Using FEMTIC on NCI

Geophysical Research Data Processing and Modelling for 2030 Computation workshop

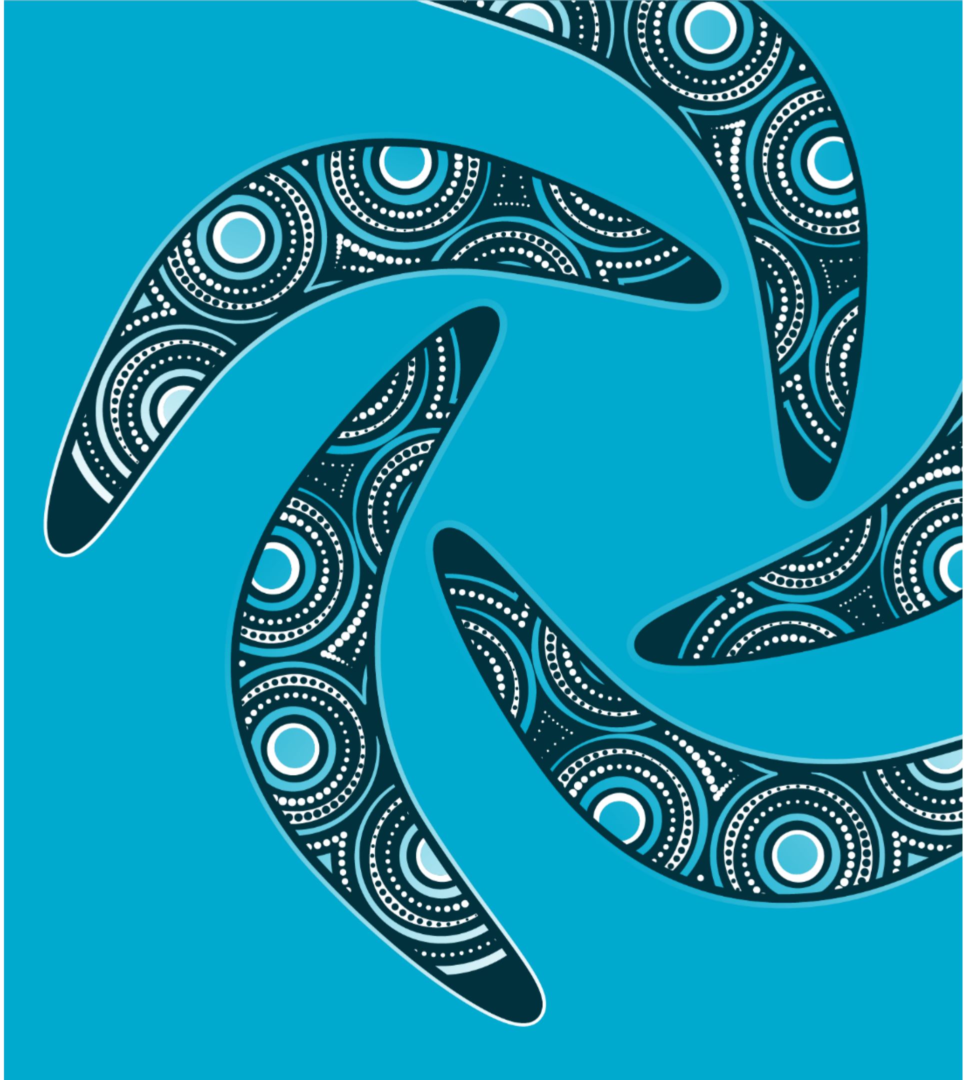
National Computational Infrastructure (NCI) Canberra, Australia

Hoël Seillé - Research Scientist

CSIRO Mineral Resources

22/11/2023

I would like to begin by acknowledging the Traditional Owners of the land that we’re meeting on today, and pay my respect to their Elders past and present.



Overview

FEMTIC

- Overview of the code
- Workflow to prepare and run inversions using *femticpy*:
  - MT data preparation
  - Mesh generation
  - Inversion on GADI
  - Results QC and visualization (Paraview)
- Synthetic example and jupyter notebook
- Test with an Australian dataset

Overview of the FEMTIC code

Geophysical Journal International

Geophys. J. Int. (2015) **202,** 828–849 doi: 10.1093/gji/ggv186

GJI Geomagnetism, rock magnetism and palaeomagnetism

3-D inversion of magnetotelluric data using unstructured tetrahedral elements: applicability to data affected by topography

Yoshiya Usui[1,2]

[1] *Department of Earth and P*

[2] *Volcanic Fluid Research C*

Geophysical Journal International

Geophys. J. Int. (2017) **208,** 1359–1372 doi: 10.1093/gji/ggw459

Advance Access publication 2016 December 9

GJI Geomagnetism, rock magnetism and palaeomagnetism

Three-dimensional resistivity structure of Asama Volcano revealed by data-space magnetotelluric inversion using unstructured tetrahedral elements

Yoshiya Usui,[1,2] Yas

Takao Koyama,[5] Yu

[1] *Department of Earth and Planeta*

[2] *Volcanic Fluid Research Center, T*

[3] *Institute of Seismology and Volca*

[4] *Institute of Seismology and Volca*

[5] *Volcano Research Center, Earthqu*

[6] *Fukushima Renewable Energy Ins*

[7] *Aso Volcanological Laboratory, In*

Geophysical Journal International

Geophys. J. Int. (2018) **214,** 952–974 doi: 10.1093/gji/ggy171

Advance Access publication 2018 May 05

GJI Marine geosciences and applied geophysics

Marine magnetotelluric inversion with an unstructured tetrahedral mesh

Yoshiya Usui,[1,2] Takafumi Kasaya,[3,4] Yasuo Ogawa[2] and Hisanori Iwamoto[4]

[1] *Department of Earth and Planetary Sciences, Tokyo Institute of Technology, Tokyo 152-8551, Japan. E-mail: yoshiya.usui@gmail.com*

[2] *Volcanic Fluid Research Center, Tokyo Institute of Technology, Tokyo 152-8551, Japan*

[3] *Research and Development Center for Earthquake and Tsunami, Japan Agency for Marine–Earth Science and Technology, Yokosuka, Kanagawa 237-0061, Japan*

[4] *Project Team for Development of New-generation Research Protocol for Submarine Resources, Japan Agency for Marine–Earth Science and Technology, Yokosuka, Kanagawa 237-0061, Japan*

