d.models.VolumeModel().
```

hx, hy, hz [ndarray] Cell widths in x-, y-, and z-directions.

nu [int] Number of Gauss-Seidel iterations.

gauss seidel x

```
emg3d.core.gauss_seidel_x (ex, ey, ez, sx, sy, sz, eta_x, eta_y, eta_z, zeta, hx, hy, hz, nu) Gauss-Seidel method with line relaxation in x-direction.
```

This is the equivalent to <code>gauss_seidel()</code>, but with line relaxation in the x-direction. See <code>gauss_seidel()</code> for more details.

The resulting system A x = b to solve consists of n unknowns (x-vector), and the corresponding matrix A is a banded matrix with the main diagonal and five upper and lower diagonals:

The matrix A is complex and symmetric $(A = A^T)$, and therefore only the main diagonal and the lower five off-diagonals are required.

- The right-hand-side b has length 5*nCx-4 (nCx even).
- The matrix A has length of b and 1+2*5 diagonals; we use for it an array of length 6*len(b).

The values are computed in rows of 5 lines, with the indicated middle and left matrices as indicated in the above scheme. These blocks are filled into the main matrix A and vector b, and subsequently solved with a non-standard Cholesky factorisation, <code>solve()</code>.

Tangential components at the boundaries are assumed to be 0 (PEC boundaries).

The result is stored in the provided electric fields ex, ey, and ez.

Parameters

```
ex, ey, ez [ndarray] Electric fields in x-, y-, and z-directions, as obtained from emg3d. fields.Field.
```

sx, sy, sz: Source fields in x-, y-, and z-directions, as obtained from emg3d.fields. Field.

eta_x, eta_y, eta_z, zeta: VolumeModel parameters (multiplied by volumes) as obtained from emg3d.models.VolumeModel().

hx, hy, hz [ndarray] Cell widths in x-, y-, and z-directions.

nu [int] Number of Gauss-Seidel iterations.

gauss seidel y

```
emg3d.core.gauss_seidel_y (ex, ey, ez, sx, sy, sz, eta_x, eta_y, eta_z, zeta, hx, hy, hz, nu) Gauss-Seidel method with line relaxation in y-direction.
```

This is the equivalent to <code>gauss_seidel()</code>, but with line relaxation in the y-direction. See <code>gauss_seidel()</code> for more details.

The resulting system A x = b to solve consists of n unknowns (x-vector), and the corresponding matrix A is a banded matrix with the main diagonal and five upper and lower diagonals:

```
.-0
|X|
        0
0-.-0
              left: middle: right:
\ | X | \
                                  (not used)
  0 - . - 0
              0-
                                  0
   \ | X | \
                 \
                        | X
                                   \perp
    0 - . - 0
   \ | X |
      0-
. 1*1, -4*1, |1*4, |1*4, |1*4, |1*4, |1*4, |1*4 upper or lower
```

The matrix A is complex and symmetric $(A = A^T)$, and therefore only the main diagonal and the lower five off-diagonals are required.

- The right-hand-side b has length 5*nCy-4 (nCy even).
- The matrix A has length of b and 1+2*5 diagonals; we use for it an array of length 6*len(b).

The values are computed in rows of 5 lines, with the indicated middle and left matrices as indicated in the above scheme. These blocks are filled into the main matrix A and vector b, and subsequently solved with a non-standard Cholesky factorisation, <code>solve()</code>.

Note: The smoothing with linerelaxation in y-direction is carried out in reversed lexicographical order, in order to improve speed (memory access). All other smoothers ($gauss_seidel()$, $gauss_seidel_x()$, and $gauss_seidel_z()$) use lexicographical order.

Tangential components at the boundaries are assumed to be 0 (PEC boundaries).

The result is stored in the provided electric fields ex, ey, and ez.

Parameters

```
ex, ey, ez [ndarray] Electric fields in x-, y-, and z-directions, as obtained from emg3d. fields.Field.
```

sx, sy, sz: Source fields in x-, y-, and z-directions, as obtained from emg3d.fields. Field.

eta_x, eta_y, eta_z, zeta: VolumeModel parameters (multiplied by volumes) as obtained from emg3d.models.VolumeModel().

hx, hy, hz [ndarray] Cell widths in x-, y-, and z-directions.

nu [int] Number of Gauss-Seidel iterations.

gauss_seidel_z