FEMTIC is a 3-D magnetotelluric inversion code. FEMTIC is made by object-oriented programming with C++. FEMTIC is applicable to land magnetotelluric survey data as well as ocean bottom magnetotelluric survey data.

https://github.com/yoshiya-usui/femtic

sites.google.com/view/yoshiyausui/femtic

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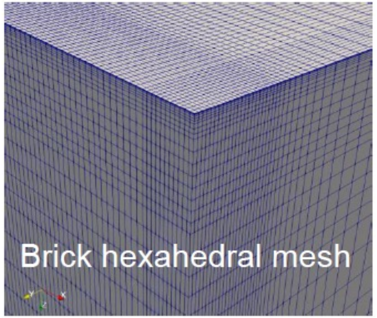
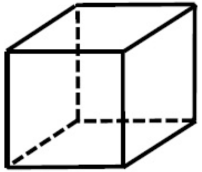
Functional overview

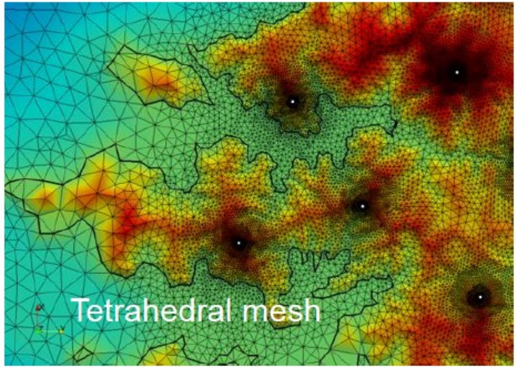
FEMTIC gives a three-dimensional electrical resistivity structure from the response functions at observation points on the Earth's surface.

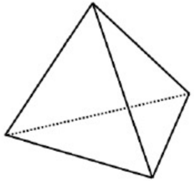
- Mesh type:
  - Tetrahedral mesh
  - Hexahedral brick mesh
  - Non-conforming deformed hexahedral mesh



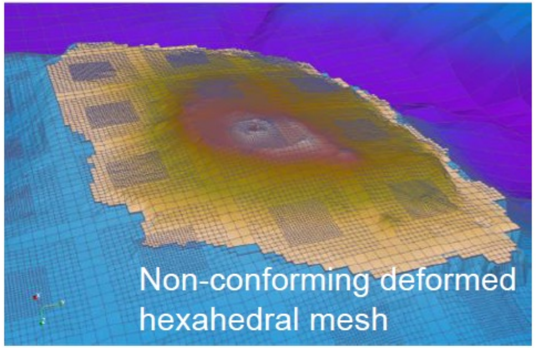


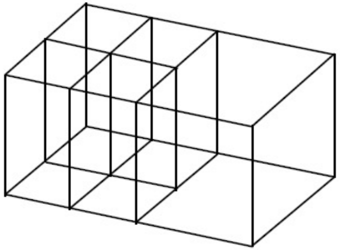
Brick hexahedral element





Tetrahedral element





Non-conforming deformed hexahedral element

Functional overview

- FEMTIC gives a three-dimensional electrical resistivity structure from the response functions at observation points on the Earth's surface.
  - Mesh type: Tetrahedral mesh / Hexahedral brick mesh / Non-conforming deformed hexahedral mesh
  - Data type: Impedance tensor / Vertical magnetic transfer function / Inter-station horizontal magnetic transfer function / Phase tensor / Apparent resistivity & Phase
  - Inversion algorithm: Model-space Gauss-Newton method / Data-space Gauss-Newton method
  - Parallel computation: Multiple processes parallel computation with MPI / Multiple threads parallel computation with OpenMP / MPI & OpenMP hybrid parallel computation
  - Model parameter: Subsurface electrical resistivity / Distortion matrix of galvanic distortion
  - Regularization: L2 / L1 regularization

Workflow

- Workflow to prepare and run inversions using *femticpy*:

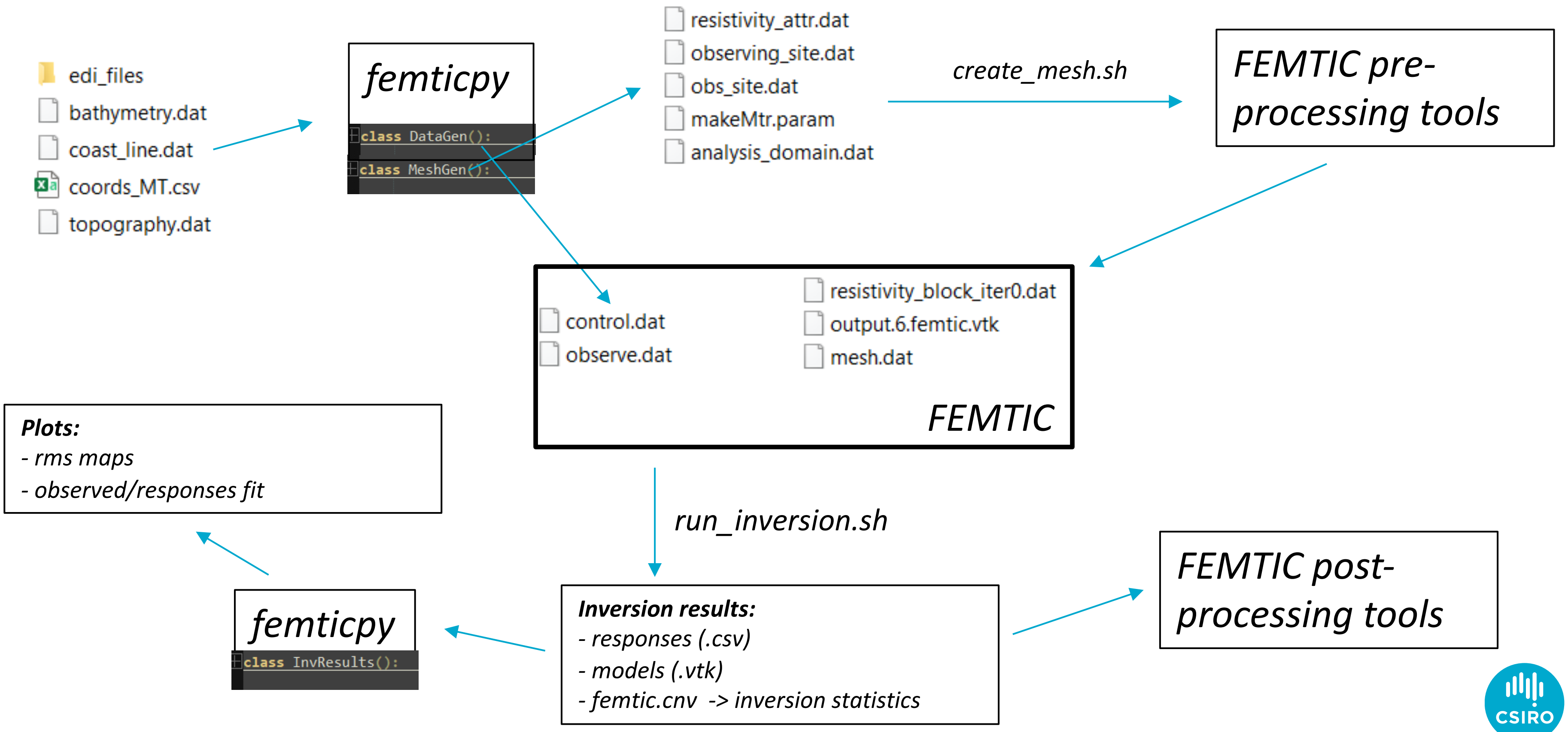
  - MT data preparation
  - Mesh generation on GADI
  - Inversion on GADI
  - Results QC and visualization (Paraview)

```
class DataGen():

class MeshGen():

class InvResults():
```

Workflow


edi_files
bathymetry.dat
coast_line.dat
coords_MT.csv
topography.dat
femticpy
class DataGen():
class MeshGen():
resistivity_attr.dat
observing_site.dat
obs_site.dat
makeMtr.param
analysis_domain.dat
create_mesh.sh
FEMTIC pre-processing tools
control.dat
observe.dat
resistivity_block_iter0.dat
output.6.femtic.vtk
mesh.dat
FEMTIC
run_inversion.sh
Plots:
- rms maps
- observed/responses fit
femticpy
class InvResults():
Inversion results:
- responses (.csv)
- models (.vtk)
- femtic.cnv -> inversion statistics
FEMTIC post-processing tools

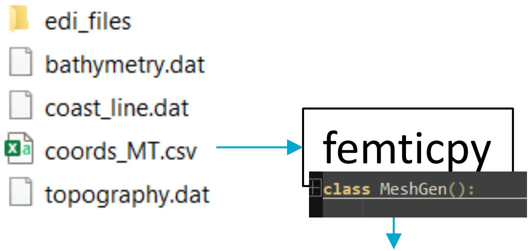
Workflow: MT data preparation with *femticpy*

- EDI files → observe.dat
  (only for impedance tensor)
- Set-up error floors
- Create Control file: Define inversion parameters

```
NUM_THREADS
1
MESH_TYPE
1
OUTPUT_PARAM_VTK
3
0 4 5
RESISTIVITY_BOUNDS
1
INV_METHOD
1
BOTTOM_RESISTIVITY
100.0
BOTTOM_ROUGHNING_FACTOR
1.0
DISTORTION
0
OUTPUT_OPTION
0 0
TRADE_OFF_PARAM
1.0
ITERATION
0 5
RETRIAL
2
CONVERGE
1.0
STEP_LENGTH
0.5 0.1 1.0
3
0.5 1.25
END
```

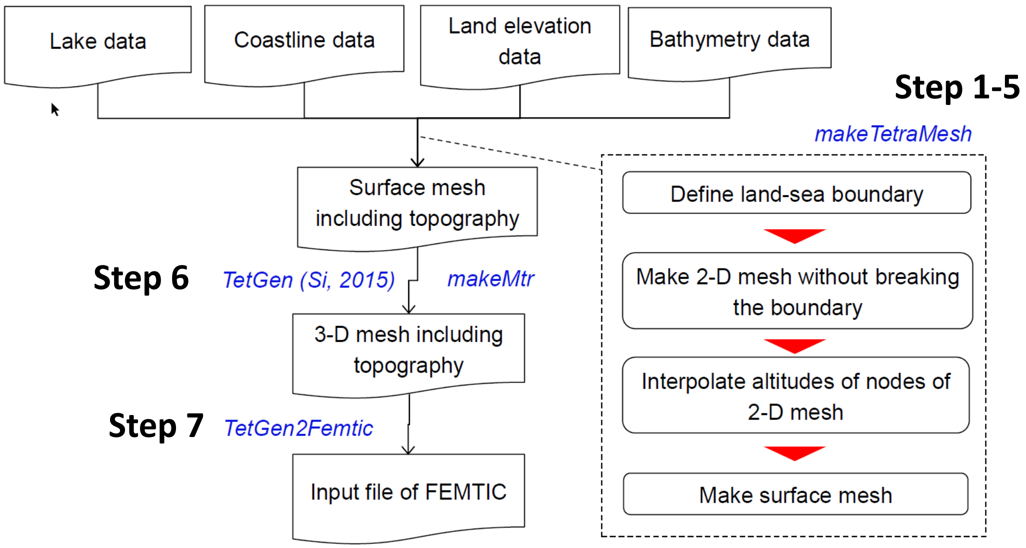
```python
def write_inversion_control(self,
                            INV_METHOD = 1,
                            NUM_THREADS = 1,
                            DISTORTION = 0,
                            TRADE_OFF_PARAM = [3],
                            ITERATION = 10,
                            ):
    file_loc = os.path.join(self.outdir, 'control.dat')
    file = open(file_loc,'w')
    file.write('NUM_THREADS\n')
    file.write('%d\n'%NUM_THREADS)
    file.write('MESH_TYPE\n')
    file.write('1\n')
    file.write('OUTPUT_PARAM_VTK\n')
    file.write('2\n')
    file.write('0 4\n')
    file.write('OFILE_TYPE\n')
    file.write('0\n')
    file.write('DISTORTION\n')
    file.write('%d\n'%DISTORTION)
    file.write('INV_METHOD\n')
    file.write('%d\n'%INV_METHOD)
    file.write('BOTTOM_RESISTIVITY\n')
    file.write('100.0\n')
    file.write('BOTTOM_ROUGHNING_FACTOR\n')
    file.write('1.0\n')
    file.write('OUTPUT_OPTION\n')
    file.write('0 0\n')
    file.write('TRADE_OFF_PARAM\n')
    for i in range(len(TRADE_OFF_PARAM)):
        file.write('%.2f '%TRADE_OFF_PARAM[i])
    file.write('\n')
    file.write('ITERATION\n')
    file.write('0 %d\n'%ITERATION)
    file.write('RETRIAL\n')
```