```
emg3d.core.gauss_seidel_z (ex, ey, ez, sx, sy, sz, eta_x, eta_y, eta_z, zeta, hx, hy, hz, nu) Gauss-Seidel method with line relaxation in z-direction.
```

This is the equivalent to <code>gauss_seidel()</code>, but with line relaxation in the z-direction. See <code>gauss_seidel()</code> for more details.

The resulting system A = b to solve consists of n unknowns (x-vector), and the corresponding matrix A is a banded matrix with the main diagonal and five upper and lower diagonals:

```
.-0
|X|
0 - . - 0
             left: middle: right:
\ | X | \
                               (not used)
 0 - . - 0
             0-
                               0
   \ | X | \
              \
                      | X
                               |\
   0 - . - 0
   \ | X |
      0-.
. 1*1, -4*1, | 1*4, X 4*4, \ 4*4 upper or lower
```

The matrix A is complex and symmetric $(A = A^T)$, and therefore only the main diagonal and the lower five off-diagonals are required.

- The right-hand-side b has length 5*nCz-4 (nCz even).
- The matrix A has length of b and 1+2*5 diagonals; we use for it an array of length 6*len(b).

The values are computed in rows of 5 lines, with the indicated middle and left matrices as indicated in the above scheme. These blocks are filled into the main matrix A and vector b, and subsequently solved with a non-standard Cholesky factorisation, <code>solve()</code>.

Tangential components at the boundaries are assumed to be 0 (PEC boundaries).

The result is stored in the provided electric fields ex, ey, and ez.

Parameters

```
ex, ey, ez [ndarray] Electric fields in x-, y-, and z-directions, as obtained from emg3d. fields.Field.
```

```
sx, sy, sz: Source fields in x-, y-, and z-directions, as obtained from emg3d.fields. Field.
```

```
eta_x, eta_y, eta_z, zeta: VolumeModel parameters (multiplied by volumes) as obtained from emg3d.models.VolumeModel().
```

hx, hy, hz [ndarray] Cell widths in x-, y-, and z-directions.

nu [int] Number of Gauss-Seidel iterations.

restrict