Workflow: Mesh generation



Input files for *meshGen.sh*:

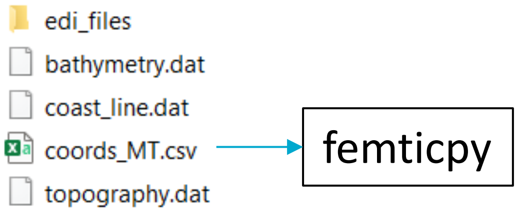
How to make 3-D mesh including topography

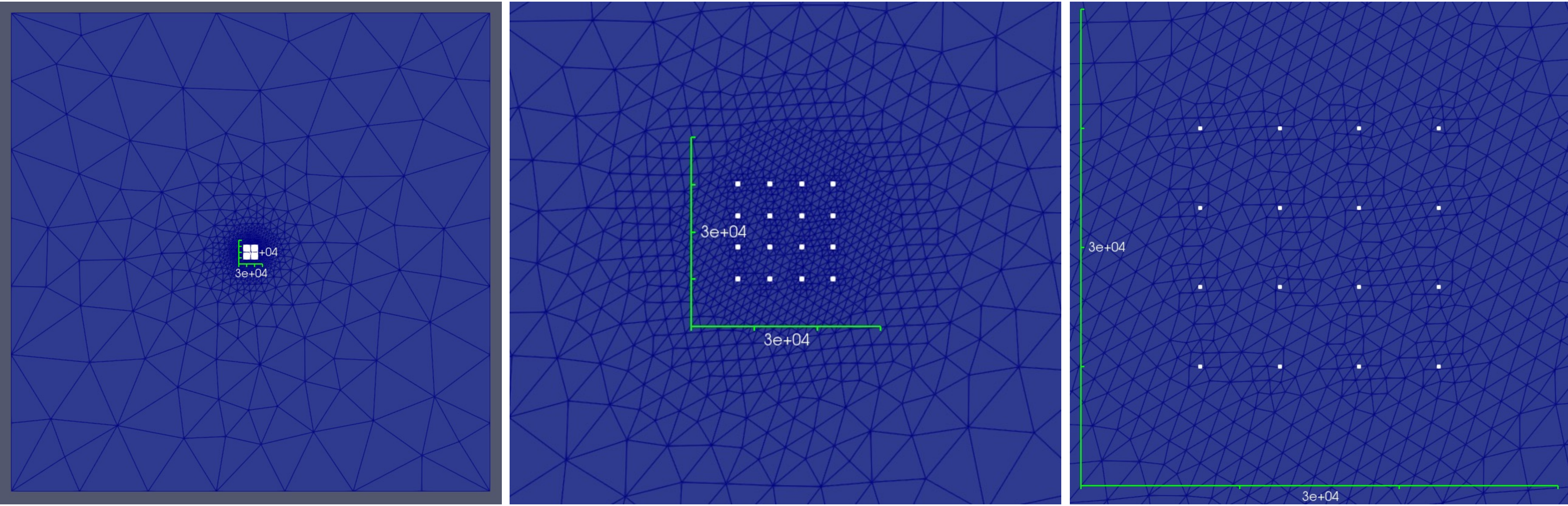


Script that sequentially runs the different pre-processing routines required to create the mesh.

meshGen.sh is ran as a job on Gadi.

Workflow: Mesh generation

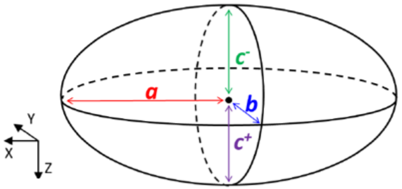




Workflow: Mesh generation

- edi_files
- bathymetry.dat
- coast_line.dat
- coords_MT.csv
- topography.dat

→ femticpy



a	len	f_h	f_v^+	f_v^-

a : *Length along x axis (km)*

len : *Edge length within the ellipsoid (km)*

f_h : *Oblateness on the X-Y plane*

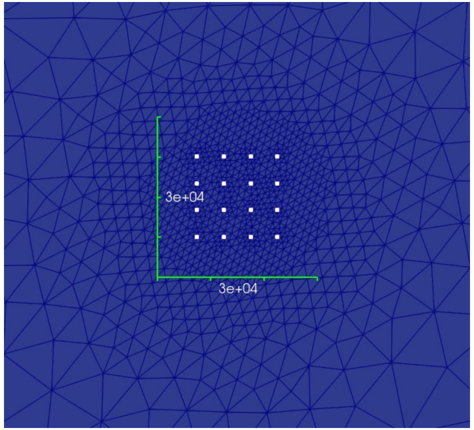
f_v^+ : *Oblateness on the Z-X plane (Upper side)*

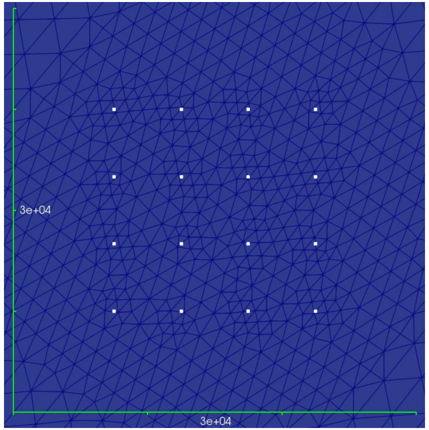
f_v^- : *Oblateness on the Z-X plane (Lower side)*

$$\frac{b}{a} = 1 - f_h$$

$$\frac{c^+}{a} = 1 - f_v^+$$

$$\frac{c^-}{a} = 1 - f_v^-$$





Step 1-5

```
mesh01.center = [0.0, 0.0, 0.0]
mesh01.rotation = 0
mesh01.ellipsoids_control = [3,
                          [15, 2, 0.0, 0.0, 0.0],
                          [30, 5, 0.0, 0.0, 0.0],
                          [200.0, 100.0, 0.0, 0.0, 0.0]]
```

```
mesh01.ellipsoids_observing_sites =  [1,
                                       1., 1.]
```

Step 6

```
mesh01.ellipsoids_obs_sites = [1,
                              [1., 0.5, 0.3]]

# and in the full mesh
mesh01.ellipsoids_mtr = [4,
                        [10, 2, 0.0, 0.0, 0.0],
                        [30, 5, 0.0, 0.0, 0.0],
                        [100.0, 100.0, 0.0, 0.0, 0.0],
                        [300, 100.0, 0.0, 0.0, 0.0]]
```

Step 7

```
mesh01.ellipsoids_resistivity_attr = [3,
                                   [15.0,  2.0,  0.0,  0.0],
                                   [30, 5.0, 0.0, 0.0],
                                   [300.0,  300.0,  0.0,  0.0]]


mesh01.ellipsoids_resistivity_attr_sites = [1,
                                   [1.0, 1.0]]
```

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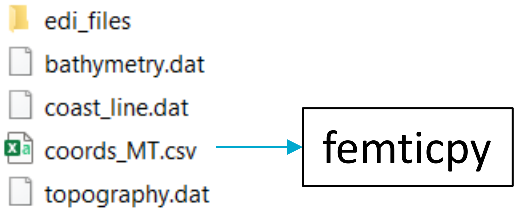
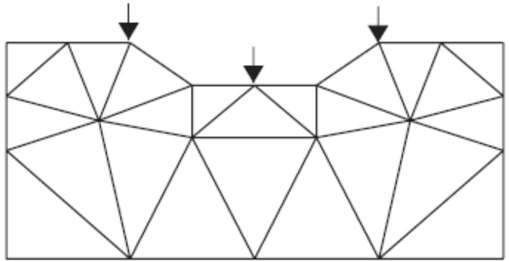
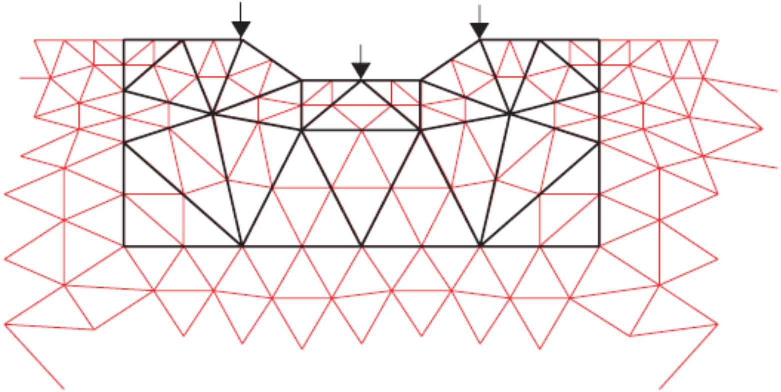
Workflow: Mesh generation





Günther, T., Rücker, C. & Spitzer, K., 2006. Three-dimensional modelling and inversion of dc resistivity data incorporating topography – II. Inversion, *Geophys. J. Int.*, **166**(2), 506–517.



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                            [30, 5, 0.0, 0.0, 0.0],
                            [200.0, 100.0, 0.0, 0.0, 0.0]]
```

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mesh01.ellipsoids_observing_sites =  [1,
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Step 6

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# and in the full mesh
mesh01.ellipsoids_mtr = [4,
                         [10, 2, 0.0, 0.0, 0.0],
                         [30, 5, 0.0, 0.0, 0.0],
                         [100.0, 100.0, 0.0, 0.0, 0.0],
                         [300, 100.0, 0.0, 0.0, 0.0]]
```

Step 7

```
mesh01.ellipsoids_resistivity_attr = [3,
                                     [15.0,  2.0,  0.0,  0.0],
                                     [30, 5.0, 0.0, 0.0],
                                     [300.0,  300.0,  0.0,  0.0]]

mesh01.ellipsoids_resistivity_attr_sites = [1,
                                           [1.0, 1.0]]
```

Workflow: Generate the mesh on GADI

```
[hs3588@gadi-login-03 hs3588]$ qsub create_mesh.sh
```

Output:

- inversion files:
    - resistivity_block_iter0.dat
    - mesh.dat

- Visualization files (Paraview):
    - output.6.femtic.vtk
    - triangles_with_height.vtk

```
#! /bin/bash

project=$1
cd $project
cp input_data/{topography.dat,bathymetry.dat,coast_line.dat} ./meshGen/files/
cd meshGen


#----------------------"
#-----    STEP 1    -----"
#----------------------"

echo "STEP 1... "
cp files/{control.dat,coast_line.dat,analysis_domain.dat,observing_site.dat} .
makeTetraMesh -stp 1
echo "   done!"
sleep 1

#----------------------"
#-----    STEP 2    -----"
#----------------------"

echo "STEP 2... "
makeTetraMesh -stp 2
```

```
[hs3588@gadi-login-03 meshGen]$ head resistivity_block_iter0.dat
     28190       3933
         0          0
         1          0
         2       1701
         3          0
         4       3559
         5       1128
         6          0
         7          0
         8          0
[hs3588@gadi-login-03 meshGen]$
```