```
emg3d.core.restrict (crx, cry, crz, rx, ry, rz, wx, wy, wz, sc_dir)
Restriction of residual from fine to coarse grid.
```

Corresponds to Equation 8 in [Muld06]. The equation for the x-direction, using the notation $\{x, y, z\}$ instead of $\{1, 2, 3\}$, is given by

$$r_{x,K+1/2,L,M}^{2h} = \sum_{j_y=-1}^{1} \sum_{j_z=-1}^{1} w_{L,j_y}^y w_{M,j_z}^z \times \left(r_{x,k+1/2,l+j_y,m+j_z}^h + r_{x,k+3/2,l+j_y,m+j_z}^h\right).$$

The superscripts h, 2h indicate quantities defined on the coarse grid and on the fine grid, respectively. The indices $\{K, L, M\}$ on the coarse grid correspond to $\{k, l, m\} = 2\{K, L, M\}$ on the fine grid. The weights w are obtained from $restrict_weights()$.

The restrictions of rx, ry, and rz are stored directly in crx, cry, and crz.

Parameters

crx, cry, crz [ndarray] Coarse grid {x,y,z}-directed residual (pre-allocated empty arrays).

 \mathbf{rx} , \mathbf{ry} , \mathbf{rz} [ndarray] Fine grid $\{x,y,z\}$ -directed residual.

wx, wy, wz: tuple Tuples containing the weights (wl, w0, wr) as returned from restrict_weights() for the x-, y-, and z-directions.

sc_dir [int] Direction of semicoarsening; 0 for no semicoarsening.

restrict_weights

emg3d.core.restrict_weights (vectorN, vectorCC, h, cvectorN, cvectorCC, ch)
Restriction weights for the coarse-grid correction operator.

Corresponds to Equation 9 in [Muld06]. A generalized version of that equation is given by

$$\begin{split} w^v_{Q,-1} &= \left(v^h_{q-1/2} - v^{2h}_{Q-1/2}\right)/d^v_{q-1},\\ w^v_{Q,0} &= 1,\\ w^v_{Q,1} &= \left(v^{2h}_{Q+1/2} - v^h_{q+1/2}\right)/d^v_{q+1}, \end{split}$$

where d are the dual grid cell widths, v is one of $\{x,y,z\}$, and Q,q the corresponding entries of $\{K,L,M\},\{k,l,m\}$. The superscripts h,2h indicate quantities defined on the coarse grid and on the fine grid, respectively. The indices $\{K,L,M\}$ on the coarse grid correspond to $\{k,l,m\}=2\{K,L,M\}$ on the fine grid.

For the dual volume cell widths at the boundaries the scheme of [MoSu94] is applied, where $d_0^x = h_{1/2}^x/2$ at k = 0, $d_{N_x}^x = h_{N_x-1/2}^x$ at $k = N_x$, and so on.

The following parameters must all be in the same direction, hence, all must be either for the x, the y, or the z direction. The returned weights are for this direction.

Parameters

vectorN, **cvectorN** [ndarray] Cell edges of the fine (vectorN) and coarse (cvectorN) grids.

vectorCC, **cvectorCC** [ndarray] Cell centers of the fine (vectorCC) and coarse (cvectorCC) grids.

h, ch [ndarray] Cell widths of the fine (h) and coarse (ch) grids.

Returns

wl, w0, wr [ndarray] Left, central, and right weights in the direction provided in the in-

solve

emg3d.core.solve(amat, bvec)

Solve A x = b using a non-standard Cholesky factorisation.

Solve the system A x = b using a non-standard Cholesky factorisation without pivoting for a symmetric, complex matrix A tailored to the problem of the multigrid solver. The matrix A (amat) is an array of length 6*n, containing the main diagonal and the first five lower off-diagonals (ordered so that the first element of the main diagonal is followed by the first elements of the off diagonals, then the second elements and so on). The vector byec has length b.

The solution is placed in b (bvec), and A (amat) is replaced by its decomposition.

1. Non-standard Cholesky factorisation.

From [Muld07]: We use a non-standard Cholesky factorisation. The standard factorisation factors a hermitian matrix A into L L^H, where L is a lower triangular matrix and L^H its complex conjugate transpose. In our case, the discretisation is based on the Finite Integration Technique ([Weil77]) and provides a matrix A that is complex-valued and symmetric: $A = A^T$, where the superscript T denotes the transpose. The line relaxation scheme takes a matrix B that is a subset of A along the line. B is a complex symmetric band matrix with eleven diagonals. The non-standard Cholesky factorisation factors the matrix B into L L^T. Because of the symmetry, only the main diagonal and five lower diagonal elements of B need to be computed. The Cholesky factorisation replaces this matrix by L, containing six diagonals, after which the line relaxation can be carried out by simple back-substitution.

 $A = LDL^T$ factorisation without pivoting:

$$\begin{split} D(j) &= A(j,j) - \sum_{k=1}^{j-1} L(j,k)^2 D(k), \ j=1,..,n; \\ L(i,j) &= \frac{1}{D(j)} \left[A(i,j) - \sum_{k=1}^{j-1} L(i,k) L(j,k) D(k) \right], \ i=j+1,..,n. \end{split}$$

A and L are in this case arrays, where $A(i, j) \rightarrow A(i + 5j)$.

2. Solve A x = b.

Solve A x = b, given L which is the result from the factorisation in the first step (and stored in A), hence, solve L x = b, where x is stored in b:

$$b(j) = b(j) - \sum_{k=1}^{j-1} L(j,k)x(k), j = 2,..,n.$$

The result is equivalent with simply using numpy.linalg.solve(), but faster for the particular use-case of this code.

Note that in this custom solver there is no pivoting, and the diagonals of the matrix cannot be zero.

Parameters

amat [ndarray] Banded matrix A provided as a vector of length 6*n, containing main diagonal plus first five lower diagonals.

bvec [ndarray] Right-hand-side vector b of length n.

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