resistivity_block_iter[Iter#].dat

Number of elements (N_e)	*Number of parameter cells (N_p)*

Workflow: Inversion on GADI

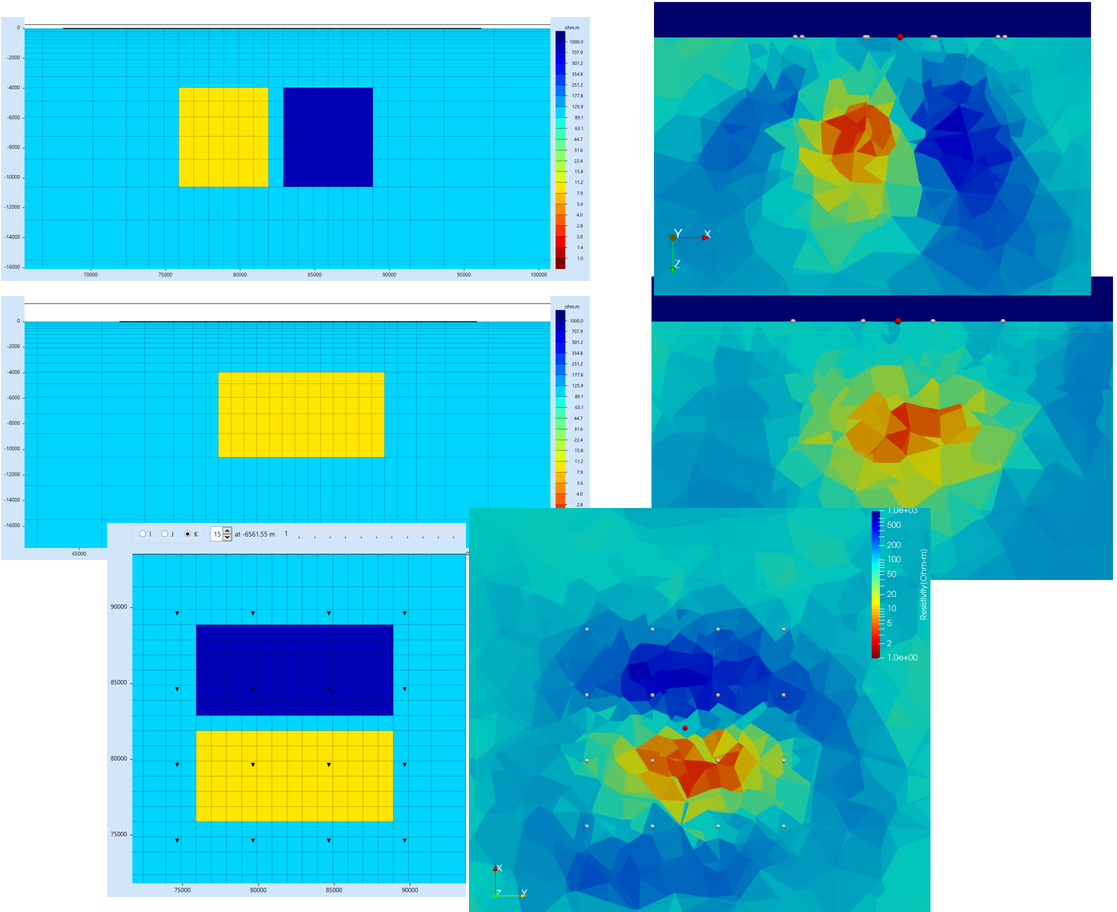
```
[hs3588@gadi-login-03 hs3588]$ qsub run_inversion.sh
```

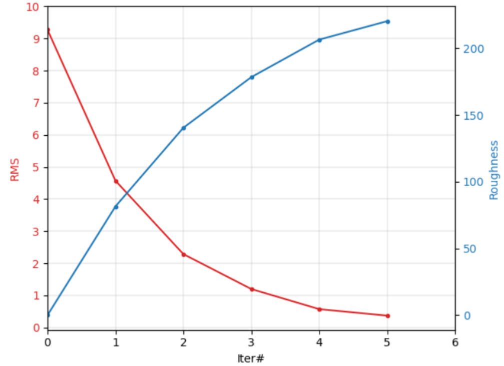
Output, for each iteration:

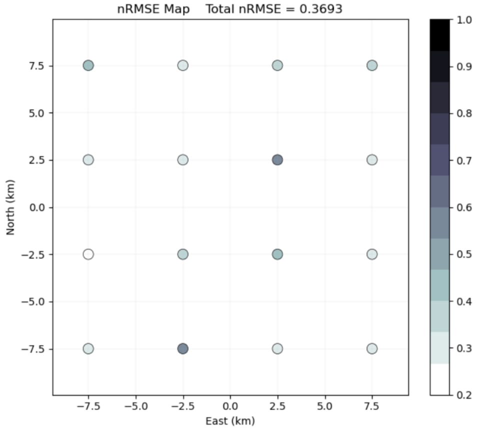
- responses (.csv)
- models (.vtk)
- obs_loc.vtk
- femtic.cnv -> inversion statistics

```
#!/bin/bash
#PBS -P nm05
#PBS -q normal
#PBS -l ncpus=8,walltime=0:30:00,mem=20GB,jobfs=1GB
#PBS -l storage=scratch/nm05+gdata/up99+gdata/nm05

module use /g/data/up99/modulefiles
module load femtic/4.1

project=synthetic

cd ${PBS_O_WORKDIR}

cd $project/inversion

mpirun -np 8 femtic
```

Workflow: Results QC and visualization (Paraview)

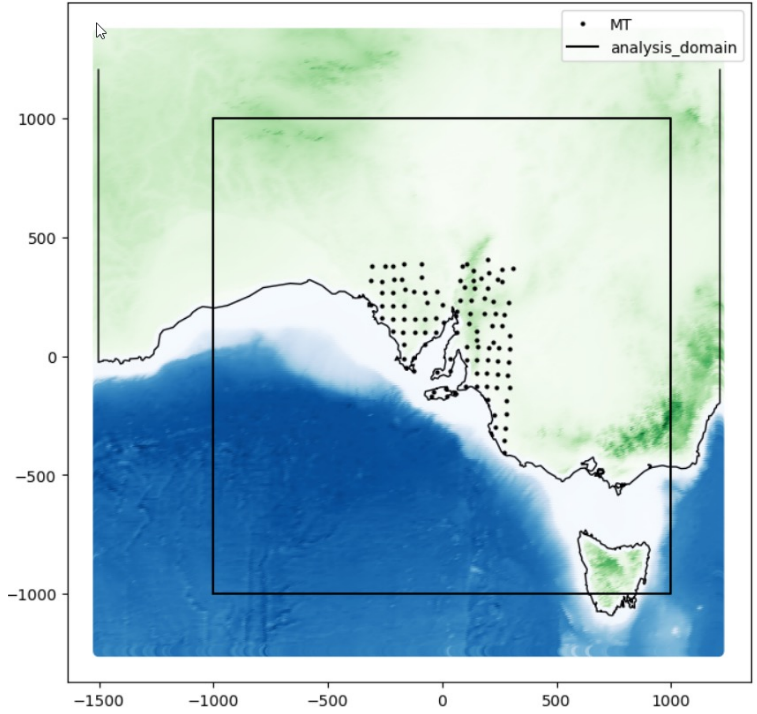






Synthetic example and jupyter notebook

Test with an Australian dataset



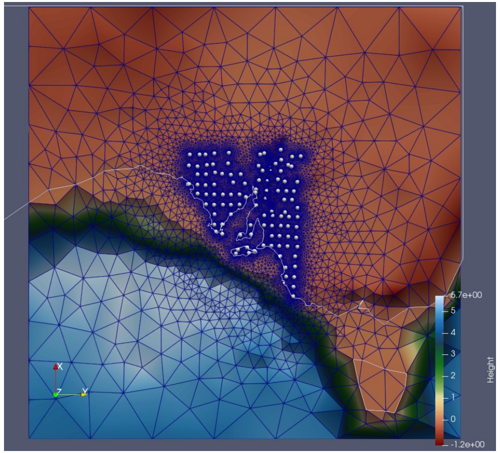

```
inversion01.error_floor_Z = [0.1, 0.05, 0.05, 0.1]
```

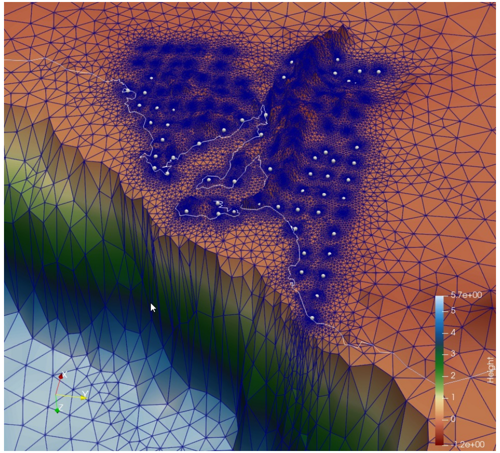
109 MT sites

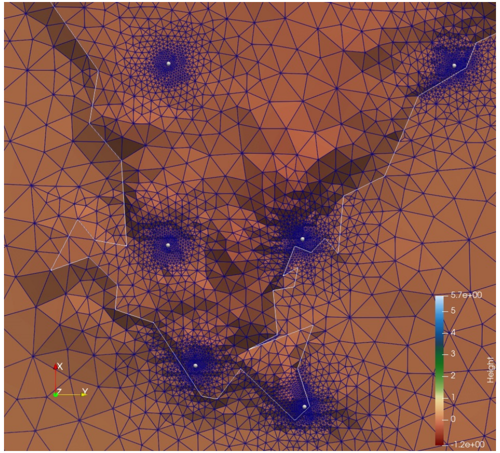
19 freqs / site, in between 0.03125 Hz and 0.00006 Hz

```
#SBATCH --ntasks-per-node=16
#SBATCH --nodes=2
#SBATCH --mem=900g

# Application specific commands:
module load intel-fc
module load intel-cc
module load intel-mkl/2020.1.217
module load openmpi/4.1.1-ofed51-intel20

mpirun -n 32 ../femtic
```

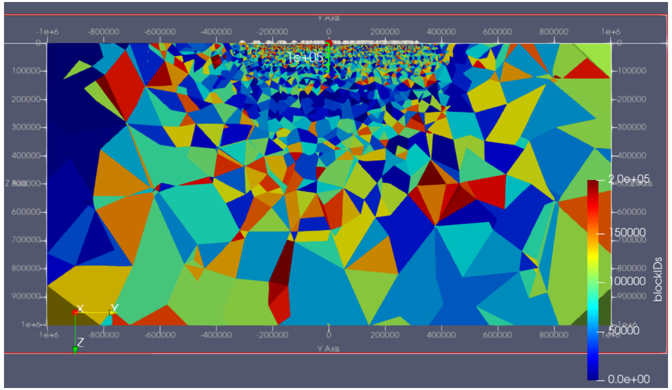
Test with an Australian dataset

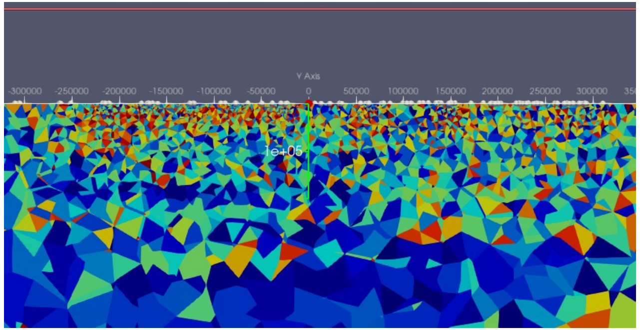




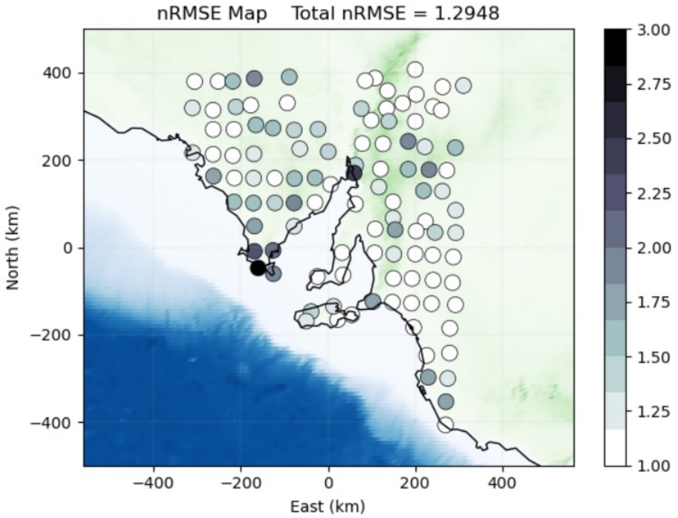


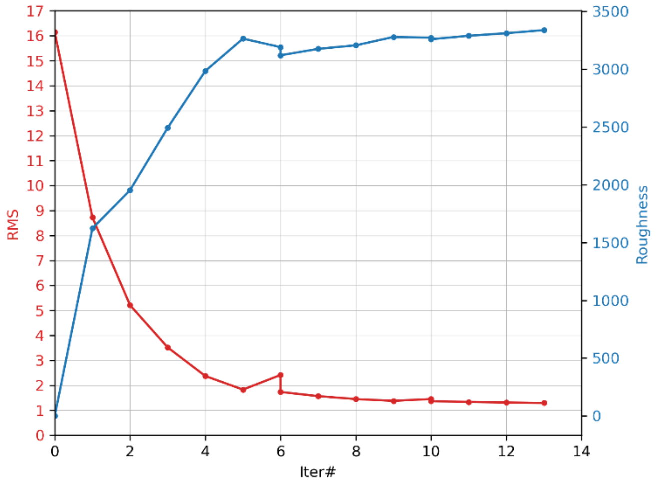
200k Cells

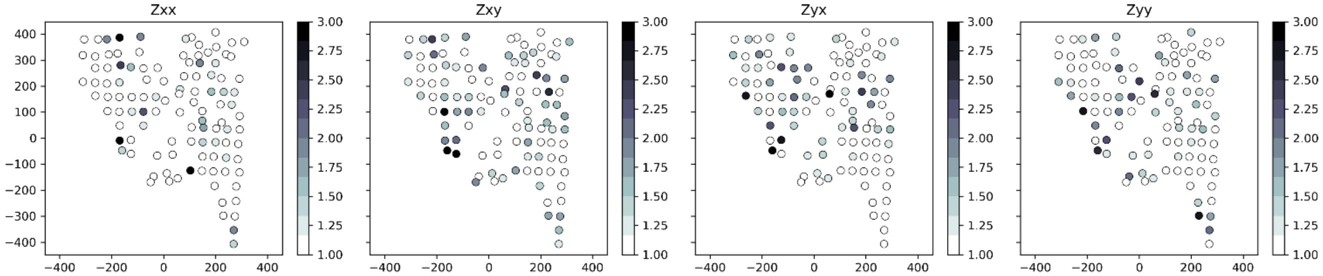


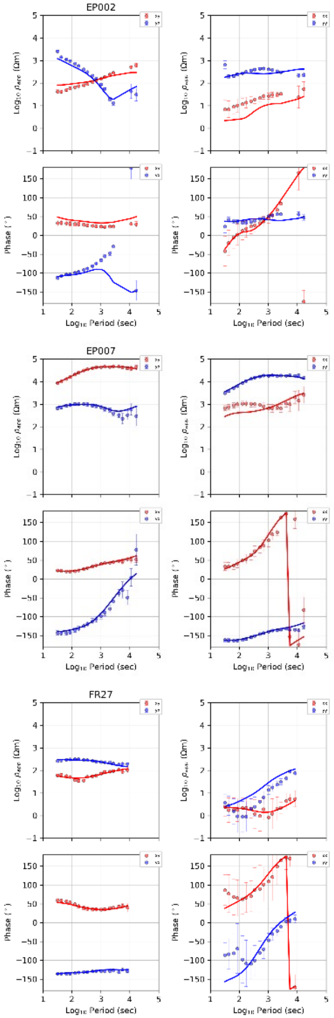


Test with an Australian dataset



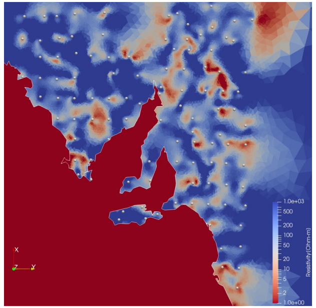




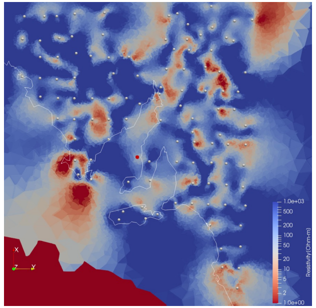


Test with an Australian dataset

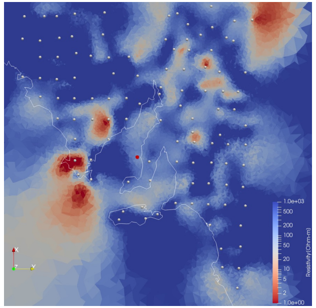
0 km



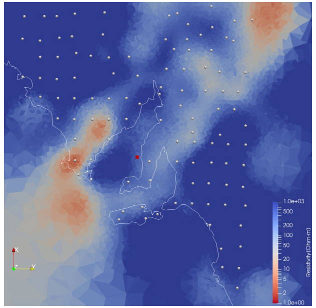
5 km



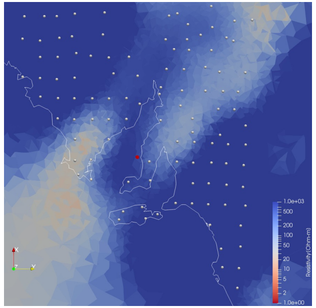
20 km

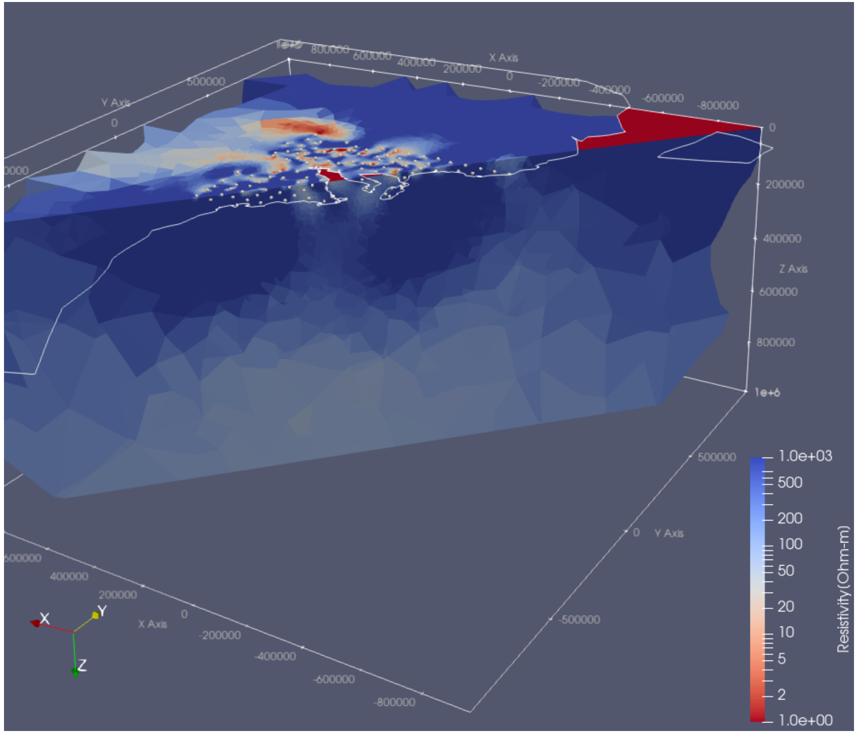


50 km



100 km





Thank you

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